SECOND ORDER BISMUT FORMULAE AND APPLICATIONS TO NEUMANN SEMIGROUPS ON MANIFOLDS

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ABSTRACT. Let $M$ be a complete connected Riemannian manifold with boundary $\partial M$, 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 $LP_t f$ and Hess $P_t f$ and present estimates of these quantities under suitable curvature conditions. In case when $P_t$ is symmetric in $L^2(\mu)$ for some probability measure $\mu$, 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 $\partial M$, and let $X_t$ be the reflecting diffusion process on $M$ generated by $\frac{1}{2}L$ where $L = \Delta + Z$; here $\Delta$ is the Laplace-Beltrami operator and $Z$ a smooth vector field on $M$. According to [12] [13] [24], the reflecting diffusion process $X_t$ starting at $x$ can be constructed as solution to the following SDE on $M$ with reflection:

$$dX_t = \mathbb{I}_t \circ dB_t + \frac{1}{2}Z(X_t) \, dt + \frac{1}{2}N(X_t) \, dl_t, \quad X_0 = x, \quad (1.1)$$

where $B_t$ is a standard Brownian motion on the tangent space $T_x M = \mathbb{R}^d$, $\mathbb{I}_t : T_x M \rightarrow T_{X_t} M$ the stochastic parallel transport along $X_t$, $N$ the inward normal unit vector field on $\partial M$, and $l_t$ the local time of $X_t$ on $\partial M$. 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

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

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

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 [11] [20] [10] using martingale arguments, and been extended to second order derivatives in [1] [11] [17] [18] [20] [23] [15].
In the case the boundary of $M$ is non-empty, Bismut type formulae have been derived in \cite{24,8} for the gradient of the Neumann semigroup $P_t$, see also \cite{16,12,25} 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 $\text{Ric}_Z := \text{Ric} - \nabla Z$ where $\text{Ric}$ is the Ricci curvature tensor, and let $\text{II}$ be the second fundamental form of the boundary:

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

A derivative formula for $P_t f$ is given in \cite{12,24} 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

$$\text{Ric}_Z := \text{Ric} - \nabla Z \geq K, \quad \text{II} \geq \sigma,$$

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

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

a Bismut type formula for $\nabla P_t f$ has been established in \cite{24} for $f \in \mathcal{B}_0(M)$ such that $\nabla P_t f$ is bounded on $[0, t] \times M$. More precisely, there exists a family of random homomorphisms $Q_t : T_x M \to T_x' M$ with the property that

$$|Q_t| \leq e^{-Kt/2 - \sigma t/2} \quad \text{and} \quad \langle N(X_t^1), Q_t(v) \rangle \mathbb{1}_{[X_t^1 \in \partial M]} = 0, \quad v \in T_x M,$$

such that

$$\nabla P_t f(v) = \mathbb{E}\left[\langle \nabla f(X_t^1), Q_t(v) \rangle\right], \quad v \in T_x M, \quad (1.3)$$

and

$$\nabla P_t f(v) = \mathbb{E}\left[f(X_t^1) \int_0^t \langle h'(s)Q_s(v), /_v dB_s \rangle\right], \quad v \in T_x M \quad (1.4)$$

for any choice of a non-negative $h \in C^1_b([0, t])$ such that $h(0) = 0$, $h(t) = 1$. When $\text{Ric}_Z$ and $\text{II}$ are bounded from below, the second part of condition (A) holds if either $\partial M$ is convex, or if $\partial M$ has strictly positive injectivity radius, the sectional curvature of $M$ being bounded above and $Z$ bounded, see \cite{24, Section 3.2}.

The aim of this paper is to extend (1.3) and (1.4) to second order derivatives and to establish Bismut type formulae for $LP_t f$ and $\text{Hess}_{P_t} f := \nabla^2 P_t f$, along with some applications. When compared to the case without boundary as in \cite{11}, the present study faces an essential new difficulty. Indeed, by formal calculations, the Bismut formula for second derivatives of $P_t f$ 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.

In Sections 2, we derive a Bismut type formula for $LP_t f$ also in terms of the multiplicative functional $Q_t$, which provides as consequence an upper estimate depending on the lower bounds of $\text{Ric}_Z$ and $\text{II}$, more precisely, condition (A) and $\|Z\|_{\infty} < \infty$. This estimate is new even in the case without boundary where the existing estimate in \cite{23} depends on the uniform norm of $\text{Ric}_Z$.

In Section 3, we establish a Bismut type formula for $\text{Hess}_{P_t} f$ 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 \cite{11,23,15,18}, 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
\[
\langle N(X_t), Q_t(v) \rangle |_{X_t \in \partial M} = 0
\]
which is reasonable since
\[
\langle \nabla P_{T>t}(X_t), N(X_t) \rangle |_{X_t \in \partial M} = 0.
\]
It follows that to express \( \nabla P_t f \) on the boundary, information on the second fundamental form
\[
\Pi^\#(P_\partial(v)) = -\langle \nabla P_\partial(v), N \rangle^\#
\]
is sufficient. However, when it comes to the second order derivative of \( P_t f \) on the boundary, no condition like
\[
\text{Hess}_{P_{T>t}}(N(X_t), \cdot) |_{X_t \in \partial M} = 0
\]
is satisfied, which naturally demands for full information on \( \nabla N \). This indicates that one not only needs to control \( \Pi \) but also \( \nabla N \). For this reason, in Section 3, two new functionals \( \tilde{Q}_t \) and \( W_t \) are introduced in (3.3) and (3.14) respectively, which our Bismut formula for \( \text{Hess}_{P_t f} \) will be based on and which then allow to derive upper bounds.

In Section 5, we apply the 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 [23] for the case without boundary.

For \( t \geq 0 \), let \( //_0^\rightarrow : T_{X_0}M \to T_{X_t}M \) denote stochastic parallel transport along the paths of the reflecting diffusion process \( X \). The covariant differential \( D \) in \( t \geq 0 \) is defined as \( D := //_0^\rightarrow d //_{1-t}^\rightarrow \) 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
\[
Dv_t = //_0^\rightarrow d //_{t-0}^\rightarrow v_t, \quad t \geq 0.
\]
For \( n \in \mathbb{N} \) and \( t \geq 0 \), let \( \tilde{Q}_t^{(n)} : T_{X_0}M \to T_{X_t}M \) solve the covariant differential equation:
\[
D\tilde{Q}_t^{(n)} = -\frac{1}{2} \left\{ \text{Ric}_Z^{\#}(\tilde{Q}_t^{(n)}) dt + \Pi^{\#}(\tilde{Q}_t^{(n)}) d\Lambda + n P_N(\tilde{Q}_t^{(n)}) d\bar{X} \right\}, \quad t \geq 0, \quad \tilde{Q}_0^{(n)} = \text{id}, \quad (2.1)
\]
where \( \text{id} \) is the identity map on \( T_{X_0}M \) and \( P_N \) the projection operator onto the normal direction \( N \) of \( \partial M \) such that when \( X_t \in \partial D \),
\[
P_N \tilde{Q}_t^{(n)} v = \langle \tilde{Q}_t^{(n)} v, N(X_t) \rangle N(X_t), \quad v \in T_{X_0}M.
\]
Furthermore for \( P_\partial : T_x M \to T_x \partial M \) being the projection operator for \( x \in \partial M \), let
\[
\langle \Pi^{\#}(\tilde{Q}_t^{(n)} v_1, v_2) \rangle := \Pi( P_\partial \tilde{Q}_t^{(n)} v_1, P_\partial v_2), \quad v_1, v_2 \in T_{X_t}M, X_t \in \partial M.
\]
By the curvature conditions (1.2), we then have
\[
\sup_{n \geq 1} |\tilde{Q}_t^{(n)}| \leq e^{-\frac{1}{2} \int_0^t K(X_s) ds - \frac{1}{2} \int_0^t \sigma^2(X_s) ds}, \quad t \geq 0, \quad (2.2)
\]
\[
\int_0^t |P_N(\tilde{Q}_s^{(n)})|^2 d\bar{X}_s \leq \frac{1}{n} \int_0^t |\tilde{Q}_s^{(n)}|^2 |K^-(X_s) ds + \sigma^-(X_s) d\bar{X}_s| \to 0 \quad \text{as } n \to \infty. \quad (2.3)
\]
Define
\[
\{\tilde{Q}_t^{(n)}\}^{-1} = //_{1-t}^\rightarrow \{\tilde{Q}_t^{(n)}//_{1-t}^\rightarrow\}^{-1} : T_{X_t}M \to T_{X_t}M \quad (2.4)
\]
where \( \{\tilde{Q}_t^{(n)}//_{1-t}^\rightarrow\}^{-1} \) is the inverse of the operator
\[
\tilde{Q}_t^{(n)}//_{1-t}^\rightarrow : T_{X_t}M \to T_{X_t}M.
\]
To show that \( \{Q_t^{(n)}\}^{-1} \) exists, let
\[
\tau_k := \inf \{ t \geq 0 : \rho_o(X_t) \geq k \}, \quad k \geq 1,
\]
where \( \rho_o \) is the Riemannian distance to a reference point \( o \in M \). Fix \( T > 0 \). By [24, Lemma 3.1.2], we have
\[
\mathbb{E}[e^{\alpha \tau_{T+1}}] < \infty, \quad \alpha > 0. \tag{2.5}
\]
Since \( \text{Ric}_Z \) and \( \Pi \) are locally bounded, (2.1) and (2.5) imply that \( Q_t^{(n)} / \tau_{T+1} \) is invertible with
\[
\mathbb{E}\left[ \sup_{t \in [0,T]} \left| (Q_t^{(n)})^{-1} \right|^p \right] = \mathbb{E}\left[ \sup_{t \in [0,T]} \left| (Q_t^{(n)})^{-1} \right|^p \right] < \infty, \quad p,k \geq 1. \tag{2.6}
\]

To derive a Bismut formula for \( LP_t f \), we need to estimate the martingales
\[
M_t^{(h,n)} := \int_0^t \left( h_s Q_s^{(n)} \int_0^s h_r (Q_r^{(n)})^{-1} / \tau_{r+1} \right) \, dB_s, \quad n \geq 1 \tag{2.7}
\]
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 \( P_N Q_t = 0 \) if \( X_t \in \partial M \). This construction has been extended in [24, 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 \( P_N Q_t = 0 \). Hence a priori, existence of the stochastic integral
\[
\int_0^t \left( h_s Q_s^{(n)} \int_0^s h_r (Q_r^{(n)})^{-1} / \tau_{r+1} \right) \, dB_s, \quad n \geq 1
\]
is not obvious.

**Lemma 2.1.** Let \( K \in C(M) \) and \( \sigma \in C(\partial M) \) such that [12] holds. Then for any adapted real process \( (h_t)_{t \in [0,T]} \) with
\[
C(h) := \mathbb{E}\left[ \int_0^T h_s^2 e^{\int_0^s K^{-1}(X_r) \, dr + \int_0^s \sigma^{-1}(X_r) \, dr} \, ds \right] < \infty, \tag{2.8}
\]
the martingales \( M_t^{(h,n)} \) in (2.7) satisfy
\[
\sup_{n \geq 1} \mathbb{E}\left[ \sup_{t \in [0,T]} |M_t^{(h,n)}| \right] \leq 3 (3 + \sqrt{10}) \left( C(h) \mathbb{E}\left[ \int_0^T h_s^2 \, ds \right] \right)^{1/2} < \infty. \tag{2.9}
\]
In addition, if there is a constant \( \alpha > 1 \) such that
\[
\mathbb{E}\left[ \left( \int_0^T h_s^2 \, ds \right)^{\alpha} \right] < \infty, \tag{2.10}
\]
then there exists a real random variable \( M_T^h \) with \( \mathbb{E}[|M_T^h|^{2\alpha}] < \infty \), and a subsequence \( n_m \to \infty \) as \( m \to \infty \), such that
\[
\lim_{m \to \infty} \mathbb{E}[\eta M_T^{(h,n_m)}] = \mathbb{E}[\eta M_T^h], \quad \eta \in L^{2\alpha}(\mathbb{P}). \tag{2.11}
\]
In case (2.10) holds for \( \alpha = 1 \) as well, one has
\[
\mathbb{E}[|M_T^h|] \leq 3 (3 + \sqrt{10}) \left( C(h) \mathbb{E}\left[ \int_0^T h_s^2 \, ds \right] \right)^{1/2}.
\]

**Proof.** (a) We first prove (2.9). By Fatou’s lemma, it suffices to show
\[
I_{k,n} := \mathbb{E}\left[ \sup_{t \in [0,T]} \left| \int_0^t (h_s Q_s^{(n)} \int_0^s h_r (Q_r^{(n)})^{-1} / \tau_{r+1}) \, dB_s \right| \right] \leq 3 (3 + \sqrt{10}) \sqrt{C(h)} \left( \mathbb{E}\left[ \int_0^T h_s^2 \, ds \right] \right)^{1/2}, \quad k,n \geq 1. \tag{2.12}
\]
For fixed $n \geq 1$ let

$$\xi_s := Q_s^{(n)} \int_0^s h_r(Q_r^{(n)})^{-1} \, dB_r, \quad s \geq 0.$$ 

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

$$I_{k,n} \leq 3E \left[ \left( \int_0^{T \wedge \tau_k} |\xi_s|^2 h_s^2 \, ds \right)^{1/2} \right] \leq 3E \left[ \sup_{s \in [0, T \wedge \tau_k]} |\xi_s|^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \left( \int_0^{T \wedge \tau_k} h_s^2 e^{\int_0^s K(X_r)dr + \int_0^s \sigma(X_r) \, dl} \, ds \right)^{1/2} \right]$$

Furthermore, by Itô’s formula we have

$$d|\xi_s|^2 = 2\langle \xi_s, h_s \rangle dB_s + \{Ric_{\mathbb{Z}}(\xi_s, \xi_s)ds + II(\xi_s, \xi_s)dl_s \} - n|P_N \xi_s|^2 dl_s + d[\xi, \xi]_s$$

which implies

$$d|\xi_s|^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \left( \int_0^{T \wedge \tau_k} h_s^2 e^{\int_0^s K(X_r)dr + \int_0^s \sigma(X_r) \, dl} \, ds \right)^{1/2} \leq (2+\alpha) \int_0^{T \wedge \tau_k} h_s^2 \, ds + E \left[ \int_0^{T \wedge \tau_k} h_s^2 \, ds \right]$$

(2.13)

By the condition $\xi_0 = 0$ and Lenglart’s inequality, we have

$$E \left[ \sup_{s \in [0, T \wedge \tau_k]} |\xi_s|^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \right] \leq 6E \left[ \left( \int_0^{T \wedge \tau_k} h_s^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \, ds \right)^{1/2} \right] + E \left[ \int_0^T h_s^2 \, ds \right]$$

(2.14)

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

$$E \left[ \sup_{s \in [0, T \wedge \tau_k]} |\xi_s|^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \right] \leq (3 + \sqrt{10})^2 E \left[ \int_0^T h_s^2 \, ds \right].$$

Combining this with (2.13), estimate (2.12) follows by letting $k$ tend to $\infty$.

(b) Assume that (2.10) holds for some $\alpha > 1$. By estimate (2.14) and the Burkholder-Davis-Gundy inequality, we can find constants $c_1, c_2 > 0$ such that

$$E \left[ \sup_{s \in [0, T \wedge \tau_k]} \left( |\xi_s|^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \right)^\alpha \right] \leq c_1 E \left[ \left( \int_0^{T \wedge \tau_k} h_s^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \, ds \right)^{\alpha/2} \right] + c_1 E \left[ \left( \int_0^T h_s^2 \, ds \right)^{\alpha/2} \right]$$

$$\leq c_1 E \left[ \left( \sup_{s \in [0, T \wedge \tau_k]} |\xi_s|^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \right) \left( \int_0^{T \wedge \tau_k} h_s^2 \, ds \right)^{\alpha/2} \right] + c_1 E \left[ \left( \int_0^T h_s^2 \, ds \right)^{\alpha/2} \right]$$

$$\leq \frac{1}{2} E \left[ \left( \sup_{s \in [0, T \wedge \tau_k]} \left( |\xi_s|^2 e^{-\int_0^s 2K(X_r)dr - \int_0^s \sigma(X_r) \, dl} \right)^{\alpha} \right) \right] + \frac{c_1^2}{2} E \left[ \left( \int_0^T h_s^2 \, ds \right)^{\alpha/2} \right] + c_2 E \left[ \left( \int_0^T h_s^2 \, ds \right)^{\alpha/2} \right].$$

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Together with (2.10) this implies
\[ G := \mathbb{E} \left[ \sup_{t \in [0,T]} \left( \xi_t^2 e^{-\int_0^t K^{-}(X_s) e^{\int_0^s \sigma^-(X_u) \mathrm{d}u} \right) \right] < \infty. \]

On the other hand, by Burkholder-Davis-Gundy’s inequality, there exists a constant \( c_3 > 0 \) such that
\[ \mathbb{E} \left[ |M_T^{(h,O)}|^{2n} \right] \leq c_3 \mathbb{E} \left[ \left( \int_0^T \left| \xi_t^2 e^{-\int_0^t K^{-}(X_s) e^{\int_0^s \sigma^-(X_u) \mathrm{d}u} \right|^n \right) \right] \]
\[ \leq c_3^n G^{\frac{2n}{n+1}} \left( \int_0^T \mathbb{E} \left[ h_t^2 e^{\int_0^t K^{-}(X_s) e^{\int_0^s \sigma^-(X_u) \mathrm{d}u} \right] \right)^{\frac{n}{n+1}} < \infty, \quad n \geq 1. \]

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

**Theorem 2.2.** Let \( K \in C(M) \) and \( \sigma \in C(\partial M) \) such that (1.2) holds. For \( T > 0 \) and \( x \in M \), let \( h_t \) be an adapted real process such that \( \int_0^T h_s \mathrm{d}s = -1 \) and
\[ \mathbb{E} \left[ \int_0^T h_t^2 \left( e^{\int_0^t K^{-}(X_s) e^{\int_0^s \sigma^-(X_u) \mathrm{d}u} \right) + |Z(X_s)^2| \right] < \infty. \]
(2.15)
Then, for any \( f \in \mathcal{B}_b(M) \),
\[ L(P_T f)(x) = 2 \mathbb{E} \left[ f(X_T^x) \left( M_T^h + \int_0^T \langle \tilde{h}_tZ(X_t^x), \mathrm{d}B_t \rangle \right) \right], \]
(2.16)
where \( \tilde{h}_t := 1 + \int_0^t h_s \mathrm{d}s. \) Consequently,
\[ |L(P_T f)(x)| \leq \frac{3}{2} \|f\|_{\infty} \left\{ \mathbb{E} \left[ \left( \int_0^T \left| \tilde{h}_t\right|^2 \right] \right] \right\}^{1/2} \left\{ 3 + \sqrt{10} \left( C(h) \mathbb{E} \int_0^T \tilde{h}_s^2 \mathrm{d}s \right)^{1/2} \right\}. \]
(2.17)
**Proof.** (1) We first assume \( f \in C^\infty_0(L) \), the class of functions \( f \in C^\infty(M) \) such that \( N f |_{\partial M} = 0 \) and \( \|L f\|_{\infty} < \infty \). In this case, we have the Kolmogorov equations (see [24] Theorem 3.1.3)),
\[ \partial_t P_{T-t} f = -P_{T-t} L f, \quad NP_{T-t} f |_{\partial M} = 0, \quad t \in [0,T]. \]
(2.18)
In the sequel, we write for simplicity
\[ X_t = X_t^x, \quad N_t = N(X_t), \quad Z_t = Z(X_t), \quad M_t := L P_{T-t} f(X_t), \quad t \in [0,T]. \]
Furthermore, we write \( A_t \equiv B_t \) for two processes \( A_t \) and \( B_t \) if the difference \( A_t - B_t \) is a local martingale. By Itô’s formula and (2.18), we obtain
\[ \mathrm{d}M_t = \langle \nabla (L P_{T-t} f)(X_t) , \mathrm{d}B_t \rangle + 2\tilde{h}_t M_t \mathrm{d}t + \frac{1}{2} N(L P_{T-t} f)(X_t) \mathrm{d}t, \]
which together with \( \tilde{h}_0 = 1 \) implies
\[ (L P_{T-t} f)(X_t) \tilde{h}_t^2 - L P_T f(x) = \int_0^t (L P_{T-t} f)(X_s) \tilde{h}_s \mathrm{d}s. \]
(2.19)
With \( \Delta = -\mathrm{d}^* \mathrm{d} \) and \( L = \Delta + Z \), we have
\[ -(L P_{T-t} f)(X_t) = \{ \mathrm{d}^* (M_{P_{T-t} f})(X_t) \} (X_t) \]
(2.20)
Combined with (2.19), this further yields
\[ (L P_{T-t} f)(X_t) \tilde{h}_t^2 - L P_T f(x) = \int_0^t (L P_{T-s} f)(X_s) \tilde{h}_s \mathrm{d}s \]
we observe that by Itô's formula

\[ \mathbb{E} \left[ T \int_0^T \frac{\partial f}{\partial x} (X_t) \, dB_t \right] = \mathbb{E} \left[ T \int_0^T \frac{\partial f}{\partial t} (X_t) \, dx \right]. \tag{2.21} \]

Let \( Q^{(n)}_t \) be the adjoint operator to \( Q^{(n)}_t \). By Itô's formula and the Weitzenböck formula, we obtain

\[ \mathbb{E} \left[ (dP_{T-t}) f(X_t) Q^{(n)}_t \right] = \mathbb{E} \left[ \left( \nabla \cdot dB_t \right) (dP_{T-t}) f(X_t) \right] (Q^{(n)}_t) + \mathbb{E} \left[ \text{Hess}_{P_{T-t}} (N_t) Q^{(n)}_t \right] \right) (X_t) dB_t. \]

Combining this with

\[ \text{Hess}_{P_{T-t}} (N_t) Q^{(n)}_t \]

and using Itô's formula, we derive

\[ \int_0^T (dP_{T-t}) \, dB_t = - \int_0^T \left( \nabla f \right) \, dB_t + \int_0^T \left( \text{Hess}_{P_{T-t}} (N_t) Q^{(n)}_t \right) \, dB_t. \tag{2.22} \]

To deal with the last term of the above equation and the second term on the right-hand side of (2.21), we observe that by Itô's formula

\[ dP_{T-t} f(X_t) = \langle \nabla P_{T-t} f(X_t), \, dW_t \rangle = (dP_{T-t} f)(W_t), \]

so that

\[ \int_0^T (dP_{T-t}) f(Z_t) \, dB_t = \int_0^T \left( \nabla f \right) \, dB_t + \int_0^T \left( \text{Hess}_{P_{T-t}} (N_t) Q^{(n)}_t \right) \, dB_t. \tag{2.23} \]

Combining these equations with (2.22) and (2.20), we obtain

\[ \int_0^T (LP_{T-t}) f(X_t) \, dB_t = \int_0^T \left( \nabla f \right) \, dB_t + \int_0^T \left( \text{Hess}_{P_{T-t}} (N_t) Q^{(n)}_t \right) \, dB_t. \]

The last equation and Eq. (2.19) yield

\[ (LP_{T-t}) f(X_t) = \int_0^T \left( \nabla f \right) \, dB_t + \int_0^T \left( \text{Hess}_{P_{T-t}} (N_t) Q^{(n)}_t \right) \, dB_t. \tag{2.24} \]
To get rid of the local martingales in the above calculations, we consider the diffusion process up to exit times from bounded balls. Since Hess$_{P,f}$ is locally bounded, for any $k \geq 1$ we find a constant $c_k > 0$ such that

$$\frac{1}{c_k} \left[ \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \text{Hess}_{P_{T \wedge \tau_k},f}(N_s, N_s) \left( N_s, \frac{Q_s^\langle \rangle}{\langle \rangle} \right) \right] \int_0^s h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_r \rangle ds \right] \leq \mathbb{E} \left[ \int_0^{T \wedge \tau_k} |(Q_s^\langle \rangle)^* N_s|^2 \right]^{1/2} \mathbb{E} \left[ \int_0^s h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_r \rangle ds \right]^{1/2}. \tag{2.24}$$

Next, we observe from (2.22), (2.3) and (2.5) that

$$\lim_{n \to \infty} \mathbb{E} \left[ \int_0^{T \wedge \tau_k} |(Q_s^\langle \rangle)^* N_s|^2 \right] = \lim_{n \to \infty} \mathbb{E} \left[ \int_0^{T \wedge \tau_k} |P_N Q_s^\langle \rangle (Q_s^\langle \rangle)^* N_s|^2 \right] \leq \lim_{n \to \infty} \mathbb{E} \left[ \sup_{\tau \in [0, T \wedge \tau_k]} |Q_s^\langle \rangle^2 \right] \mathbb{E} \left[ \int_0^{T \wedge \tau_k} |P_N Q_s^\langle \rangle|^2 ds \right] = 0,$$

and by Burkholder-Davis-Gundy’s inequality,

$$\mathbb{E} \left[ \int_0^{T \wedge \tau_k} |h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_r \rangle ds \right] \leq \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \left( \sup_{s \in [0, T \wedge \tau_k]} |h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_r \rangle ds \right)^2 \right] < \infty.$$

Using these estimates when taking the upper bound of (2.24), we arrive at

$$\lim_{n \to \infty} \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \text{Hess}_{P_{T \wedge \tau_k},f}(N_s, N_s) \left( N_s, \frac{Q_s^\langle \rangle}{\langle \rangle} \right) \int_0^s h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_r \rangle ds \right] = 0. \tag{2.25}$$

On the other hand, since the process in (2.23) is a martingale up to time $T \wedge \tau_k$, its expectation at time $T \wedge \tau_k$ vanishes, so that

$$L(P_T f)(x) - \mathbb{E} \left[ \frac{T \wedge \tau_k}{T \wedge \tau_k} \int_0^{T \wedge \tau_k} f(X_T) \right] - 2dP_{T \wedge \tau_k} f \left( \frac{T \wedge \tau_k}{T \wedge \tau_k} \int_0^{T \wedge \tau_k} h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_s \rangle \right) = 2 \mathbb{E} \left[ \int_0^{T \wedge \tau_k} h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_s \rangle \right] + 2 \mathbb{E} \left[ f(X_T) \int_0^{T \wedge \tau_k} h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_s \rangle \right] + 2 \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \text{Hess}_{P_{T \wedge \tau_k},f}(N_s, N_s) \left( N_s, \frac{Q_s^\langle \rangle}{\langle \rangle} \right) \int_0^s h_r(Q_{s}^{\langle \rangle})^{-1} \langle , dB_r \rangle ds \right].$$

By $h_T = 0$, Lemma 2.1 (2.23) and (2.15), we may first take $k \to \infty$ and then choose a subsequence $n_m \to \infty$ to derive (2.16) for $f \in C^\infty_N(L)$.

(2) To extend the formula to $f \in B_0(M)$, we let $h_t = 0$ for $t \geq T$ and define finite signed measures $\mu_\varepsilon$ on $M$ as

$$\mu_\varepsilon(A) := 2 \mathbb{E} \left[ 1_A (X_{T+\varepsilon}^T) \left( M^\mu_T + \int_0^T \langle \tilde{h}_t h_s Z_s , \langle , dB_s \rangle \rangle \right) \right], \quad \varepsilon \geq 0,$$

for measurable subsets $A \subset M$. By step (1) and (2.18), we have

$$\frac{P_{T+\varepsilon} f(x) - P_T f(x)}{\varepsilon} = \frac{1}{\varepsilon} \int_0^\varepsilon L_{P+\varepsilon} f(x) dr = \frac{1}{\varepsilon} \int_0^\varepsilon dr \int_0^T df \mu_\varepsilon = \int_M f d\mu_\varepsilon, \quad f \in C^\infty_N(L), \quad \varepsilon > 0,$$

where $\mu_\varepsilon := \frac{1}{\varepsilon} \int_0^\varepsilon \mu_\varepsilon dr$ is a finite signed measure on $M$. Since functions in $C^\infty_N(L)$ determine finite measures, according to Lemma 2.1 and condition (2.18), $\mu_\varepsilon$ is a finite measure, and this implies (we have in particular $M^\mu_T = M^\mu_T$ since $h_t = 0$ for $t \geq T$),

$$\frac{P_{T+\varepsilon} f(x) - P_T f(x)}{\varepsilon} = \int_M f d\mu_\varepsilon, \quad f \in B_0(M), \quad \varepsilon > 0.$$
Since the law of $X_T$ is absolutely continuous and $P_t f \to f$ a.e. as $r \downarrow 0$, we get by the strong Markov property $\mathbb{E}^{x_T} f(X_{T+r}) = P_t f(X_T) \to f(X_T)$ a.s. as $r \downarrow 0$. By the dominated convergence theorem we may let $\varepsilon \downarrow 0$ to arrive at
\[
\frac{dP_t f(x)}{dt} \bigg|_{t=T} = 2\mathbb{E} \left[ f(X_T) \left( M^h_T + \int_0^T \langle \dot{h}_s, \dot{Z}_s \rangle \, ds \right) \right], \quad f \in \mathcal{B}_b(M).
\] (2.26)

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 $(\phi P_{t+\varepsilon} f)(X_t)$ for some cut-off function $\phi$ at $x$, the proof of (3.1.5) in [24] implies
\[
LP_t f(x) = \frac{d}{dt} P_t f(x), \quad t > 0, \quad f \in \mathcal{B}_b(M).
\] (2.27)

Combining (2.26) and (2.27), we prove (2.16) 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 [23]. Moreover, compared to the estimate in [23], 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 and $||Z||_{\infty} < \infty$. Let $x \in M$ and $T > 0$. Then

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

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

\[
|L(P_T f)(x)| \leq (P_T f^2)^{1/2}(x) \left( \frac{2 \sqrt{3} ||Z||_{\infty}}{3\sqrt{T}} + \frac{\sqrt{2} e^{K^{-T}/2}}{T} \right).
\] (2.28)

**Proof.** The first assertion is a direct consequence of inequality (2.17). It hence suffices to show inequality (2.28). Note that

\[
\mathbb{E}^{x_T} \left[ f(X_T) M_T^{(h,n)} \right] \leq (P_T f^2)^{1/2}(x) \left[ \mathbb{E} [M_T^{(h,n)}]^2 \right]^{1/2},
\] (2.29)

where $M_T^{(h,n)}$ is defined as in (2.27). Let $h_s = -1/T$. Then,

\[
\mathbb{E} [M_T^{(h,n)}]^2 \leq \frac{1}{T^2} \left[ \int_0^T \mathbb{E} \left[ Q^{(n)}_{\lambda T_k} \int_0^{\lambda T_k} |Q_r^{(n)}|^{-1} \, |\dot{B}_r| \, ds \right]^2 \right]^{1/2}.
\]

By Itô’s formula, we see that

\[
d \left( e^{-K_s} \int_0^s (Q_r^{(n)})^{-1} \, |\dot{B}_r| \, ds \right)^2 \leq 2 e^{-K_s} \int_0^s (Q_r^{(n)})^{-1} \, |\dot{B}_r| \, ds + ds.
\] (2.30)

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

\[
\mathbb{E} \left[ e^{-K_{s \wedge T_k}} \int_0^{s \wedge T_k} (Q_r^{(n)})^{-1} \, |\dot{B}_r| \, ds \right]^2 \leq s.
\]

Letting $k$ tend to $\infty$ yields

\[
\mathbb{E} \left[ \left( \int_0^{s \wedge T_k} (Q_r^{(n)})^{-1} \, |\dot{B}_r| \, ds \right)^2 \right] \leq s e^{K^{-s}}.
\]

Combining this with (2.30) and (2.29), we see that $(M_T^{(h,n)})_{n \geq 1}$ 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

\[
\mathbb{E} [M_T^h]^2 \leq \frac{e^{K^{-T}}}{2T^2}.
\]

By this and the Bismut formula (2.16), the second assertion (2.28) holds. \qed
3. Hessian formula for $P_t f$ and its application

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

$$\langle \text{Ric}_Z^v(v_1), v_2 \rangle := \text{Ric}_Z(v_1, v_2) = \text{Ric}(v_1, v_2) - \langle \nabla_v Z, v_2 \rangle, \quad v_2 \in T_x M.$$  

Let $R$ denote the Riemann curvature tensor. Then $d^* R(v_1)$ is the linear operator on $T_x M$ determined by

$$\langle d^* R(v_1, v_2), v_3 \rangle = \langle (\nabla_v \text{Ric}_Z^v)(v_1), v_2 \rangle - \langle (\nabla_v \text{Ric}_Z^v)(v_3), v_1 \rangle, \quad v_3 \in T_x M,$$

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

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

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

$$\text{Ric}_Z := \text{Ric} - \nabla Z \geq K, \quad -\nabla N \geq \sigma, \quad (3.1)$$

where the second condition means $-\langle \nabla X N, X \rangle \geq \sigma(x)|X|^2$ for $x \in \partial M$ and $X \in T_x M$. Moreover, assume that there exist three non-negative functions $\alpha, \beta$ and $\gamma$, such that

$$|R|_{\text{HS}}(x) \leq \alpha(x), \quad |d^* R + \nabla \text{Ric}_Z^v - R(Z)(x) < \beta(x), \quad |\nabla(\nabla N)^v + R(N)(x) < \gamma(x), \quad (3.2)$$

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

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

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

$$D \tilde{Q}_t = -\frac{1}{2} \text{Ric}_Z^v(\tilde{Q}_t) dt + \frac{1}{2} (\nabla N)^v(\tilde{Q}_t) d_1, \quad \tilde{Q}_0 = \text{id.} \quad (3.3)$$

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

$$D W^h_t(v, v) = R((\cdot), dB_t, \tilde{Q}_t(\tilde{h}(t) v), \tilde{Q}_t(v))$$

$$-\frac{1}{2} (d^* R - R(Z) + \nabla \text{Ric}_Z^v)(\tilde{Q}_t(\tilde{h}(t) v), \tilde{Q}_t(v)) dt$$

$$-\frac{1}{2} (\nabla N - R(N))^v(\tilde{Q}_t(\tilde{h}(t) v), \tilde{Q}_t(v)) d_1$$

$$-\frac{1}{2} \text{Ric}_Z^v(W^h_t(v, v)) dt + \frac{1}{2} (\nabla N)^v(W^h_t(v, v)) d_1$$

with initial condition $W^h_0(v, v) = 0$.

**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 $\tilde{h}(\cdot)$ be an adapted and bounded real process such that $\int_0^T \tilde{h}_s ds = -1$ for $t \geq T \wedge \tau_D$, and such that

$$\mathbb{E} \left[ \int_0^{T \wedge \tau_D} \left( \tilde{h}_s^2 + h_s^2 (\alpha^2(X_s) + \beta^2(X_s)) \right) e^{\int_0^t K^{-}(X_s) dr + \int_0^t \sigma^{-}(X_s) dl_s} ds + \int_0^{T \wedge \tau_D} h_s^2 \gamma^2(X_s) e^{\int_0^t K^{-}(X_s) dr + \int_0^t \sigma^{-}(X_s) dl_s} dl_s \right] < \infty \quad (3.4)$$

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

$$
\text{Hess}_{\mathcal{P}_T} f(v, v)(x) = -\mathbb{E}^x \left[ f(X_T) \left( \int_0^T \langle W^h_s(v, h_s v), \mathcal{P}_s \rangle ds \right) \right] + \mathbb{E}^x \left[ f(X_T) \left( \int_0^T \langle \tilde{Q}_s(h_s v), \mathcal{P}_s \rangle ds \right) - \int_0^T |\tilde{Q}_s(h_s v)|^2 ds \right].
$$

Moreover,

$$
|\text{Hess}_{\mathcal{P}_T} f| \leq 3||f||_\infty C(h)^{1/2} \left\{ (3 + \sqrt{10}) \mathbb{E} \left( \int_0^{T + \tau_D} t \nu(X_t) e^{\int_0^t K^{-1}(X_s) dt + \int_0^t \nu(X_s) dt} \mathcal{L}_s^2 \right) \right\}^{1/2} + \frac{1}{2} \mathbb{E} \left( \int_0^{T + \tau_D} \nu(X_t) e^{\int_0^t K^{-1}(X_s) dt + \int_0^t \nu(X_s) dt} \mathcal{L}_s^2 \right)^{1/2} + \frac{2}{3} C(h)^{1/2},
$$

where $C(h)$ is defined as in (2.8).

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 estimates 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 $\int_0^T h_s ds = -1$, which imply $\tilde{h}_s = 0$ for $s \geq T \wedge \tau_D$. Then the functions $K$, $\sigma$, $\alpha$, $\beta$, and $\gamma$ are all bounded on $D$ and $|\tilde{h}_s| \leq 1$. Moreover, condition (3.4) can be simplified to

$$
\mathbb{E} \left[ \int_0^T h_s^2 e^{\int_0^s \nu(X_t) dt} ds \right] < \infty.
$$

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

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

4) Assume $\Pi \geq \sigma_1$ and $|\nabla N| \leq \sigma_2$. 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 $X_2 = \langle X, N \rangle N$,

$$
-\langle \nabla X, X \rangle = -\langle \nabla X_1, X_1 \rangle - \langle X, N \rangle^2 - \langle X, N \rangle \langle \nabla X_1, N \rangle - \langle X, N \rangle \langle \nabla N, X_1 \rangle
$$

$$
= -\langle \nabla X_1, X_1 \rangle - \langle X, N \rangle \langle \nabla N, X_1 \rangle
$$

$$
\geq \sigma_1 |X_1|^2 - \sigma_2 |X_1| \cdot |X, N| \geq \min \left\{ \sigma_1, -\frac{\sigma_2}{2} \right\} |X|^2.
$$

In particular, if $\nabla N = 0$ and $\Pi \geq \sigma$, then it is easy to see that for $x \in \partial M$,

$$
-\langle \nabla X, X \rangle \geq -\sigma^{-2} |X|^2, \quad \text{for} \quad X \in T_xM \text{ and } x \in \partial M.
$$

5) Naturally, one might try to work with $Q_t^{(n)}$ instead of $\tilde{Q}_t$ to define $M_t(v, v)$, in order to avoid the term $\nabla N$. But we have already seen that $Q_t$ is the limit of $Q_t^{(n)}$, see the proof of [24, Theorem 3.2.1], which satisfy the covariant Itô equation (2.1). We have

$$
d \left( \nabla dP_{T-t}(Q_t^{(n)}(v), Q_t^{(n)}(v))(X_t) \right)
$$

$$
= \langle \nabla_{\mathcal{P}_{T-t}} \mathcal{P}_{T-t}, \nabla dP_{T-t} \rangle \left( Q_t^{(n)}(v), Q_t^{(n)}(v) \right) - \langle \nabla dP_{T-t} \rangle \left( \text{Ric}_{\mathcal{P}_{T-t}}^2(Q_t^{(n)}(v), Q_t^{(n)}(v)) \right) dt
$$

$$
- \langle \nabla dP_{T-t} \rangle \left( Q_t^{(n)}(v), \Pi \nu(Q_t^{(n)}(v)) \right) dl_t + \partial_t \langle \nabla dP_{T-t} \rangle(Q_t^{(n)}(v), Q_t^{(n)}(v)) dt
$$

$$
+ \frac{1}{2} \nabla N \langle \nabla dP_{T-t} \rangle(Q_t^{(n)}(v), Q_t^{(n)}(v)) dl_t + \frac{1}{2} \left( \text{tr} \nabla^2 + \nabla Z \right) \langle \nabla dP_{T-t} \rangle(Q_t^{(n)}(v), Q_t^{(n)}(v)) dt
$$
\[-n(Q_t^{(n)}(v), N(X_t)) \nabla dP_{T-t} f(N(X_t), Q_t^{(n)}(v)) \, dt \]
\[\equiv -n(Q_t^{(n)}(v), N(X_t)) \nabla dP_{T-t} f(Q_t^{(n)}(v), N) \, dt \]
\[= - \langle Q_t^{(n)}(v), N(X_t) \rangle \nabla dP_{T-t} f(\nabla_N f(N), Q_t^{(n)}(v)) \, dt \]
\[+ \frac{1}{2} (dP_{T-t} f)((\nabla(\nabla_N f(N)) + R(N))(Q_t^{(n)}(v), Q_t^{(n)}(v))) \, dt \]
\[- \nabla dP_{T-t} f(R^{\ast}(Q_t^{(n)}(v), Q_t^{(n)}(v))) \, dt. \tag{3.6} \]

The main difficulty is to clarify the limit of
\[n(Q_t^{(n)}(v), N(X_t)) \nabla dP_{T-t} f(Q_t^{(n)}(v), N),\]
as \(n\) tends to \(\infty\). In addition, information on \(\nabla_N N\) is required to deal with the term
\[\langle Q_t^{(n)}(v), N(X_t) \rangle \nabla dP_{T-t} f(\nabla_N f(N), Q_t^{(n)}(v)) \, dt.\]

To this end, we even need information concerning \(\nabla N\) on the full vector bundle of the boundary if we use \(\tilde{Q}_r\) in the definition of \(M_r(v, v)\) in the above proof, and then it is still non-trivial to check the martingale property. In this respect, working with the functional \(\tilde{Q}_r\) 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
\[
\mathbb{E} \left[ \sup_{t \in [0, T]} \left| \int_0^T h_s \langle W^h_s(v, v), \mathcal{L}_s B_s \rangle \right| \right] \leq 3C(h)^{1/2} \left\{ (3 + \sqrt{10}) \mathbb{E} \left[ \int_0^T \alpha^2(X_s) e^{\int_0^t \kappa^- (X_r) dr + \int_0^t \kappa^+(X_r) \, d\tau_r} \frac{\beta_r^2}{\alpha_r} \, ds \right]^{1/2} \right. \\
+ \frac{1}{2} \mathbb{E} \left[ \int_0^T \beta^2(X_s) e^{\int_0^t \kappa^- (X_r) dr + \int_0^t \kappa^+(X_r) \, d\tau_r} \frac{\beta_r^2}{\alpha_r} \, ds \right]^{1/2} \\
+ \frac{1}{2} \mathbb{E} \left[ \int_0^T \gamma^2(X_s) e^{\int_0^t \kappa^- (X_r) dr + \int_0^t \kappa^+(X_r) \, d\tau_r} \frac{\gamma_r^2}{\alpha_r} \, ds \right]^{1/2} \left. \right\}. \tag{3.7} \]

**Proof.** By the Lenglart inequality and the Minkowski inequality, we have
\[
\mathbb{E} \left[ \sup_{t \in [0, T]} \left| \int_0^T h_s^{(1)} \langle W^h_s(v, v), \mathcal{L}_s B_s \rangle \right| \right] \leq 3 \mathbb{E} \left[ \int_0^T h_s^{(1)} \langle W^h_s(v, v), \mathcal{L}_s B_s \rangle^2 \, ds \right]^{1/2} \tag{3.8} \]
\[
\leq 3 \mathbb{E} \left[ \int_0^T \left| \int_0^T \tilde{Q}_s \tilde{R}(\mathcal{L}_s B_s, \tilde{Q}_s(v)) \, ds \right|^2 \right]^{1/2} \\
+ \frac{3}{2} \mathbb{E} \left[ \int_0^T \left| \int_0^T \tilde{Q}_s (\mathcal{L}_s B_s, \tilde{Q}_s(v)) \, ds \right|^2 \right]^{1/2} \\
+ \frac{3}{2} \mathbb{E} \left[ \int_0^T \left| \int_0^T \tilde{Q}_s \tilde{R}(\mathcal{L}_s B_s, \tilde{Q}_s(v)) \, ds \right|^2 \right]^{1/2} \tag{3.8}. \]

Let
\[\xi_s^{(1)} = \tilde{Q}_s \int_0^T \tilde{Q}_s^{-1} \left( \mathcal{L}_s B_s, \tilde{Q}_s(v) \right) \, ds.\]
\[
\xi_s^{(2)} = \tilde{Q}_s \int_0^s \tilde{Q}_r^{-1} (d'R - R(Z) + \triangledown \text{Ric}_{\tilde{g}})(\tilde{Q}_r(\tilde{h}(r)v), \tilde{Q}_r(v)) \, dr;
\]
\[
\xi_s^{(3)} = \tilde{Q}_s \int_0^s \tilde{Q}_r^{-1} (\triangledown^2 N - R(N)) \tilde{g}(\tilde{Q}_r(\tilde{h}(r)v), \tilde{Q}_r(v)) \, dl_r.
\]

Then, we have
\[
\mathbb{E} \left[ \left( \int_0^{T \wedge \tau_k} h_s^2 |\xi_s^{(1)}|^2 \, ds \right)^{1/2} \right] \leq \mathbb{E} \left[ \sup_{s \in [0, T \wedge \tau_k]} |\xi_s^{(1)}|^2 e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \right]^{1/2} \mathbb{E} \left[ \int_0^{T \wedge \tau_k} h_s^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, ds \right]^{1/2},
\]
and
\[
d\left| e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \xi_s^{(1)} \right|^2 = 2 e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \left( R(//_s dB_s, \tilde{Q}_s(\tilde{h}_s v)) \tilde{Q}_s(v), \xi_s^{(1)} \right) + e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \left[ R^{\#}(\tilde{Q}_s(\tilde{h}_s v), \tilde{Q}_s(v))^2 \right]_{\text{HS}} \, ds
\]
\[
- e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \, \text{Ric}_g(\xi_s^{(1)}, \xi_s^{(1)}) \, ds - e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \left\langle -\nabla_{\xi_s^{(1)}} N, \xi_s^{(1)} \right\rangle \, dl_s
\]
\[
- K^-(X_s) e^{\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \xi_s^{(1)} \right|^2 \, ds - \sigma^-(X_s) \left| e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \xi_s^{(1)} \right|^2 \, dl_s
\]
\[
\leq 2 e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \left( R(//_s dB_s, \tilde{Q}_s(\tilde{h}_s v)) \tilde{Q}_s(v), \xi_s^{(1)} \right) + e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \left[ R^{\#}(\tilde{Q}_s(\tilde{h}_s v), \tilde{Q}_s(v))^2 \right]_{\text{HS}} \, ds
\]
\[
\leq 2 e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \left( R(//_s dB_s, \tilde{Q}_s(\tilde{h}_s v)) \tilde{Q}_s(v), \xi_s^{(1)} \right) + \alpha(X_s)^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, h_s^2 \, ds, \quad s < \tau_k,
\]
which implies
\[
\mathbb{E} \left[ \sup_{s \in [0, T \wedge \tau_k]} |\xi_s^{(1)}|^2 e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \right] \leq \mathbb{E} \left[ \left( \int_0^{T \wedge \tau_k} |\xi_s^{(1)}|^2 \alpha(X_s)^2 \, ds \right)^{1/2} \right] + \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \alpha(X_s)^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, h_s^2 \, ds \right]
\]
\[
\leq 6 \mathbb{E} \left[ \left( \int_0^{T \wedge \tau_k} |\xi_s^{(1)}|^2 \alpha(X_s)^2 \, ds \right)^{1/2} \right] + \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \alpha(X_s)^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, h_s^2 \, ds \right]^{1/2}
\]
\[
\leq 6 \mathbb{E} \left[ \sup_{s \in [0, T \wedge \tau_k]} |\xi_s^{(1)}|^2 e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \right]^{1/2} \left( \int_0^{T \wedge \tau_k} \alpha(X_s)^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, h_s^2 \, ds \right)^{1/2}
\]
\[
+ \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \alpha(X_s)^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, h_s^2 \, ds \right]
\]
\[
\leq \frac{1}{2 \delta} \mathbb{E} \left[ \sup_{s \in [0, T \wedge \tau_k]} |\xi_s^{(1)}|^2 e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \right] + 18 \delta \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \alpha(X_s)^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, h_s^2 \, ds \right]
\]
\[
+ \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \alpha(X_s)^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, h_s^2 \, ds \right], \quad \delta > 0.
\]

Substituting the optimal choice \( \delta = \frac{1}{6} (3 + \sqrt{10}) \), we get
\[
\mathbb{E} \left[ \sup_{s \in [0, T \wedge \tau_k]} |\xi_s^{(1)}|^2 e^{-\int_0^s K^-(X_s) \, dr - \int_0^s \sigma^-(X_s) \, dl_r} \right] \leq (3 + \sqrt{10})^2 \mathbb{E} \left[ \int_0^{T \wedge \tau_k} \alpha(X_s)^2 e^\int_0^s K^-(X_s) \, dr + \int_0^s \sigma^-(X_s) \, dl_r \, h_s^2 \, ds \right].
\]
Combining this with (3.9) and letting $k$ tend to $\infty$ yields

$$
\mathbb{E}\left(\int_0^T h_s^2 (\xi_s^{(1)})^2 \, ds\right)^{1/2}
\leq \mathbb{E}\left[\sup_{s \in [0, T]} |\xi^{(1)}_s|^2 \right]^{1/2} \mathbb{E}\left[\int_0^T h_s^2 e^{\int_0^t K^2(-X_r) \, dr - \int_0^t \sigma^2(-X_r) \, dl} \, ds\right]^{1/2}
\leq (3 + \sqrt{10})\mathbb{E}\left[\int_0^T \alpha(X_s)^2 e^{\int_0^t K^2(-X_r) \, dr - \int_0^t \sigma^2(-X_r) \, dl} \, ds\right]^{1/2} C(h)^{1/2}.
$$

Moreover, for any $\varepsilon > 0$,

$$
d\left(\left|\left|e^{-\frac{1}{2} \int_0^t K^2(-X_r) \, dr - \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \xi_t^{(2)}\right|^2 + \varepsilon\right|\right)^{1/2}
= e^{-\int_0^t K^2(-X_r) \, dr - \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \left(\left|\left|e^{-\frac{1}{2} \int_0^t K^2(-X_r) \, dr - \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \xi_t^{(2)}\right|^2 + \varepsilon\right|\right)^{-1/2}
\times \left(\left(\mathbf{d}^* R - R(Z) + \nabla R\nabla Z\right)\tilde{h}(\tilde{h}(t)v) \tilde{h}(t), \xi_t^{(2)}\right) dt
\leq e^{-\int_0^t K^2(-X_r) \, dr - \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \left(\left|\left|e^{-\frac{1}{2} \int_0^t K^2(-X_r) \, dr - \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \xi_t^{(2)}\right|^2 + \varepsilon\right|\right)^{-1/2}
\times \left(\left(\mathbf{d}^* R - R(Z) + \nabla R\nabla Z\right)\tilde{h}(\tilde{h}(t)v) \tilde{h}(t), \xi_t^{(2)}\right) dt
\leq \beta(X_t) \epsilon_t^{1/2} \int_0^t K^2(-X_r) \, dr + \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \tilde{h}_s \, ds, t < \tau_k.
$$

Taking the integral on both sides, letting $\varepsilon$ tend to 0 and $k$ tend to $\infty$, we then conclude that

$$
\left|\xi_t^{(2)}\right| \leq e^{\frac{1}{2} \int_0^t K^2(-X_r) \, dr + \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \int_0^t \beta(X_s) \epsilon_s^{1/2} \int_0^t K^2(-X_r) \, dr + \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \tilde{h}_s \, ds. \tag{3.11}
$$

With a similar argument, we have

$$
\left|\xi_t^{(3)}\right| \leq e^{\frac{1}{2} \int_0^t K^2(-X_r) \, dr + \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \int_0^t \gamma(X_s) e^{\frac{1}{2} \int_0^t K^2(-X_r) \, dr + \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \tilde{h}_s \, ds. \tag{3.12}
$$

These estimates together imply

$$
\mathbb{E}\left[\sup_{t \in [0, T]} \int_0^t h_s^2 \left(W_s^h(v, v), \left|\% dB_s\right|\right)\right]
\leq 3C(h)^{1/2}\left\{\left(3 + \sqrt{10}\right)\left(\mathbb{E}\left[\int_0^T \alpha(X_s)^2 e^{\int_0^t K^2(-X_r) \, dr - \int_0^t \sigma^2(-X_r) \, dl} \, ds\right]^{1/2}
\frac{1}{2} \left(\mathbb{E}\left[\int_0^T \beta(X_s)^2 e^{\int_0^t K^2(-X_r) \, dr + \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \tilde{h}_s^2 \, ds\right]^{1/2}
\frac{1}{2} \left(\mathbb{E}\left[\int_0^T \gamma(X_s)^2 e^{\int_0^t K^2(-X_r) \, dr + \frac{1}{2} \int_0^t \sigma^2(-X_r) \, dl} \tilde{h}_s^2 \, ds\right]^{1/2}
\right)\right)\right\}.
$$

\textbf{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 $f \in B_b(M)$ and $v \in T_x M$,

$$
(\nabla \mathbf{d} P_{T-t} f)(\tilde{Q}((\tilde{h}(t)v), \tilde{Q}(\tilde{h}(t)v))) + (\mathbf{d} P_{T-t} f)(W_s^h(v, \tilde{h}(t)v))
$$

where $\tilde{Q}((\tilde{h}(t)v), \tilde{Q}(\tilde{h}(t)v))$ is the Cameron-Martin space.
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 \(v \in T_x M\),

\[
M_t(v, v) = \nabla_d P_{T-t} f(\tilde{Q}_t(v), \tilde{Q}_t(v)) + (dP_{T-t} f)(W_t(v, v))
\]

is a local martingale where

\[
W_t(v, v) = \tilde{Q}_t \int_0^t \tilde{Q}_s^{-1} R(\nabla d\tilde{B}_s, \tilde{Q}_s(v)) \tilde{Q}_s(v) \nabla d\tilde{Q}_s(v) \nabla_t \tilde{Q}_s(v) \tilde{Q}_s(v) \nabla R(Z) + \nabla \text{Ric}_Z(\tilde{Q}_s(v), \tilde{Q}_s(v)) ds
\]

\[
- \frac{1}{2} \tilde{Q}_t \int_0^t \tilde{Q}_s^{-1} (d^* R - R(Z) + \nabla \text{Ric}_Z(\tilde{Q}_s(v), \tilde{Q}_s(v)) ds
\]

(3.13)

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

\[
dL f = (\text{tr} \nabla^2 + \nabla_Z \nabla d f - d f(\text{Ric}^Z - \nabla Z)^\sharp); \quad (3.15)
\]

\[
\nabla d(\Delta f) = (\nabla d(\nabla d f)) (\nabla d f) + (\nabla d f) \nabla d(\nabla d f) + (d f(\text{Ric}^Z - \nabla Z)^\sharp) - (d f(\text{Ric}^Z - \nabla Z)^\sharp); \quad (3.16)
\]

\[
\nabla d(Z(f)) = \nabla N(\nabla d f) + (\nabla d f) \nabla d(Z(f)) + (d f(\text{Ric}^Z - \nabla Z)^\sharp) + (d f(\text{Ric}^Z - \nabla Z)^\sharp); \quad (3.17)
\]

\[
\nabla d(N(f)) = \nabla N(\nabla d f) + (\nabla d f) \nabla d(N(f)) + (d f(\text{Ric}^Z - \nabla Z)^\sharp) + (d f(\text{Ric}^Z - \nabla Z)^\sharp); \quad (3.18)
\]

where \(\nabla d f(\nabla N \circ d(\nu, v)) = \nabla d f(\nabla N \circ d(\nu, v)).\) Let

\[
M_t(v, v) = \nabla d P_{T-t} f(\tilde{Q}_t(v), \tilde{Q}_t(v)) + (dP_{T-t} f)(W_t(v, v)). \quad (3.19)
\]

Then by Itô’s formula we have

\[
dM_t(v, v) = (\nabla d d_B \nabla d P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v)) + (\nabla d d_B d P_{T-t} f)(W_t(v, v))
\]

\[
+ (\nabla d P_{T-t} f)(D \tilde{Q}_t(v), \tilde{Q}_t(v)) + (\nabla d P_{T-t} f)(\tilde{Q}_t(v), D \tilde{Q}_t(v))
\]

\[
+ \partial_t (\nabla d P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v)) \text{dt} + \frac{1}{2} (\text{tr} \nabla^2 + \nabla Z)(\nabla d P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v)) \text{dt}
\]

\[
+ \frac{1}{2} \nabla N(\nabla d P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v)) \text{d}l_t + \frac{1}{2} \nabla N(\nabla d P_{T-t} f)(W_t(v, v)) \text{d}l_t
\]

\[
+ (d P_{T-t} f)(D W_t(v, v)) + (\nabla d P_{T-t} f)(W_t(v, v)) \nabla d P_{T-t} f)(W_t(v, v)) \text{dt} + \frac{1}{2} (\text{tr} \nabla^2 + \nabla Z)(d P_{T-t} f)(W_t(v, v)) \text{dt}
\]

(3.20)

Taking into account the commutation properties \([3.16, 3.18]\) and according to the definition of \(\tilde{Q}_t\), for the terms on the right side of \((3.20)\), we observe that

\[
\partial_t (\nabla d P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v)) \text{dt} + (\nabla d P_{T-t} f)(D \tilde{Q}_t(v), \tilde{Q}_t(v)) + (\nabla d P_{T-t} f)(\tilde{Q}_t(v), D \tilde{Q}_t(v))
\]

\[
= - \frac{1}{2} (\text{tr} \nabla^2 + \nabla Z)(\nabla d P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v)) \text{dt}
\]

\[
+ (\nabla d P_{T-t} f)(\nabla d P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v)) \text{dt}
\]

\[
- \nabla d P_{T-t} f((d^* R - R(Z) + \nabla \text{Ric}_Z)\nabla \tilde{Q}_t(v), \tilde{Q}_t(v)) \text{dt} + \frac{1}{2} (d P_{T-t} f)(D W_t(v, v)) \text{dt}
\]
According to the definition of $W_t$, we calculate the quadratic covariation of $\mathbf{d}P_{T-t}f$ and $W_t(v, v)$ as

\[
[D(\mathbf{d}P_{T-t}f), DW_t(v, v) - \mathbf{d}P_{T-t}f(W_t(v, v)) \mathbf{d}t
= \frac{1}{2} \left( \frac{\| \mathbf{d}^2 R - R(Z) + \nabla \text{Ric}_Z \|^2}{\| v_1 \|^2} \right) d_t,
\]

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

\[
[D(\mathbf{d}P_{T-t}f), DW_t(v, v)] = \left[ \mathbf{d}_{/dZ} \mathbf{d}P_{T-t}f, R(\mathbf{d}B_t, \mathbf{d}B_t) \right] d_t,
= \text{tr} \left( \mathbf{d}P_{T-t}f, R(\mathbf{d}B_t, \mathbf{d}B_t) \right) d_t
= \mathbf{d}P_{T-t}f(\mathbf{R}^{\frac{d}{d}}(\mathbf{Q}_t(v), \mathbf{Q}_t(v))) d_t.
\]

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

\[
(\mathbf{d}P_{T-t}f)(DW_t(v, v)) = \left( \frac{1}{2} \left( \frac{\| \mathbf{d}^2 R - R(Z) + \nabla \text{Ric}_Z \|^2}{\| v_1 \|^2} \right) \right) d_t,
\]

We conclude that

\[
\mathbf{d}P_{T-t}f \left( \mathbf{D} \mathbf{Q}_t(v), \mathbf{Q}_t(v) \right) + \left( \nabla \mathbf{d}P_{T-t}f \right) \left( \mathbf{Q}_t(v), D \mathbf{Q}_t(v) \right) + \frac{1}{2} \left( \frac{\| \mathbf{d}^2 R - R(Z) + \nabla \text{Ric}_Z \|^2}{\| v_1 \|^2} \right) d_t
\]

On the other hand, for the terms in (3.20) related to the normal vector on the boundary, we have

\[
\nabla_N(\mathbf{d}P_{T-t}f)(\mathbf{Q}_t(v), \mathbf{Q}_t(v)) d_t + \mathbf{d}P_{T-t}f(W_t(v, v)) d_t
\]

\[
= -\mathbf{d}P_{T-t}f((\nabla N)^2(\mathbf{Q}_t(v), \mathbf{Q}_t(v)) d_t - \mathbf{d}P_{T-t}f((\nabla N)^2(\mathbf{Q}_t(v), \mathbf{Q}_t(v))) d_t
\]

Combining this with (3.20) and (3.21), we obtain

\[
dM_t(v, v) = \frac{1}{2} \mathbf{d}P_{T-t}f \left( \mathbf{V}^2 N + R(N)(\mathbf{Q}_t(v), \mathbf{Q}_t(v))(X_t) d_t - (\nabla N)^2(W_t(v, v))(X_t) d_t \right)
\]

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

Let

\[
M_t^{\hat{h}}(v, v) = \nabla \mathbf{d}P_{T-t}f(\mathbf{Q}_t(h(t)v), \mathbf{Q}_t(v)) + \mathbf{d}P_{T-t}f(W_t^{\hat{h}}(v, v)).
\]
From the definition of $W^h_T(v,v)$, resp. $W^2_T(v,v)$, and in view of the fact that $M_t(v,v)$ is a local martingale, we see that

$$M^h_T(v,v) - \int_0^t (\nabla dP_{T-s,f})(\tilde{Q}_s(h,v), \tilde{Q}_s(v)) \, ds$$

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

$$M^h_T(v,\tilde{h}(t)v) - \int_0^t (\nabla dP_{T-s,f})(\tilde{Q}_s(h,v), \tilde{Q}_s(\tilde{h}(t)v)) \, ds$$

$$- \int_0^t \nabla dP_{T-s,f}(\tilde{Q}_s(h,v), \tilde{Q}_s(\tilde{h}(t)v)) \, ds - \int_0^t (dP_{T-s,f})(W^h_s(v, h,v)) \, ds$$

$$+ \int_0^t \int_0^s (\nabla dP_{T-r,f})(\tilde{Q}_r(h(r)v), \tilde{Q}_r(h,v)) \, dr \, ds$$

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

$$M^h_T(v, \tilde{h}(t)v) - \int_0^t (\nabla dP_{T-s,f})(\tilde{Q}_s(h,v), \tilde{Q}_s(\tilde{h}(t)v)) \, ds$$

$$- \int_0^t \nabla dP_{T-s,f}(\tilde{Q}_s(h,v), \tilde{Q}_s(\tilde{h}(t)v)) \, ds - \int_0^t (dP_{T-s,f})(W^h_s(v, h,v)) \, ds$$

$$+ \int_0^t \int_0^s (\nabla dP_{T-r,f})(\tilde{Q}_r(h(r)v), \tilde{Q}_r(\tilde{h}(t) - \tilde{h}(r)v)) \, dr$$

$$= M^h_T(v,\tilde{h}(t)v) - \int_0^t (dP_{T-s,f})(W^h_s(v, h,v)) \, ds - 2 \int_0^t \nabla dP_{T-s,f}(\tilde{Q}_s(h,v), \tilde{Q}_s(\tilde{h}(t)v)) \, ds$$

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

$$P_{T-s,f}(X_t) = P_{T-f}(x) + \int_0^t dP_{T-s,f}(/ /s dB_s).$$

(3.25)

The usual integration by parts yields

$$\int_0^t (dP_{T-s,f})(W^h_s(v, h,v)) \, ds - P_{T-s,f}(X_t) \int_0^t (W^h_s(v, h,v), / /s dB_s)$$

(3.26)

is a local martingale.

On the other hand, from the Itô formula and the commutation rule (3.15), we obtain

$$d(dP_{T-s,f}(\tilde{Q}_t(v))) = \nabla dP_{T-s,f}(/ /s dB_t, \tilde{Q}_t(v)) - \frac{1}{2} d(\Delta P_{T-s,f})(\tilde{Q}_t(v)) \, dt$$

$$+ \frac{1}{2} (\text{tr} \nabla^2 dP_{T-s,f})(\tilde{Q}_t(v)) \, dt + \frac{1}{2} \nabla_N(dP_{T-s,f})(\tilde{Q}_t(v)) \, dl_t$$

$$- \frac{1}{2} dP_{T-s,f}(\text{Ric}^h(\tilde{Q}_t(v))) \, dl_t - \frac{1}{2} dP_{T-s,f}(\langle \nabla N \rangle^h(\tilde{Q}_t(v))) \, dl_t$$

$$= \nabla dP_{T-s,f}(/ /s dB_t, \tilde{Q}_t(v)) + \frac{1}{2} \nabla_N(dP_{T-s,f})(\tilde{Q}_t(v)) \, dl_t$$

$$- \frac{1}{2} dP_{T-s,f}(\langle \nabla N \rangle^h(\tilde{Q}_t(v))) \, dl_t$$

$$= \nabla dP_{T-s,f}(/ /s dB_t, \tilde{Q}_t(v)) + \frac{1}{2} d(N(P_{T-s,f}))(\tilde{Q}_t(v)) \, dl_t$$

$$= \nabla dP_{T-s,f}(/ /s dB_t, \tilde{Q}_t(v)).$$
It thus follows that
\[
\mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}(t)v)) = \mathbf{d}P_Tf(v) + \int_0^t (\nabla \mathbf{d}P_{T-s}f(\tilde{Q}_s(\tilde{h}_s v))) ds + \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) ds.
\]
Integration by parts yields that
\[
\int_0^t (\nabla \mathbf{d}P_{T-s}f(\tilde{Q}_s(\tilde{h}_s v))) ds - \mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}(t)v)) + \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) ds \int_0^t \langle \tilde{Q}_s(h_s v), \langle /s dB_s \rangle \rangle ds
\]
(3.27)
is also a local martingale. Concerning the last term in (3.27), we note that
\[
\int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) ds \int_0^t \langle \tilde{Q}_s(h_s v), \langle /s dB_s \rangle \rangle - \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) \left( \int_0^s \langle \tilde{Q}_s(h_s v), /r dB_r \rangle ds \right) \right) ds
\]
is also a local martingale. Combining this with (3.27) we conclude that
\[
\int_0^t (\nabla \mathbf{d}P_{T-s}f(\tilde{Q}_s(\tilde{h}_s v))) ds - \mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}(t)v)) + \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) ds \int_0^t \langle \tilde{Q}_s(h_s v), \langle /r dB_r \rangle \rangle ds
\]
(3.28)
is a local martingale.

Using the local martingales (3.26) and (3.28) to replace the last two terms in (3.24), we conclude that
\[
(\nabla \mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}(t)v), \tilde{Q}_t(\tilde{h}(t)v))) + (\mathbf{d}P_{T-t}f(W^h_t(v, \tilde{h}(t)v)) - P_{T-t}f(X_t) \int_0^t \langle W^h_t(v, h_s v), \langle /s dB_s \rangle \rangle ds \]
\[
- 2 \mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}(t)v)) \int_0^t \langle \tilde{Q}_s(h_s v), \langle /s dB_s \rangle \rangle ds
\]
(3.29)
is a local martingale as well. On the other hand, by the product rule for martingales, we have
\[
\left( \int_0^t \langle \tilde{Q}_s(h_s v), \langle /s dB_s \rangle \rangle \right)^2 - \int_0^t |\tilde{Q}_s(h_s v)|^2 ds = 2 \int_0^t \left( \int_0^s \langle \tilde{Q}_r(h(r)v), \langle /s dB_s \rangle \rangle \right) \langle \tilde{Q}_s(h_s v), \langle /s dB_s \rangle \rangle \right) ds \]
(3.30)
which along with (3.25) implies that
\[
P_{T-t}f(X_t) \left( \left( \int_0^t \langle \tilde{Q}_s(h_s v), \langle /s dB_s \rangle \rangle \right)^2 - \int_0^t |\tilde{Q}_s(h_s v)|^2 ds \right)
\]
\[
- 2 \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) \int_0^s \langle \tilde{Q}_r(h(r)v), \langle /r dB_r \rangle \rangle ds
\]
is a local martingale. Applying this observation to (3.29), we finally see that
\[
(\nabla \mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}(t)v)), \tilde{Q}_t(\tilde{h}(t)v))) + (\mathbf{d}P_{T-t}f(W^h_t(v, \tilde{h}(t)v))
\]
\[
- 2 \mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}(t)v)) \int_0^t \langle \tilde{Q}_s(h_s v), \langle /s dB_s \rangle \rangle
\]
\[
- P_{T-t}f(X_t) \int_0^t \langle W^h_t(v, h_s v), \langle /s dB_s \rangle \rangle
\]
\[
+ P_{T-t}f(X_t) \left( \left( \int_0^t \langle \tilde{Q}_s(h_s v), \langle /s dB_s \rangle \rangle \right)^2 - \int_0^t |\tilde{Q}_s(h_s v)|^2 ds \right)
\]
is a local martingale. This completes the proof. □

With the Lemmas 3.3 and 3.4 we are now in position to prove Theorem 3.1.

Proof of Theorem 3.1 Let \( h^\varepsilon_s = 0 \) for \( s \geq (T - \varepsilon) \wedge \tau_k \). Let \( B_k := \{ x : \rho_\alpha(x) \leq k \} \) for \( k \geq 1 \). By the strong Markov property, the boundedness of \( P_f \) on \([\varepsilon, T] \times B_k \) and the boundedness of \(|\mathbf{d}P_f|\) and \(|\text{Hess}_{P_f}|\) on \([\varepsilon, T] \times B_k \) for \( f \in \mathbb{B}(M) \), it follows from Lemma 3.3 that

\[
(\nabla \mathbf{d}P_T) (v, v) = -\mathbb{E} \left[ f(X_T^v) \int_0^{T \wedge \tau_k} \langle W^\varepsilon_s (h^\varepsilon_s v), v \rangle \mathbf{d}B_s \right] + \mathbb{E} \left[ f(X_T^v) \left( \left( \int_0^{T \wedge \tau_k} \langle \tilde{Q}_s (h^\varepsilon_s v), v \rangle \mathbf{d}B_s \right)^2 - \int_0^{T \wedge \tau_k} |\tilde{Q}_s (h^\varepsilon_s v)|^2 \mathbf{d}s \right].
\]

Letting \( \varepsilon \downarrow 0 \), we have

\[
(\nabla \mathbf{d}P_T) (v, v) = -\mathbb{E} \left[ f(X_T^v) \int_0^{T \wedge \tau_k} \langle W^\varepsilon_s (h_s v), v \rangle \mathbf{d}B_s \right] + \mathbb{E} \left[ f(X_T^v) \left( \left( \int_0^{T \wedge \tau_k} \langle \tilde{Q}_s (h_s v), v \rangle \mathbf{d}B_s \right)^2 - \int_0^{T \wedge \tau_k} |\tilde{Q}_s (h_s v)|^2 \mathbf{d}s \right].
\]

By Lemma 3.3 and the observation that there exists a constant \( c > 0 \) such that

\[
\mathbb{E} \left[ \sup_{t \in [0, T]} \left( \left( \int_0^{T \wedge \tau_k} \langle \tilde{Q}_s (h_s v), v \rangle \mathbf{d}B_s \right)^2 - \int_0^{T \wedge \tau_k} |\tilde{Q}_s (h_s v)|^2 \mathbf{d}s \right) \right] \leq c \mathbb{E} \left[ \int_0^T e^{\int_0^s K^- (X_t) \mathbf{d}s + \int_0^s \alpha^- (X_t) \mathbf{d}s + \int_0^s \gamma^- (X_t) \mathbf{d}s} \right],
\]

we complete the proof by Fatou’s lemma. □

3.1. Global Hessian estimates of the semigroup. In this subsection, we continue the discussion on explicit global estimates for \( \text{Hess}_{P_f} \) under suitable conditions.

For \( \varepsilon > 0 \), let

\[
\mathcal{D}_\varepsilon := \{ \phi \in C^2_b (M) : \inf \phi = 1, N \log \phi \geq \sigma^- + \epsilon \}.
\]

(B) The functions \( K, \sigma \) in (3.1) and \( \alpha, \beta, \gamma \) in (3.2) are constant, and there exists \( \phi \in \mathcal{D}_\varepsilon \) for some \( \varepsilon > 0 \) such that

\[
K_{\phi, \xi} := \sup_{x \in M} \{ -L \log \phi + 2q \| \nabla \log \phi \|^2 \} < \infty \tag{3.31}
\]

for some positive constant \( q > 1 \).

By [24, Section 3.2], such \( \phi \) can be constructed if \( \partial M \) 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 is met automatically. Under the global bounds of condition (B), it holds that

\[
\text{Ric}_Z + L \log \phi - 2\| \nabla \log \phi \|^2 \geq K - K_\phi,
\]

where we write \( K_\phi := K_{\phi, 1} \) for simplicity. By [6, Theorem 2.2], we obtain

\[
\| \nabla P_t f \|_\infty \leq \| f \|_\infty e^{-(K-K_{\phi, 1})t}, \quad t > 0, \tag{3.32}
\]

which implies that \( |\nabla P_t f| \) is bounded on \([0, T] \times M \) for \( f \in C^1_b (M) \).

Next local Bismut formulae, as the one in Theorem 3.1 for \( \text{Hess}_{P_f} \), permit us to show that for any \( \varepsilon > 0 \),

\[
|\text{Hess}_{P_f}| \text{ is bounded on } [\varepsilon, T] \times M. \tag{3.33}
\]
This requires for \( x \in M \) and a given relatively compact open neighbourhood \( D \) of \( x \), the construction of an adapted real process \( h_t \) such that \( h_t = 0 \) for \( t \geq T \wedge \tau_D \) and \( \int_0^{T \wedge \tau_D} h_t \, dt = -1 \) with the property that
\[
\mathbb{E} \left[ \int_0^T h_t^2 \, dt \right] < \infty, \quad \text{and} \quad \sup_{x \in M} \mathbb{E}[\|e^{\phi (\sigma^- + \varepsilon) h}\|] < \infty
\]
for \( 1/p + 1/q = 1 \) and \( p, q > 1 \), where \( \tau_D := \inf\{ t \geq 0 : X_t \notin D \} \) denotes the first exit time of \( D \), see estimate (3.5). In Remark 3.6 below we briefly sketch the construction of processes \( h \) with the required properties. Before this, let us introduce the conformal change of the metric such that the boundary under the new metric is convex.

**Remark 3.5** (Conformal change of the metric). We start with a conformal change of the metric \( g \). Since \( \phi \in \mathcal{D}_e \), we have \( \Pi \geq \sigma \geq -(\sigma^- + \varepsilon) \geq -N \log \phi \) and the boundary \( \partial M \) is convex under the metric \( g' := \phi^{-2} g \). Let \( \Delta' \) and \( \nabla' \) 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
\[
U_i = \phi^{-1} (\gamma(s)) P_{\gamma(0), \gamma(s)} P_i V_i, \\
J_i (s) = f(s) U_i, \quad 1 \leq i \leq d,
\]
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 \( f(s) = 1 \wedge \frac{s}{\rho(s, y) / \Delta} \). Then \( J_i (0) = 0 \) and \( J_i (\rho') = \phi^{-1} (\gamma) P'_{\gamma(s), \gamma(s)} V_i, \ 1 \leq i \leq d, \)
\[
\phi^{-2} (\Delta' + Z') \rho' (x, \cdot) (y)
\]
\[
\leq \sum_{i=1}^d \int_0^{\rho'} \left( |[\nabla' \gamma_i] (s) |^2 - \langle R' (\gamma, J_i) J_i, \gamma' \rangle (s) \right) ds + \phi^{-2} (\gamma) Z' \rho' (x, \cdot) (y)
\]
\[
\leq \sum_{i=1}^d \int_0^{\rho'} \left( f(s)^2 \phi^{-2} (\gamma(s)) + f(s)^2 |[\nabla' U_i] (s) |^2 - f(s)^2 \langle R' (\gamma, U_i) U_i, \gamma' \rangle (s) \right) ds + \phi^{-2} (\gamma) Z' \rho' (x, \cdot) (y).
\]
(3.34)

On the other hand,
\[
\phi^{-2} (\gamma) Z' \rho' (x, \cdot) (y)
\]
\[
= \int_0^{\rho'} \frac{d}{ds} \left( \frac{f(s)^2 \phi^{-2} (\gamma(s)) (Z' (\gamma(s)), \gamma') (s)}{d} \right) ds
\]
\[
= 2 \int_0^{\rho'} f(s) f(s) \phi^{-2} (\gamma(s)) (Z'(\gamma(s), \gamma') (s) + f(s)^2 \frac{d}{ds} \left( \phi^{-2} (\gamma) (Z'(\gamma), \gamma') (s) \right) ds
\]
\[
= 2 \int_0^{\rho'} f(s) f(s) \phi^{-2} (\gamma(s)) (Z'(\gamma), \gamma') (s) ds
\]
\[
+ \int_0^{\rho'} f(s)^2 \phi^{-2} (\gamma(s)) ([\nabla' Z' \circ \gamma, \gamma'] (s) ds
\]
\[
- 2 \int_0^{\rho'} f(s)^2 \phi^{-2} (\gamma(s)) (\nabla \log \phi (\gamma(s)), \gamma(s)) (Z'(\gamma(s)), \gamma') (s) ds
\]
(3.35)

Note that \( |\gamma| = \phi \). We then conclude from (3.34) and (3.35) that
\[
\phi^{-2} (\gamma (\Delta' + Z') \rho' (x, \cdot) (y)
\]
Remark 3.6 which proves (3.36) and (3.37).

The next step is to check that for \( \alpha > 0 \),

\[
\sup_{x \in M} \mathbb{E}^x \left[ e^{\sigma \phi - \varepsilon t} \right] < \sup_{x \in M} \mathbb{E}^x \left[ e^{\sigma (\phi - \varepsilon) t} \right] < \| \phi \|_\infty \exp \left( \frac{\alpha}{2} K_{\phi, \alpha} t \right) < \infty, \tag{3.36}
\]

\[
\sup_{x \in M} \mathbb{E}^x \left[ e^{(\sigma \phi - \varepsilon) t} \right] < \| \phi \|_\infty \exp \left( K \phi t \right) < \infty, \tag{3.37}
\]

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,

\[
d\phi^{-\alpha}(X_t) = \langle \nabla \phi^{-\alpha}(X_t), \mu d\mathbf{B}_t \rangle + \frac{1}{2} L\phi^{-\alpha}(X_t) dt + \frac{1}{2} N\phi^{-\alpha}(X_t) d\mathbf{L}_t
\]

\[
\leq \langle \nabla \phi^{-\alpha}(X_t), \mu d\mathbf{B}_t \rangle - \alpha \phi^{-\alpha}(X_t) \left(-\frac{1}{2} K_{\phi, \alpha} dt + \frac{1}{2} N \log \phi(X_t) d\mathbf{L}_t \right)
\]

\[
\leq \langle \nabla \phi^{-\alpha}(X_t), \mu d\mathbf{B}_t \rangle - \alpha \phi^{-\alpha}(X_t) \left(-\frac{1}{2} K_{\phi, \alpha} dt + \frac{1}{2} (\sigma^- + \varepsilon) d\mathbf{L}_t \right),
\]

then

\[ \phi^{-\alpha}(X_t) \exp \left( -\frac{\alpha}{2} K_{\phi, \alpha} t + \frac{\alpha}{2} (\sigma^- + \varepsilon) t \right) \]

is a local submartingale. Therefore, by Fatou’s lemma and taking into account that \( \phi \geq 1 \), we get

\[ \mathbb{E} \left[ \phi^{-\alpha}(X_T) \exp \left( -\frac{\alpha}{2} K_{\phi, \alpha} t + \frac{\alpha}{2} (\sigma^- + \varepsilon) t \right) \right] \leq 1, \]

which proves (3.36) and (3.37).

Remark 3.6 (Construction of \( h \)). Let \( D = B'(x, k) \) where \( B'(x, k) := \{ y \in M : \rho'(x, y) \leq k \} \) for some \( k > 0 \). We search for an adapted real process \( h = h_k \) satisfying \( \int_0^T (h_k)_s ds = -1 \) for \( t \geq T \wedge \tau_k \) and

\[ \mathbb{E}^x \left[ \int_0^T (h_k^2)_s ds \right] < \infty \]

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

\[ (h_k)_t = 1 + \int_0^t (h_k)_s ds \]

so that \( (h_k)_0 = 1 \) and \( (h_k)_t = 0 \) for \( t \geq T \wedge \tau_k \). For \( k > 0 \) let

\[ \theta_k(p) = \cos \left( \frac{\pi \rho'(x, p)}{2k} \right), \quad p \in B(x, k). \]
Then set \((\bar{h}_k)_s = (h \circ \ell_k)_s\) where a function \(h \in C^1([0, T])\) is chosen so that \(\bar{h}(0) = 1, \bar{h}(T) = 0\) with \((\bar{h})' = h\) and
\[
\ell_k(s) = \int_0^s \theta_k^{-2}(X_r(x)) \mathbf{1}_{\{r < \sigma_k(T)\}} \, dr,
\]
\[
\sigma_k(s) = \inf \left\{ r \geq 0 : \int_0^r \theta_k^{-2}(X_u(x)) \, du \geq s \right\}.
\]
This construction is due to [21], the claim follows from [22, 21], see the proof of [7, Lemma 2.1] for the details. For this \(\bar{h}_k\), we have
\[
\mathbb{E} \left[ \int_0^{t \wedge t_k} h_k^2(s) \, ds \right] = \mathbb{E} \left[ \int_0^{\theta_k(t)} (h \circ \ell_k)^2(s) \theta_k^{-4p}(X_s(x)) \, ds \right] = \int_0^t h^2(s) \mathbb{E} [\theta_k^{-4p+2}(X_s'(x))] \, ds
\]
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 [21] 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 \(N p'(x, \cdot) \leq 0\), that
\[
\mathbb{E} [\theta_k^{-4p+2}(X'_k(x))] \leq \theta_k(x)^{-4p+2} e^{c(\theta_k)s},
\]
where
\[
c(\theta_k) = (2p - 1) \sup_{B'(x, k)} \left\{ \left( \frac{4p - 1}{2} |\nabla \theta_k|^2 - \theta_k L \theta_k \right) \right\}.
\]
Using \(\theta_k(x) = 1\) and taking
\[
\bar{h}(t) = 1 - \frac{c(\theta_k)}{p(1 - e^{-c(\theta_k)t/p})} \int_0^t e^{-c(\theta_k)r/p} \, dr
\]
we obtain
\[
\mathbb{E} \left[ \int_0^{T \wedge t} h_k^2(s) \, ds \right] \leq \int_0^T \left( \frac{c(\theta_k)}{p} \right)^{2p} \frac{e^{-c(\theta_k)s}}{(1 - e^{-c(\theta_k)t/p})^{2p}} \, ds \leq \left( \frac{c(\theta_k)}{p} \right)^{2p} \frac{T}{(1 - e^{-c(\theta_k)t/p})^{2p}} \leq \frac{e^{c(\theta_k)t}}{T^{2p-1}}.
\]
Indeed, according to the definition of \(\theta_k\), we have
\[
|\nabla \theta_k| \leq \frac{\pi}{2k},
\]
and by the Laplacian comparison theorem
\[
-(\theta_k L \theta_k)(p) \leq \cos \left( \frac{\pi p'(x, p)}{2k} \right) \sin \left( \frac{\pi p'(x, p)}{2k} \right) \frac{\pi}{2k} L p'(x, \cdot)(p) + \cos \left( \frac{\pi p'(x, p)}{2k} \right) \frac{\pi^2}{4k^2}
\]
\[
\leq \frac{\pi^2}{4k^2} \left( c(x) + \frac{d}{\rho'(x, p)} + (K - K_0)p'(x, p) \right) + \frac{\pi^2}{4k^2}
\]
\[
\leq \frac{c(x)^2}{4k} + \frac{(d + 1)^2}{4k^2} + \frac{(K - K_0)^2}{4}, \quad \rho'(x, p) \leq k
\]
for some constant \(c(x) > 0\), where
\[
\text{Ric}_Z + L \log \phi - 2|\nabla \log \phi|^2 \geq K - K_0.
\]
We then conclude that
\[ c(\theta_k) \leq (2p - 1) \left( \frac{c(x)\pi^2}{2k} + \frac{(2d + 4p + 1)\pi^2}{4k^2} + \frac{(K - K_\phi)^2}{2} \right). \]

Then by the local version of the Bismut type Hessian formula, we have
\[
|\operatorname{Hess}_{P_T} f(x)| \leq 3 e^{K_T} \|f\|_0 \left[ \mathbb{E} \int_0^T h_k^2(s) e^{\sigma^\top l_s} \, ds \right]^{1/2} \left\{ (3 + \sqrt{10})\alpha + \frac{\beta}{2} \right\} \left( \mathbb{E} \int_0^T e^{\sigma^\top l_s} \, ds \right)^{1/2} \]
\[ + \frac{\gamma}{2} \left( \mathbb{E} \int_0^T e^{\sigma^\top l_s} \, ds \right)^{1/2} + \frac{2}{3} \left( \mathbb{E} \int_0^T h_k^2(s) e^{\sigma^\top l_s} \, ds \right)^{1/2} \]
\[ \leq 3 e^{K_T} \|f\|_0 \left( e^{K_{\phi}T} T^{1/q} \left( \frac{e^{2\alpha(\theta_k)T} T^{1/p}}{T^{2p-1}} \right)^{1/2} \right) \left\{ (3 + \sqrt{10})\alpha + \frac{\beta}{2} \right\} \left( e^{K_{\phi}T} T \right)^{1/2} \]
\[ + \frac{\gamma}{2} \left( \frac{\|\phi\|_0 e^{K_{\phi}T}}{\sigma^\top + \epsilon} \right)^{1/2} + \frac{2}{3} \left( \frac{\|\phi\|_0 e^{K_{\phi}T}}{\sigma^\top + \epsilon} \right)^{1/2} \left( \frac{T^{2p-1}}{T^{2p-1}} \right)^{1/2} \right\} \cdot \]

When the manifold is non-compact, letting \( k \) tend to \( \infty \) yields
\[
|\operatorname{Hess}_{P_T} f(x)| \leq 3 e^{K_T} \|f\|_0 \left( e^{K_{\phi}T + \frac{2p-1}{p-1}(K - K_\phi)^2 T^{-1}} \right)^{1/2} \left\{ (3 + \sqrt{10})\alpha + \frac{\beta}{2} \right\} \left( e^{K_{\phi}T} T \right)^{1/2} \]
\[ + \frac{\gamma}{2} \left( \frac{e^{K_{\phi}T}}{\sigma^\top + \epsilon} \right)^{1/2} + \frac{2}{3} \left( \frac{e^{K_{\phi}T + \frac{2p-1}{p-1}(K - K_\phi)^2 T^{-1}}}{\sigma^\top + \epsilon} \right)^{1/2} \right\} \cdot \]

for \( T > 0. \)

**Theorem 3.7.** Assume that condition \((B)\) holds. Let \( h \) be a non-positive and adapted process satisfying \( \int_0^T h_s \, ds = -1 \) and
\[
\mathbb{E}^x \left[ \int_0^T (h_s^2 + \bar{h}_s^2) e^{\sigma^\top l_s} \, ds \right] < \infty,
\]
where \( \bar{h}_t = 1 + \int_0^t h_s \, ds. \) Then, for \( f \in \mathcal{B}_b(M) \) and \( v \in T_x M, \)
\[
\operatorname{Hess}_{P_T f}(v, v)(x) = - \mathbb{E}^x \left[ f(X_T) \int_0^T \langle W_s^h(v, h_s v), \mathbb{I}_s \rangle dB_s \right] \]
\[ + \mathbb{E}^x \left[ f(X_T) \left( \int_0^T \langle \bar{Q}_s(h_s v), \mathbb{I}_s \rangle dB_s \right)^2 - \int_0^T |\bar{Q}_s(h_s v)|^2 \, ds \right].
\]
Moreover, for \( T > 0 \) and \( f \in \mathcal{B}_b(M), \)
\[
|\operatorname{Hess}_{P_T f}(x)| \leq \left( \alpha + \frac{\beta}{2} \sqrt{T} + \frac{2}{T} \right) e^{K_T} \mathbb{E}^x \left[ e^{\sigma^\top l_T} \right] (P_T f^2)^{1/2} \]
\[ + \frac{\gamma}{2} \left( \frac{e^{K_T}}{\sqrt{T}} \right)^{1/2} \left( \mathbb{E}^x \left( \int_0^T e^{\sigma^\top l_s} \, ds \right)^2 \right)^{1/2} \left( P_T f^2 \right)^{1/2}. \]

**Proof.** For the adapted process \( h, \) we see from Lemma 3.3 that
\[
\mathbb{E} \left[ \sup_{|v| \leq 0.7} \int_0^T h_s \langle W_s^h(v, v), \mathbb{I}_s \rangle dB_s \right] \]
\[ \leq e^{K_T} \left( \mathbb{E}^x \int_0^T e^{\sigma^\top l_s} h_s^2 \, ds \right)^{1/2} \left\{ \alpha(3 + \sqrt{10}) \left( \mathbb{E} \int_0^T e^{\sigma^\top l_s} \bar{h}_s^2 \, ds \right)^{1/2} \right\} \]
\[ + \frac{\beta}{2} \left( \mathbb{E} \int_0^T e^{\sigma^\top l_s} \bar{h}_s^2 \, ds \right)^{1/2} + \frac{\gamma}{2} \left( \mathbb{E} \int_0^T e^{\sigma^\top l_s} \bar{h}_s^2 \, ds \right)^{1/2} < \infty, \]
and
\[
\mathbb{E} \left[ \left( \int_0^T \langle \tilde{Q}_s(h_s v), /, dB_s \rangle \right)^2 - \int_0^T |\tilde{Q}_s(h_s v)|^2 \, ds \right] \\
\leq 2 e^{K^T} \mathbb{E} \left( \int_0^T e^{\sigma l_t} h_t^2 \, ds \right) < \infty.
\]

Moreover, by (3.33) both \(|\nabla f|\) and \(|\text{Hess}_{P_{\epsilon} f}|\) are bounded on \([\epsilon, T] \times M\). We complete the proof by following the steps as in the proof of Theorem 3.1 to obtain from (3.13) \(Hess_{P_{\epsilon} f}(v, v)(x) = -\mathbb{E}^x \left[ f(X_T) \int_0^T \langle W_{\alpha}^\beta(v, h(s)v), /, dB_s \rangle \right] \]
\[+ \mathbb{E}^x \left[ f(X_T) \left( \int_0^T \langle \tilde{Q}_s(h_s v), /, dB_s \rangle \right)^2 - \int_0^T |\tilde{Q}_s(h_s v)|^2 \, ds \right]. \quad (3.38)\]

Indeed, using the mentioned boundedness on \([\epsilon, T] \times M\), we get (3.38) first for \(f\) replaced by \(P_{\epsilon} f\) and from this (3.38) is obtained by letting \(\epsilon\) 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
\[|\text{Hess}_{P_{\epsilon} f}|(x) \leq (P_T|f|^2)^{1/2} \left[ \mathbb{E} \left( \int_0^T \langle W_{\alpha}^\beta(v, h(s)v), /, dB_s \rangle \right)^2 \right]^{1/2} \]
\[+ 2(P_T|f|^2)^{1/2} \int_0^T e^{\sigma l_t} h_t^2(s) \, ds \]
\[\leq \frac{1}{T} (P_T|f|^2)^{1/2} \left[ \mathbb{E} \left( \int_0^T \langle \tilde{Q}_s \int_0^s \tilde{Q}_r^{-1}(\nabla R - R(Z) + \nabla \text{Ric}_2) \tilde{Q}_r(h(r)v), \tilde{Q}_r(v) \rangle \, dr \right)^2 \, ds \right]^{1/2} \]
\[+ \frac{1}{2T} (P_T|f|^2)^{1/2} \left[ \mathbb{E} \left( \int_0^T \langle \tilde{Q}_s \int_0^s \tilde{Q}_r^{-1} \nabla^2 N - \nabla(N) \tilde{Q}_r(h(r)v), \tilde{Q}_r(v) \rangle \, dr \right)^2 \, ds \right]^{1/2} \]
\[+ \frac{1}{T^2} (P_T|f|^2)^{1/2} e^{KT} \int_0^T \mathbb{E}[e^{\sigma l_t}] \, ds \]
\[\leq \left( \alpha + \frac{\beta}{2\sqrt{T}} + \frac{2}{T} \right) e^{KT} \mathbb{E}^x[e^{\sigma l_t}] (P_T|f|^2)^{1/2} \]
\[+ \frac{\gamma}{2\sqrt{T}} e^{KT} \mathbb{E}^x[e^{\sigma l_t}]^{1/2} \left[ \mathbb{E}^x \left( \int_0^T e^{l_t} \, dl_t \right)^2 \right]^{1/2} \]
\[\left( P_T|f|^2 \right)^{1/2}. \quad \Box\]

**Corollary 3.8.** Assume that condition (B) holds with \(\sigma = \gamma = 0\). Then
\[|\text{Hess}_{P_{\epsilon} f}|(x) \leq \left( \alpha + \frac{\sqrt{T}}{2} + \frac{2}{T} \right) e^{KT} (P_T|f|^2)^{1/2} \]
for \(T > 0\) and \(f \in \mathcal{B}_b(M)\).

**Proof.** This is a direct consequence of the estimate in Theorem 3.7 \(\Box\)

**Remark 3.9.** Note that the condition \(-\nabla N \geq 0\), i.e. \(\sigma = 0\) implies \(\Pi \geq 0\). It has been proved in [24], that then
\[|\nabla P_{\epsilon} f|(x) \leq \frac{e^{KT}}{\sqrt{T}} (P_T|f|^2)^{1/2} < \infty \quad (3.39)\]
for any $t > 0$, see also \[8\].

4. Hessian formula with gradient terms

The main theorem in this section relies on the fact that under (B), along with suitable conditions, the local martingale $M_t$ defined in (3.19) is a true martingale. This fact will be exploited for further applications.

**Theorem 4.1.** Assume that condition (B) holds. For $T > 0$ let $h \in C([0, T])$ such that $\int_0^T h(t)\,dt = -1$. Then, for $v \in T_xM$ and $f \in C^1_b(M)$ such that $|\nabla f|$ is bounded,

$$
\text{Hess}_{P_t,f}(v,v) = \mathbb{E} \left[ -df(Q_t(v)) \int_0^T \langle \tilde{Q}_t(h(s)v), \|v\|d\mathbb{B}_s \rangle + df(W^h_t(v,v)) \right] 
$$

where $h(t) = 1 + \int_0^t h(s)\,ds$. Moreover,

$$
|\text{Hess}_{P_t,f}| \leq \left( \alpha \sqrt{T} + \frac{\beta}{2} T + \frac{1}{\sqrt{T}} \right) \mathbb{E} \left[ e^{\sigma^2 - \sigma T} \right] e^{K - T} \|\nabla f\|_\infty 
+ \frac{\gamma}{2} \mathbb{E} \left[ e^{\frac{1}{2} \sigma^2 - \sigma T} \int_0^T e^{\frac{1}{2} \sigma^2 - \sigma T} \,dl_s \right] e^{K - T} \|\nabla f\|_\infty.
$$

**Proof.** Recall that by (5.22)

$$
\nabla dP_{T-t}f(\tilde{Q}_t(h(t)v), \tilde{Q}_t(v)) + (dP_{T-t}f)(W^h_t(v,v)) - \int_0^T (\nabla dP_{T-s}f)(\tilde{Q}_s(h(s)v), \tilde{Q}_s(v))\,ds
$$

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

$$
\int_0^T (\nabla dP_{T-s}f)(\tilde{Q}_s(h(s)v), \tilde{Q}_s(v))\,ds - dP_{T-t}f(\tilde{Q}_t(v)) \int_0^T \langle \tilde{Q}_s(h(s)v), \|v\|d\mathbb{B}_s \rangle
$$

is a local martingale as well. We conclude that

$$
\nabla dP_{T-t}f(\tilde{Q}_t(h(t)v), \tilde{Q}_t(v)) + (dP_{T-t}f)(W^h_t(v,v)) - dP_{T-t}f(\tilde{Q}_t(v)) \int_0^T \langle \tilde{Q}_s(h(s)v), \|v\|d\mathbb{B}_s \rangle
$$

is a local martingale. As $\|R\|_{\infty} < \infty$, Ric $\geq K$ for some constant $K$, and $-\nabla N \geq \sigma$ for some non-positive constant $\sigma$,

$$
\|d^*R + \nabla \text{Ric}_{\text{g}} - R(Z)\|_{\infty} < \infty \quad \text{and} \quad \|\nabla^2 N + R(N)\|_{\infty} < \infty,
$$

we first get

$$
\sup_{s \in [0,T]} \mathbb{E}[\tilde{Q}_s(v)^2] \leq \sup_{s \in [0,T]} e^{-Ks} \mathbb{E}[e^{\sigma T}] < \infty,
$$

and then

$$
\mathbb{E}\left[ W^h_{T-t}(v,v) \right]
\leq \mathbb{E}\left[ e^{K^{-1} + \sigma h_T} \right]^{1/2} \mathbb{E}\left[ e^{-K^{-1} + \sigma h_T} \left[ e^{\xi (1)} \right]^{1/2} \right] + \frac{1}{2} \mathbb{E}\left[ \xi (2) \right] + \frac{1}{2} \mathbb{E}\left[ \xi (3) \right]
\leq \alpha \mathbb{E}\left[ e^{K^{-1} + \sigma h_T} \right]^{1/2} \int_0^T \mathbb{E}\left[ e^{-K^{-1} + \sigma h_T} \right]^{1/2} \left[ e^{\xi (1)} \right]^{1/2} + \frac{\beta}{2} \mathbb{E}\left[ e^{K^{-1} + \sigma h_T} \right] \int_0^T e^{\xi (1)} \,dl_s
\leq \frac{\gamma}{2} \mathbb{E}\left[ e^{K^{-1} + \sigma h_T} \right] \int_0^T e^{\xi (1)} \,dl_s
$$

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

$$
\mathbb{E}\left[ W^h_{T-t}(v,v) \right] < \infty.
$$
Recall that $|\nabla P.f|$ is bounded on $[0, T] \times M$ and $|\nabla d P.f|$ is bounded on $[\varepsilon, T] \times M$ for $0 < \varepsilon < T$, see Remark 3.6. 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 $|\nabla P.f|$ and $|\nabla d P.f|$ are bounded on $[0, T] \times M$, so that (3.22) is a true martingale. By taking expectations and passing to the limit as $\varepsilon \downarrow 0$, inequality (4.1) is obtained.

Let now $\bar{h}_s = \frac{t-s}{T-s}$ for $s \in [0, T]$. It is straightforward to deduce from (4.1) and (4.2) that

$$\mathbb{E}[|\nabla f|^2] \leq \frac{1}{\sqrt{\int_0^t e^{K_r} dr}} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} e^{-Kt/2} (P_{\varepsilon} |\nabla f|^2)^{1/2}.$$  

(ii) If $\text{Ric}_V \geq K$, $\nabla N \leq 0$, then for $f \in C^1_b(M)$,

$$|\text{Hess}_{P_{\varepsilon} f}| \leq \left(\frac{1}{\sqrt{\int_0^t e^{K_r} dr}} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right) e^{-Kt/2} (P_{\varepsilon} |\nabla f|^2)^{1/2}.$$  

Proof. If $\nabla N \leq 0$ and $\nabla^2 N + R(N) = 0$, then $\Pi \geq 0$, which together with $\text{Ric}_Z \geq K$, implies by [24] Corollary 3.2.6] that $|\nabla P.f|$ is bounded on $[0, t] \times M$. Choosing $\bar{h}$ such that $|\bar{h}| \leq 1$, we have

$$\mathbb{E}[|\nabla f|^2] \leq \frac{\alpha}{\sqrt{K}} e^{-Kt/2} \left(\int_0^t e^{-K_r} ds \right)^{1/2}.$$

Combining this with Theorem 4.1, we conclude that

$$|\text{Hess}_{P_{\varepsilon} f}| \leq (P_{\varepsilon} |\nabla f|^2)^{1/2} e^{-Kt/2} \left(\int_0^t e^{-K_r} h^2(s) ds \right)^{1/2} + (P_{\varepsilon} |\nabla f|^2)^{1/2} \left(\frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right) e^{-Kt/2}.$$  

The following choice of $h$:

$$h(s) = -\frac{e^{K_s}}{\int_0^t e^{K_r} dr}, \quad s \in [0, t],$$  

then leads to the first inequality.

If $\nabla N = 0$ and $\text{Ric}_V = K$, then $\tilde{Q}_t = e^{-Kt/2} f$, and

$$\text{Hess}_{P_{\varepsilon} f}(v, v)$$

$$= e^{-Kt/2} \mathbb{E} \left[ -d f (f_{\varepsilon} v) \int_0^t e^{-K_r} h(s)(v, d B_s) + d f \left( \int_0^t e^{-K_r} R(\tilde{h}(s)v, s) ds \right) \right]$$

$$- \frac{1}{2} e^{-Kt/2} \mathbb{E} \left[ d f \left( \int_0^t e^{-K_r} \tilde{h}(s)v, s \right) ds \right].$$
This implies
\[
|\text{Hess}_{P_t}f|_{\text{HS}} \leq e^{-Kt/2} (P_t |\nabla f|^2)^{1/2} \left( \int_0^t e^{-Ks} h(s)^2 \, ds \right)^{1/2} + \alpha (P_t |\nabla f|^2)^{1/2} \left( \int_0^t e^{-Ks} \, ds \right)^{1/2} + \frac{n\beta}{2} e^{-Kt/2} (P_t |\nabla f|^2)^{1/2} \int_0^t e^{-Ks/2} \, ds.
\]

Choosing \( h \) as in (4.3) then yields item (ii).

5. Stein method and log-Sobolev inequality

In this section, we consider \( L = \Delta - \nabla V \) for \( V \in C^2(M) \) such that
\[
\mu(dx) = e^{-V(x)} \text{vol}(dx)
\]
is a probability measure where \( \text{vol}(dx) \) denotes the volume measure on \( M \). Let \( P_t = e^{tL_\mu} \) be the contraction semigroup generated by \( L \) on \( L^2(\mu) \) with Neumann boundary conditions. In \cite{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 kind of 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 \( \tau_\nu: M \to T^*M \times T^*M \) on \( M \) is said to be a Stein kernel for a probability measure \( \nu \) on \( M \) if
\[
\int \langle \nabla V, \nabla f \rangle \, d\nu = \int \langle \tau_\nu, \text{Hess} f \rangle_{\text{HS}} \, d\nu, \quad f \in C^\infty_N(L),
\]
where \( \nabla V \) is the first order part of the operator \( L \) and where
\[
C^\infty_N(L) = \{ f \in C^\infty(M): Nf|_{\partial M} = 0, Lf \in B_b(M) \}.
\]
Since
\[
\int Lf \, d\mu = \int N(f) \, d\mu = 0
\]
for \( f \in C^\infty_N(L) \), it is easy to see that the identity map \( \text{id} \) is a Stein kernel for \( \mu \).

**Definition 5.1.** Let \( \tau_\nu \) be a Stein kernel for \( \nu \). The Stein discrepancy is defined as
\[
S(\nu|\mu)^2 = \inf \int_M |\tau_\nu - \text{id}|^2_{\text{HS}} \, d\nu,
\]
where the infimum is taken over all Stein kernels of \( \nu \), 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
\[
\text{Ric}_V := \text{Ric} + \text{Hess}_V \geq K, \quad II \geq 0
\]
holds for some positive constant \( K \). Then the classical logarithmic Sobolev inequality with respect to the measure \( \mu \) indicates that for every probability measure \( d\nu = h \, d\mu \) with smooth density \( h : M \to \mathbb{R}_+ \),
\[
H(\nu|\mu) \leq \frac{1}{2K} I(\nu|\mu), \quad (5.2)
\]
where
\[
H(\nu|\mu) = \int h \log h \, d\mu = \text{Ent}_\mu(h)
\]
is the relative entropy of \( dv = h \, d\mu \) with respect to \( \mu \) and
\[
I(\nu|\mu) = \int \frac{\nabla h^2}{h} \, d\mu = I_\mu(h)
\]
the Fisher information of \( \nu \) (or \( h \)) with respect to \( \mu \). This result is known as the Bakry-Émery criterion due to [2] for the logarithmic Sobolev inequality. Let us recall the following observations.

**Lemma 5.2.** Assume that
\[
\text{Ric}_V \geq K \quad \text{and} \quad \nu \geq 0
\]
for some positive constant \( K \), and let \( \tau_V \) be a Stein kernel for \( dv = h \, d\mu \) where \( h \in C^\infty_0(M) \). For \( t > 0 \) let \( dv = \nu \, d\mu \). Then

(i) (Integrated de Bruijn's formula)
\[
H(\nu|\mu) = \text{Ent}_\mu(h) = \frac{1}{2} \int_0^\infty I_\mu(P_t h) \, dt;
\]

(ii) (Exponential decay of Fisher information)
\[
I_\mu(P_t h) = I(\nu|\mu) = \frac{1}{2} \nu \text{Ent}_\mu(h) = e^{-Kt} I_\mu(h), \quad t \geq 0.
\]

**Proof.** Since \( N(P_t f \log P_t f) = 0 \) and \( \left(\frac{1}{2}L - \frac{\partial}{\partial t}\right) (P_t h \log P_t h) = \frac{\|P_t h\|^2}{2P_t h} \), we have
\[
H(\nu|\mu) = \int_M h \log h \, d\mu - \int_M \int_0^\infty \frac{d(P_t h \log P_t h)}{dt} \, dt \, d\mu
\]
\[
= \int_0^\infty \left( \int_M \left( \frac{1}{2}L - \frac{\partial}{\partial t} \right) (P_t h \log P_t h) \right) \, dt
\]
\[
= \frac{1}{2} \int_0^\infty \int_M \frac{\|P_t h\|^2}{P_t h} \, d\mu \, dt.
\]
The second assertion can be checked by observing first from the derivative formula that
\[
\|\nabla P_t h\|^2 \leq e^{-Kt} \left( \int_M \|\nabla (\sqrt{h})\|^2 \right) \leq 4 e^{-Kt} (P_t h) P_t |\nabla \sqrt{h}|^2
\]
which implies
\[
I_\mu(P_t h) = \int_M \|\nabla P_t h\|^2 \, d\mu \leq 4 \int_M e^{-Kt} (P_t h) P_t |\nabla \sqrt{h}|^2 \, d\mu
\]
\[
= 4 \int_M e^{-Kt} P_t |\nabla \sqrt{h}|^2 \, d\mu = 4 e^{-Kt} \int_M |\nabla \sqrt{h}|^2 \, d\mu
\]
\[
= e^{-Kt} I(\nu|\mu) = e^{-Kt} I_\mu(h). \quad \Box
\]

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 5.3.** Assume that \( \alpha := \|R\|_\infty < \infty \), \( \beta := \|\nabla \text{Ric}_V^0 + d^* R + R(\nabla V)\|_\infty < \infty \) and
\[
\nabla^2 N + R(N) = 0.
\]

Let \( dv = h \, d\mu \) for \( h \in C^\infty_0(M) \).

(i) If \( \text{Ric}_V \geq K \), \( \nabla N \leq 0 \), then
\[
I_\mu(P_t h) \leq h^2 \left( \frac{1}{\int_0^\infty e^{Kr} \, dr} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right)^2 e^{-Kt} S^2(\nu|\mu).
\]
(ii) If $\text{Ric}_V = K$, $\nabla N = 0$, then

$$I_\mu(P,h) \leq \left( \frac{1}{\sqrt{\int_0^2 e^{Kr} dr}} + \frac{n\alpha}{\sqrt{K}} + \frac{n\beta}{K} \right)^2 e^{-Kt} S^2(\nu|h).$$

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

$$I_\mu(P,h) = - \int (g_t)P_t h \, d\mu = - \int (LP_t g_t)h \, d\mu = - \int L P_t g_t, \, dv.$$ 

Hence according to the definition of Stein kernel and since $P_t g_t \in C_0^\infty(L)$, we have

$$I_\mu(P,h) = - \int \langle \text{id}, \text{Hess}_{P_t g_t} \rangle_{\text{HS}} \, dv - \int \langle \nabla V, \nabla P_t g_t \rangle \, dv$$

$$= \int \langle \tau - \text{id}, \text{Hess}_{P_t g_t} \rangle_{\text{HS}} \, dv.$$ 

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

$$I_\mu(P,h) = \int \langle \tau - \text{id}, \text{Hess}_{P_t g_t} \rangle_{\text{HS}} \, dv$$

$$\leq \left( \int |\tau - \text{id}|_{\text{HS}}^2 \, dv \right)^{1/2} \left( \int |\text{Hess}_{P_t g_t}|_{\text{HS}}^2 \, dv \right)^{1/2}$$

$$\leq n \left( \int |\tau - \text{id}|_{\text{HS}}^2 \, dv \right)^{1/2} \left( \frac{1}{\sqrt{\int_0^2 e^{Kr} dr}} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right)^2 e^{-Kt} \int P_t |\nabla g_t|^2 \, dv$$

where Corollary 4.2 is used for the function $g_t = \log P_t h$. Since

$$\int P_t |\nabla g_t|^2 \, dv = \int \frac{P_t |\nabla g_t|^2 h \, d\mu}{P_t h} = \int |\nabla g_t|^2 P_t h \, d\mu = \int |\nabla P_t h|^2 \, d\mu = I_\mu(P,h),$$

it then follows that

$$I_\mu(P,h) \leq n \left( \frac{1}{\sqrt{\int_0^2 e^{Kr} dr}} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right)^2 e^{-Kt} \int |\tau - \text{id}|_{\text{HS}}^2 \, dv.$$ 

Taking the infimum over all Stein kernels of $\nu$, we finish the proof of (i). Along the same steps, item (ii) can be proved by means of Corollary 4.2 as well. \hfill \Box

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

**Theorem 5.4.** Assume that $\alpha := \|R\|_\infty < \infty$, $\beta := \|\nabla \text{Ric}_V^\beta + d^* R + 2R(\nabla V)\|_\infty < \infty$ and $\nabla^2 N + R(N) = 0.$

Let $dv = h \, d\mu$ with $h \in C_0^\infty(M)$.

(i) If $\text{Ric}_V \geq K$, $\nabla N \leq 0$, then

$$H(\nu|h) \leq \frac{1}{2K} \left[ n^2 (1 + \varepsilon) \left( \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right)^2 S^2(\nu|h) \right] I(\nu|h)$$

$$- \frac{n^2}{2} \left( 1 + \frac{1}{\varepsilon} \right) S^2(\nu|h) \ln \left[ \frac{n^2 (1 + \frac{1}{\varepsilon}) K S^2(\nu|h)}{I(\nu|h) - n^2 (1 + \varepsilon) \left( \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right)^2 S(\nu|h)} \right] 0 + n^2 (1 + \frac{1}{\varepsilon}) K S^2(\nu|h)$$
for every $\varepsilon > 0$. Moreover, if $\alpha = 0$ and $\beta = 0$, then
\[ H(\nu|\mu) \leq \frac{n^2}{2}S^2(\nu|\mu)\ln\left(1 + \frac{I}{n^2KS^2(\nu|\mu)}\right). \]

(ii) If $\text{Ric}_V = K$, $\nabla N = 0$, then
\[ H(\nu|\mu) \leq \frac{1}{2K} \left( n^2(1+\varepsilon)\left(\frac{\alpha}{\sqrt{K}} + \frac{\beta}{K}\right)^2 S(\nu|\mu) \right) \wedge I(\nu|\mu) \]
\[ - \frac{1}{2} \left( 1 + \frac{1}{\varepsilon} \right) S^2(\nu|\mu) \ln \left( \frac{(1+\frac{1}{\varepsilon})KS^2(\nu|\mu)}{I(\nu|\mu) - n^2(1+\varepsilon)\left(\frac{\alpha}{\sqrt{K}} + \frac{\beta}{K}\right)^2 S(\nu|\mu)} \right) \]
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 5.3 and Lemma 5.2, we have
\[ H(\nu|\mu) \leq \frac{1}{2} \inf_{u>0} \left\{ A \int_0^u e^{-Kt} dt + B \int_0^\infty \frac{K}{e^{Kt}(e^{Kt} - 1)} dt + C \int_0^\infty e^{-Kt} dt \right\} \]
\[ = \frac{1}{2} \inf_{u>0} \left\{ \frac{A(1-e^{-Ku}) + C e^{-Ku}}{K} + B \int_0^\infty \frac{r}{1-r} dr \right\} \]
where
\[ A = I(\nu|\mu); \quad B = n^2 \left( 1 + \frac{1}{\varepsilon} \right) S^2(\nu|\mu); \]
\[ C = n^2(1+\varepsilon)\left(\frac{\alpha}{\sqrt{K}} + \frac{\beta}{K}\right)^2 S^2(\nu|\mu). \]
It is easy to see that if $A \leq C$, then inf is reached when $u$ tends to $\infty$; if $A > C$, then inf is reached for $e^{ou} = \frac{A-C+BK}{A-C}$ 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 $\text{Hess}_V = K > 0$, then by Obata’s Rigidity Theorem (see [19] Theorem 2) or [26] 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 5.5.** Let $(M, g)$ be a connected complete Riemannian manifold with boundary. Assume that $\text{Hess}_V = K > 0$, $\nabla N = 0$, and $\nabla^2 N = 0$. Let $dv = h d\mu$ with $h \in C_0^\infty(M)$. Then,
\[ I(\nu|\mu) \leq \frac{1}{2} S^2(\nu|\mu) \log \left( 1 + \frac{I(\nu|\mu)}{KS^2(\nu|\mu)} \right). \]
Proof. From the condition $\text{Hess}_Y = K > 0$, we know that the manifold $M$ is isometric to $\mathbb{R}^n$, i.e. $\|R\|_\infty = 0$, $\nabla \text{Ric} \equiv 0$ and $d^* R = 0$. Then by Theorem 5.3(ii),

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

The assertion can be obtained by a same arguments as in the proof of Theorem 5.4. □

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.

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