Gradient Estimates and Applications for Neumann Semigroup on Narrow Strip

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Abstract

By using local and global versions of Bismut type derivative formulas, gradient estimates are derived for the Neumann semigroup on a narrow strip. Applications to functional/cost inequalities and heat kernel estimates are presented. Since the narrow strip we consider is non-convex with zero injectivity radius, and does not satisfy the volume doubling condition, existing results in the literature do not apply.

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1 Introduction

Let $\phi_1, \phi_2 \in C^2(\mathbb{R}^d)$ with $\phi_1 < \phi_2$ and $\lim_{|x|\to \infty}\{|\phi_2(x) - \phi_1(x)|\} = 0$. We investigate gradient estimates and applications for the Neumann semigroup on the strip

$$D := \{(x, y) \in \mathbb{R}^{d+1} : \phi_1(x) \leq y \leq \phi_2(x)\}.$$

As the condition $\lim_{|x|\to \infty}\{|\phi_2(x) - \phi_1(x)|\} = 0$ means that the strip is extremely narrow at infinity, we call $D$ a narrow strip. This feature leads to essential difficulties in the study of the Neumann semigroup:

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(a) The domain is non-convex with injectivity zero, so that existing results on gradient estimates and applications derived in [10, 11, 12, 13, 16] using Li-Yau’s maximum principle and probabilistic arguments do not apply.

(b) The domain does not satisfy the volume doubling condition, so that the argument for heat kernel estimates developed by Grigoryan (see [5, 3] and references therein) using the doubling condition does not work.

As far as we know, the study of gradient and heat kernel estimates for the Neumann semigroup on a narrow strip remains new.

Let \( L = \Delta + Z \) for some \( C^1 \)-vector field \( Z \) on \( \mathbb{R}^d \). We consider the Neumann semigroup \( P_t \) generated by \( L \) on the narrow strip \( D \). Throughout the paper, we use \( \Delta \) and \( \nabla \) to denote the Laplacian and the gradient operators on the underlying Euclidean space. The main tools of our study are local/global derivative formulas addressed in Section 4. To apply these formulas, we need the following conditions on \( \phi_i (i = 1, 2) \) and \( Z \).

(i) \( \phi_1, \phi_2 \in C^2 (\mathbb{R}^d), \phi_1 < \phi_2, \lim_{|x| \to \infty} \{ \phi_2 (x) - \phi_1 (x) \} = 0, \lim \inf_{|x| \to \infty} \langle \nabla \phi_1, \nabla \phi_2 \rangle > -1, \)
and \( \langle \nabla \phi_1, \nabla \phi_2 \rangle (x) \leq (|\nabla \phi_1|^2 \wedge |\nabla \phi_2|^2) (x) \) for large \( |x| > 0 \).

(ii) \( \sup \{ \langle \nabla v, Z (x,y) \rangle : v \in \mathbb{R}^{d+1}, |v| \leq 1, (x,y) \in D \} < \infty. \)

(iii) For \( i = 1, 2, \)
\[
\sup \left\{ \frac{(-1)^i \text{Hess}_{\phi_i} (a,a)}{\phi_2 - \phi_1} (x) : x, a \in \mathbb{R}^d, |a| = 1 \right\} < \infty.
\]

(iv) For \( i = 1, 2, \)
\[
\sup_{(x,y) \in D} \left\{ (\phi_i (x) - y) \{ \Delta \phi_i (x) + \langle (\nabla \phi_i (x), -1), Z (x,y) \rangle \} + |\nabla \phi_i|^2 (x) \right\} < \infty.
\]

(v) \( \lim \sup_{|x| \to \infty} \sup_{y \in [\phi_1 (x), \phi_2 (x)]} \frac{-L (\phi_2 - \phi_1)}{\phi_2 - \phi_1} (x,y) < \infty, \lim \sup_{|x| \to \infty} |\nabla \log (\phi_2 - \phi_1) (x)| < \infty. \)

In the first condition of (v), and also in the sequel, a function \( \phi \) on \( \mathbb{R}^d \) is naturally extended to \( \mathbb{R}^{d+1} \) by setting \( \phi (x,y) := \phi (x), (x,y) \in \mathbb{R}^{d+1}. \)

Under these conditions, the reflecting diffusion process generated by \( L \) on \( D \) is non-explosive. More precisely, consider the following stochastic differential equation with reflection:

\[
(1.1) \quad d (X_t, Y_t) = \sqrt{2} dB_t + Z (X_t, Y_t) dt + N (X_t, Y_t) dl_t,
\]
where \( B_t \) is the \((d + 1)\)-dimensional Brownian motion, \( N \) is the unit inward normal vector field of \( \partial D \), and \( l_t \) is the local time of the solution \((X_t, Y_t)\) on \( \partial D \). Under the
above conditions, for any initial data \((x, y) \in D\), the equation has a unique solution \(\{(X_t, Y_t)(x, y)\}_{t \geq 0}\) which is non-explosive (see Proposition 2.1 below). Then the Neumann semigroup generated by \(L\) is formulated as

\[
P_t f(x, y) = \mathbb{E} f((X_t, Y_t)(x, y)), \quad (x, y) \in D, t \geq 0, f \in \mathcal{B}_b(D).
\]

**Theorem 1.1.** Assume (i)-(v). For any initial data \((X_0, Y_0) \in D\), the equation \((1.1)\) has a unique solution which is non-explosive. Moreover, there exists a constant \(c > 0\) such that the associated Neumann semigroup \(P_t\) satisfies the following gradient estimates.

1. For any \(p > 1\),

\[
|\nabla P_t f| \leq (P_t|\nabla f|^p)\frac{1}{p} \exp\left[ c + \frac{c p t}{p - 1}\right], \quad t \geq 0, f \in C^1_b(D).
\]

2. For any \(p \in (1, 2], t > 0\) and \(f \in \mathcal{B}_b(D)\),

\[
|\nabla P_t f|^2 \leq \frac{c p}{2(p - 1)^2(1 - \exp[-c p t/(p - 1)])}(P_t|f|^p)^{\frac{2}{p}}.
\]

Next, we present some applications of Theorem 1.1. Let \(\rho_D\) be the intrinsic distance on \(D\), i.e. for any \(x, y \in D\),

\[
\rho_D(x, y) := \inf \left\{ \int_0^1 |\gamma'(s)| ds : \gamma \in C^1([0, 1]; D), \gamma(0) = x, \gamma(1) = y \right\}.
\]

Moreover, for any probability measures \(\mu\) and \(\nu\) on \(D\),

\[
W^2_2(\rho_D) := \inf_{\pi \in \mathcal{C}(\mu, \nu)} \left( \int_{D \times D} \rho_D^2 d\pi \right)^{\frac{1}{2}}
\]

is the corresponding \(L^2\)-Wasserstein distance between \(\mu\) and \(\nu\), where \(\mathcal{C}(\mu, \nu)\) is the set of all couplings of \(\mu\) and \(\nu\). The following assertions are more or less standard consequences of the gradient estimates in Theorem 1.1.

**Corollary 1.2.** Assume (i)-(v). There exists a constant \(c > 0\) such that the following assertions hold.

1. For any \(t > 0\), the following Poincaré inequality holds:

\[
P_t f^2 \leq (P_t f)^2 + e^{c(e^c t - 1)} P_t|\nabla f|^2, \quad f \in C^1_b(D).
\]

2. For any \(t > 0\), the following log-Harnack inequality holds:

\[
P_t(\log f)(x) \leq \log P_t f(y) + \frac{e^c \rho_D(x, y)^2}{1 - e^{-c t}}, \quad x, y \in D, 0 < f \in \mathcal{B}_b(D).
\]
(3) For any measure $\mu$ which is equivalent to the Lebesgue measure on $D$, the density $p_t(x, y)$ of $P_t$ with respect to $\mu$ satisfies the following entropy inequality:
\[
\int_D p_t(x, z) \log \frac{p_t(x, z)}{p_t(y, z)} \mu(dz) \leq \frac{c e^c \rho_D(x, y)^2}{1 - e^{-ct}}, \quad x, y \in D, t > 0.
\]

(4) The invariant probability measure $\mu$ of $P_t$ is unique, and if it exists then the adjoint operator $P_t^*$ of $P_t$ on $L^2(\mu)$ satisfies the following entropy-cost inequality:
\[
\int_D (P_t^* f) \log P_t^* f d\mu \leq \frac{c e^c}{1 - e^{-ct}} W_2^p(f \mu, \mu), \quad t > 0, f \geq 0, \mu(f) = 1.
\]

(5) Let $\mu$ be the invariant probability measure of $P_t$. Then the density $p_t(x, y)$ of $P_t$ with respect to $\mu$ satisfies
\[
\int_D p_t(x, z)p_t(y, z)\mu(dz) \geq \exp \left[-\frac{\rho_D(x, y)^2c e^c}{1 - e^{-ct}} \right], \quad t > 0, x, y \in D.
\]

If $P_t$ is symmetric in $L^2(\mu)$, then
\[
p_t(x, y) \geq \exp \left[-\frac{\rho_D(x, y)^2c e^c}{1 - e^{-ct/2}} \right], \quad t > 0, x, y \in D.
\]

To illustrate the above results, we consider the following example where $\phi_i(i = 1, 2)$ are functions of $|x|$ for large $|x|$.

Example 1.1. Let $\phi_i(x) = \lambda_i \varphi(|x|) (i = 1, 2)$ for large $|x|$, where $\lambda_1 < \lambda_2$ with $\lambda_1 \leq 0 \leq \lambda_2$ are two constants, and $\varphi \in C^2_b([0, \infty))$ with $\varphi > 0, \varphi(r) \downarrow 0$ as $r \uparrow \infty$, and
\[
\limsup_{r \to \infty} \frac{|\varphi''(r)| + |\varphi'(r)|}{\varphi(r)} < \infty.
\]

Moreover, let $Z = (Z_1, Z_2) \in C^1(\mathbb{R}^{d+1}, \mathbb{R}^d \times \mathbb{R})$ satisfy (ii) and
\[
\limsup_{|x| \to \infty} \sup_{y \in [\lambda_1 \varphi(x), \lambda_2 \varphi(x)]} \left( \frac{|\varphi'(|x|)| \cdot |Z_1(x, y)|}{\varphi(|x|)} + \varphi(|x|)|Z_2(x, y)| \right) < \infty.
\]

Then it is easy to see that conditions (i)-(v) also hold, so that Theorem 1.1 and Corollary 1.2 apply.

Typical choices of $\varphi(r)$ for large $r$ meeting the above requirements include $\varphi(r) = e^{-\lambda r^\delta}$ for some $\lambda > 0$ and $\delta \in (0, 1]$, $\varphi(r) = r^{-\delta}$ for some $\delta > 0$, and $\varphi(r) = \log^{-\delta}(e + r)$ for some $\delta > 0$.

The remainder of the paper is organized as follows. In Section 2, we present some preparations, which include the non-explosion of the reflecting diffusion process, exponential estimates on the local time, and a prior gradient estimate on $P_t$. In Section 3, we prove Theorem 1.1 and Corollary 1.2. Finally, in Section 4, we introduce the local/global derivative formulas of the Neumann semigroup, which are used in Sections 2-3 as fundamental tools.
2 Preparations

The main tool in our study of gradient estimates is the following derivative formula (see Theorem 4.1 below):

\begin{equation}
\nabla P_t f = \mathbb{E}\left\{ Q_t^* \nabla f(X_t, Y_t) \right\} = \frac{1}{\sqrt{2}} \mathbb{E}\left\{ f(X_t, Y_t) \int_0^t h_s^* Q_s^* dB_s \right\},
\end{equation}

where \( h \in C^1([0, t]) \) is such that \( h_0 = 0 \) and \( h_t = 1 \), \( Q_s \) is an adapted process on \( \mathbb{R}^d \otimes \mathbb{R}^d \) satisfying

\begin{equation}
\|Q_s\| \leq e^{\int_0^s K(X_r, Y_r) dr + \int_0^s \sigma(X_r, Y_r) dl_r},
\end{equation}

and \(-\sigma\) is a lower bound of the second fundamental form of the boundary \( \partial D \). So, to apply this formula, we need to calculate the second fundamental form, and to estimate the exponential moment of the local time. Moreover, to ensure the validity of the above derivative formula, we also need to prove the non-explosion of the reflecting diffusion process generated by \( L \), and to verify the boundedness of \( \nabla P_t f \) on \([0, t] \times D\) for a reasonable class of functions \( f \). These will be done in the following three subsections respectively.

2.1 The second fundamental form

Let \( \partial_i = \{(x, \phi_i(x)) : x \in \mathbb{R}^d\} \). We have \( \partial D = \partial_1 \cup \partial_2 \). Let \( N \) be the unit inward normal vector field on \( \partial D \). Then

\begin{equation}
N(x, \phi_i(x)) = \frac{(-1)^i(\nabla \phi_i(x), -1)}{\sqrt{1 + |\nabla \phi_i(x)|^2}}, \quad x \in \mathbb{R}^d, i = 1, 2.
\end{equation}

Recall that the second fundamental form of \( \partial D \) is the following symmetric two-tensor defined on \( T \partial D \), the tangent space of \( \partial D \):

\[ \mathbb{I}(u, v) := -\langle \nabla_u N, v \rangle = -\langle \nabla_v N, u \rangle, \quad u, v \in T\partial D. \]

We say that the second fundamental form is bounded below by a function \(-\sigma\) on \( \partial D \) and denote \( \mathbb{I} \geq -\sigma \), if

\[ \mathbb{I}(v, v) \geq -\sigma(z)|v|^2, \quad z \in \partial D, v \in T_z\partial D. \]

Below, we calculate the lower bound of the second fundamental form.

For any unit tangent vector \( v \) of \( \partial D \) at point \( (x, \phi_i(x)) \in \partial_i \), there exists \( a \in \mathbb{R}^d \) with \( |a| = 1 \) such that

\[ v = \frac{(a, \nabla_a \phi_i(x))}{\sqrt{1 + |\nabla_a \phi_i(x)|^2}}. \]

Combining this with (2.3), we obtain

\[ \mathbb{I}(v, v) = -\langle \nabla_v N, v \rangle = -\frac{(-1)^i \text{Hess}_{\phi_i}(a, a)}{\sqrt{1 + |\nabla_a \phi_i|^2}(1 + |\nabla_a \phi_i|^2)}(x). \]
Therefore, letting

\[
\sigma_i(x) = \sup_{a \in \mathbb{R}^d, |a| = 1} \frac{(-1)^i \text{Hess}_{\phi_i}(a, a)}{\sqrt{1 + |\nabla \phi_i|^2 (1 + |\nabla a|)}^2}(x), \quad x \in \mathbb{R}^d, \quad i = 1, 2,
\]

\[
\sigma(x, y) = \sigma_1(x)1_{\{y = \phi_1(x)\}} + \sigma_2(x)1_{\{y = \phi_2(x)\}}, \quad (x, y) \in \partial D,
\]

we obtain \( \mathbb{I} \geq -\sigma \).

### 2.2 Non-explosion and exponential estimates on \( l_t \)

To investigate the non-explosion, we introduce the following Lyapunov function:

\[
W_0(x, y) = W_0(x) = \frac{1}{(\phi_2 - \phi_1)(x)}, \quad (x, y) \in D.
\]

By (2.3) and (i), there exists \( r_0 > 0 \) such that

\[
NW_0(x, \phi_i(x)) = \frac{\langle \nabla \phi_2, \nabla \phi_1 \rangle - |\nabla \phi_i|^2}{(\phi_2 - \phi_1)^2 \sqrt{1 + |\nabla \phi_i|^2}}(x) \leq 0, \quad i = 1, 2, W_0(x) \geq r_0.
\]

Thus, \( NW_0 \leq 0 \) holds on \( \partial D \cap \{W_0 \geq r_0\} \). We modify \( W_0 \) such that this boundary condition holds on the whole boundary \( \partial D \). Take \( \beta \in C^\infty([0, \infty)) \) with \( \beta' \geq 0, \beta|_{[0, r_0]} = r_0, \) and \( \beta(r) = r \) for \( r \geq r_0 + 1 \). Then (2.5) implies

\[
NW_{\partial D} \leq 0, \quad W := \beta \circ W_0.
\]

Moreover, by (i), \( W \) is a compact function on \( D \), i.e. \( \{x \in D : W(x) \leq r\} \) is compact for any \( r > 0 \). Define

\[
\tau_n = \inf \left\{ t \geq 0 : W(X_t, Y_t) = W(X_t) \geq n \right\}, \quad n \geq 1.
\]

Then the life time of the process can be formulated as

\[
\tau_\infty = \lim_{n \to \infty} \tau_n.
\]

**Lemma 2.1.** Assume (i)-(v).

1. For any initial data \((X_0, Y_0) \in D\), the unique solution to the equation (1.1) is non-explosive.

2. For any \( R > 0 \), there exists a constant \( c > 0 \) such that for any initial data \((X_0, Y_0) \in D\),

\[
\mathbb{E}e^{\lambda \int_0^t 1_{\{W \leq R\}}(X_s)ds} \leq e^{\lambda + c(1+\lambda)t}, \quad \lambda, t \geq 0.
\]

3. There exists a constant \( c > 0 \) such that for any initial data \((X_0, Y_0) \in D\),

\[
\mathbb{E}e^{\lambda \int_0^t \sigma(X_s, Y_s)ds} \leq e^{c(1+\lambda)t}, \quad \lambda, t \geq 0.
\]
Proof. (1) It is easy to see from (v) and the construction of \( W \) that \( LW \leq CW \) holds for some constant \( C > 0 \). Then by (2.6) and Itô’s formula, we obtain
\[
dW(X_t, Y_t) \leq dM_t + CW(X_t, Y_t)dt
\]
for some local martingale \( M_t \). This implies
\[
\mathbb{E}W(X_{t\wedge \tau_n}, Y_{t\wedge \tau_n}) \leq W(X_0, Y_0)e^{Ct}, \quad t \geq 0.
\]
Since \( W > 0 \) and \( W(X_{\tau_n\wedge t}, Y_{\tau_n\wedge t}) = n \) provided \( \tau_n \leq t \), it follows that
\[
\mathbb{P}(\tau_n \leq t) \leq \frac{\mathbb{E}W(X_{t\wedge \tau_n}, Y_{t\wedge \tau_n})}{n} \leq \frac{e^{Ct}W(X_0, Y_0)}{n}.
\]
Therefore, \( \mathbb{P}(\tau_\infty \leq t) \leq 0 \) holds for any \( t \geq 0 \), i.e. the process is non-explosive.

(2) Let \( \rho_0 = \inf_{y \in \partial D} |y| \) be the distance function to the boundary \( \partial D \). Since \( D \) is a \( C^2 \)-domain, \( \rho_0 \) is \( C^2 \)-smooth in a neighborhood of \( \partial D \). So, for any \( R > 0 \), there exists \( \varepsilon \in (0, 1) \) such that \( \rho_0 \in C^2(D \cap \{ W \leq R + 1 \} \cap \{ \rho_0 \leq \varepsilon \}) \). Let \( \alpha, \beta \in C^\infty([0, \infty)) \) such that \( \alpha(r) = r \) for \( r \leq \frac{1}{2} \), \( \alpha|_{[\varepsilon, \infty]} = \varepsilon \); and \( \beta|_{[\varepsilon, R]} = 1, \beta|_{[R+1, \infty]} = 0, \beta' \leq 0 \). Then
\[
\tilde{\rho}_\theta := (\beta \circ W)(\alpha \circ \rho_0) \in C^2(D), \quad 0 \leq \tilde{\rho}_\theta \leq 1.
\]
Moreover, since on \( \partial D \) we have \( \rho_0 = 0 \) and \( N\rho_0 = 1 \), it follows from (2.6), \( \beta' \leq 0, \alpha'(0) = 1 \) and \( \beta \circ W \geq 1 \{ W \leq R \} \) that
\[
N\tilde{\rho}_\theta = (\beta' \circ W)(\alpha \circ \rho_0)NW + (\beta \circ W)\alpha'(0)N\rho_0 \geq 1 \{ W \leq R \}
\]
holds on \( \partial D \). Thus, by Itô’s formula we obtain
\[
d\tilde{\rho}_\theta(X_t, Y_t) = \sqrt{2} \langle \nabla \tilde{\rho}_\theta(X_t, Y_t), dB_t \rangle + L\tilde{\rho}_\theta(X_t, Y_t)dt + N\tilde{\rho}_\theta(X_t, Y_t)dt
\]
\[
\geq \sqrt{2} \langle \nabla \tilde{\rho}_\theta(X_t, Y_t), dB_t \rangle - ||L\tilde{\rho}_\theta||_\infty dt + 1 \{ W(X_t) \leq R \} dt.
\]
Therefore,
\[
\mathbb{E}e^{\lambda \int_0^t 1 \{ W(X_s) \leq R \} dt} \leq e^{\lambda + \lambda ||L\tilde{\rho}_\theta||_\infty t} \mathbb{E}e^{\lambda \sqrt{2} \int_0^t \langle \nabla \tilde{\rho}_\theta(X_s, Y_s), dB_s \rangle} \leq e^{\lambda + \lambda ||L\tilde{\rho}_\theta||_\infty t + \lambda^2 ||\nabla \tilde{\rho}_\theta||^2_\infty t}.
\]

(3) Let \( g_i(x, y) = (\phi_i(x) - y)^2; (x, y) \in D \). We have \( (Ng_i)(x, \phi_i(x)) = 0 \) (i.e. \( Ng_i|_{\partial \tilde{\rho}_\varepsilon} = 0 \)) and
\[
(2.8) \quad Ng_i(x, \phi_{3-i}(x)) = -\frac{2(\phi_2 - \phi_1)(1 + \langle \nabla \phi_1, \nabla \phi_2 \rangle)}{\sqrt{1 + ||\nabla \phi_{3-i}||^2}}(x) =: -\sigma_{3-i}(x), \quad x \in \mathbb{R}^d.
\]
By (i), \( 1 + \langle \nabla \phi_1, \nabla \phi_2 \rangle(x) \geq \theta_0 \) holds for some constant \( \theta_0 > 0 \) and large enough \( |x| > 0 \). Then it follows from (2.4), (2.8) and (iii) that \( \sigma_i \leq \theta \tilde{\sigma}_i \) holds on \( \{ W \geq R \} \cap \partial D \) for some constants \( \theta, R > 0 \). Since \( \sigma_i \) is bounded on the compact set \( \partial D \cap \{ W \leq R \} \), we conclude that
\[
(2.9) \quad \sigma_i \leq \theta \tilde{\sigma}_i + c_1 1_{\{ W \leq R \}}
\]
holds on $\partial D$ for some constant $c_1 > 0$. Moreover, by (iv) we have
\[
Lg_{3-i}(x, y) = 2 - 2y \Delta \phi_{3-i}(x) + \Delta \phi_{3-i}^2(x) + 2(\phi_{3-i}(x) - y)\langle (\nabla \phi_{3-i}(x), -1), Z(x, y) \rangle \\
\leq K_{3-i}, \quad (x, y) \in D
\]
for some constant $K_{3-i} > 0$. Combining this with $N g_{3-i}|_{\partial_3-i} = 0$ and (2.8), and using Itô’s formula, we obtain
\[
dg_{3-i}(X_t, Y_t) \leq dM_t + K_{3-i}dt - \tilde{\sigma}_i(X_t)dl^t_i,
\]
where $l^t_i$ is the local time of $(X_t, Y_t)$ on $\partial t$. Due to (2.9), (2.10) and $\langle \phi_i(x) - y \rangle^2 \leq \delta^2$ on $D$, we arrive at
\[
\lambda \int_0^t \sigma_i(X_s)dl^t_s \leq \lambda \theta \int_0^t \tilde{\sigma}_i(X_s)dl^t_s + \lambda c_1 \int_0^t 1_{\{W(X_s) \leq R\}} dl^t_s
\]
\[
\leq \lambda \theta \{ \delta^2 + K_{3-i}t \} + \lambda M_t + \lambda c_1 \int_0^t 1_{\{W(X_s) \leq R\}} dl^t_s.
\]
Noting that
\[
\langle M \rangle_t = 8 \lambda^2 \theta^2 \int_0^t |\phi_{3-i}(X_s) - Y_s|^2(1 + |\nabla \phi_{3-i}(X_s)|^2)ds
\]
\[
\leq 8 \lambda^2 \theta^2 \delta^2(1 + \| \nabla \phi_{3-i} \|_{\infty}^2) t =: c_2 \lambda^2 t,
\]
this together with (2) implies
\[
E e^{\lambda \int_0^t \sigma_i(X_s)ds} \leq e^{\lambda \theta \{ \delta^2 + K_{3-i}t \} + c_2 \lambda^2 t} E M_t - \langle M \rangle_t + \lambda c_1 \int_0^t 1_{\{W(X_s) \leq R\}} dl^t_s
\]
\[
= e^{\lambda \theta \{ \delta^2 + K_{3-i}t \} + c_2 \lambda^2 t} \left( E e^{2M_t - 2\langle M \rangle_t} \right)^{\frac{1}{2}} \left( E e^{2\lambda c_1 \int_0^t 1_{\{W(X_s) \leq R\}} dl^t_s} \right)^{\frac{1}{2}}
\]
\[
\leq e^{c \lambda + c \lambda (1 + \lambda)t}
\]
for some constant $c > 0$. Therefore, we prove (3) by noting that
\[
E e^{\lambda \int_0^t \sigma_i(X_s)ds} = E e^{\lambda \int_0^t \sigma_1(X_s)ds + \lambda \int_0^t \sigma_2(X_s)ds}
\]
\[
\leq \left( E e^{2\lambda \int_0^t \sigma_1(X_s)ds} \right)^{\frac{1}{2}} \left( E e^{2\lambda \int_0^t \sigma_2(X_s)ds} \right)^{\frac{1}{2}}.
\]

**2.3 A priori gradient estimate on $P_t$**

In this subsection, we prove the boundedness of $\nabla P_t f$ on $[0, t] \times D$ for a nice reference function $f$ such that the derivative formula (2.14) is valid according to Theorem 1.1. To
this end, we use the local derivative formula presented in Theorem 4.2 below. The key point to apply this formula lies in the construction of the control process $h$, which is non-trivial due to the stopping time $\tau^x_B$. In [3] Section 4, this control process was constructed by using a time change induced by the distance function to the boundary. However, in the present case the distance of a point $x \in D$ to the boundary vanishes as $|x| \to \infty$. So, the construction from [3] Section 4 does not imply the desired boundedness of $\nabla P f$ on $[0,t] \times D$. Our trick to fix this point is to use the Lyapunov function $W$ instead of the distance function to $\partial D$, where $W$ is in (2.4).

Let

$$g_n(x) = \cos \frac{\pi W(x)}{2n}, \quad x \in \mathbb{R}^d, n \geq 1.$$  

For fixed $X_0 \in \mathbb{R}^d$, we consider $n > W(X_0) + 1 + r_0$, where $r_0 > 0$ is in (2.5). Define

$$T(t) = \int_0^t g_n(X_s \wedge \tau_n)^{-2}ds, \quad t \geq 0,$$

where $\tau_n$ is in (2.7). Then $T \in C([0, \tau_n); [1, \infty))$ is strictly increasing with $T(t) \geq t$, and $T(t) = \infty$ holds for $t \geq \tau_n$. Let

$$\tau(t) = \inf\{s \geq 0 : T(s) \geq t\}, \quad t \geq 0.$$  

We have $\tau(t) \leq t$, and $T \circ \tau(t) = t$ provided $\tau(t) < \tau_n$.

**Lemma 2.2.** Assume (i)-(v). Let $X_0 \in \mathbb{R}^d$ and $n > W(X_0) + r_0 + 1$. Then $\tau(t) < \tau_n$ holds for all $t > 0$. Moreover, for any $m \geq 1$, there exists a constant $c > 0$ independent of $n$ such that

$$\mathbb{E}g_n(X_{\tau(t)})^{-m} \leq g_n(X_0)^{-m}e^{ct}, \quad t \geq 0. \quad (2.11)$$

*Proof.* Let $\zeta_l = \inf\{t \geq 0 : g_n(X_{\tau(t)}) \leq \frac{1}{l}\}$, $l \geq 1$. By the definitions of $g_n$ and $\tau_n$, we have

$$\zeta_\infty := \lim_{l \to \infty} \zeta_l = \inf\{t \geq 0 : \tau(t) \geq \tau_n\}. \quad (2.12)$$

Moreover, by (2.6) we have $Ng_n^{-r}|_{\partial D} \leq 0$ for any $r > 0$. So, by Itô’s formula and the fact that

$$d\tau(t) = g_n(X_{\tau(t)})^2dt, \quad t \leq \zeta_l,$$

we obtain

$$dg_n(X_{\tau(t)})^{-m} = dM_t + (Lg_n^{-m})(X_{\tau(t)}, Y_{\tau(t)})d\tau(t) + Ng_n^{-m}(X_{\tau(t)}, Y_{\tau(t)})dt$$

$$= dM_t + g_n(X_{\tau(t)})^2(Lg_n^{-m})(X_{\tau(t)}, Y_{\tau(t)})dt, \quad t \leq \zeta_l \quad (2.13)$$

for some martingale $M_t$. Since $W = W_0$ for $W_0 \geq r_0 + 1$, by (v), there exists a constant $C > 0$ independent of $n$ such that

$$-(Lg_n)(x, y) = \left(\frac{\pi \sin \frac{\pi}{2n\phi_2 - \phi_1}}{2n}\right)(L(\phi_2 - \phi_1)^{-1}) + \frac{\pi^2 g_n(x)}{4n^2} |\nabla(\phi_2 - \phi_1)^{-1}|^2(x, y)$$

$$= \left(\frac{\pi \sin \frac{\pi}{2n\phi_2 - \phi_1}}{2n}\right) \left(2|\nabla \log(\phi_2 - \phi_1)|^2 - \frac{L(\phi_2 - \phi_1)}{\phi_2 - \phi_1} \right) + \frac{\pi^2 g_n |\nabla \log(\phi_2 - \phi_1)|^2}{4n^2(\phi_2 - \phi_1)^2} \right)(x, y)$$

$$\leq C, \quad \text{if} \ (x, y) \in D, \ 1 + r_0 \leq W_0(x) \leq n, \quad \text{9}$$
Thus, \( E(2.14) \)

\[ |\nabla g_n|^2(x) \leq \frac{\pi^2 |\nabla \log(\phi_2 - \phi_1)|^2}{4n^2(\phi_2 - \phi_1)^2}(x) \leq C, \quad (x, y) \in D, \quad 1 + r_0 \leq W_0(x) \leq n. \]

Moreover, it is easy to see that \( \{|Lg_n| + |\nabla g_n|\}_{n \geq 1} \) are uniformly bounded on the compact set \( D \cap \{W_0 \leq r_0 + 1\} \), we conclude that

\[
\begin{align*}
g_n(X_{\tau(t)})^2 (Lg_n^{-m})(X_{\tau(t)}, Y_{\tau(t)}) & = -m g_n(X_{\tau(t)})^{1-m}(Lg_n)(X_{\tau(t)}, Y_{\tau(t)}) + m(m+1)(g_n^{-m}|\nabla g_n|^2)(X_{\tau(t)}) \\
& \leq c g_n(X_{\tau(t)})^{-m}, \quad t \leq \tau_n
\end{align*}
\]

holds for some constant \( c > 0 \) independent of \( n \). Combining this with (2.13), we obtain

\[ \mathbb{E} g_n(X_{\tau(t \wedge \zeta)})^{-m} \leq g(X_0)^{-m} e^{ct}, \quad t \geq 0, \quad l \geq 1. \]

Thus,

\[ \mathbb{P}(\zeta \leq t) \leq \frac{\mathbb{E} g_n(X_{\tau(t \wedge \zeta)})^{-m}}{l^m} \leq \frac{e^{ct}}{g_n(X_0)^m l^m}. \]

Letting \( l \to \infty \) we obtain \( \mathbb{P}(\zeta \leq t) = 0 \) for all \( t > 0 \), so that by (2.12), \( \mathbb{P}(\tau(t) < \tau_n) = 1 \) holds for all \( t \geq 0 \). Finally, (2.11) follows from (2.14) by letting \( l \to \infty \).

Combining Lemma 2.2 with Theorem 4.2 below, we can prove the following gradient estimate on \( P_t \).

**Lemma 2.3.** Assume (i)-(v). There exists a constant \( C > 0 \) such that

\[ |\nabla P_t f|^2 \leq \frac{C}{t \wedge 1} \{P_t f^2 - (P_t f)^2\}, \quad t > 0, \quad f \in \mathcal{B}_b(D). \]

Consequently, for any \( f \in C^2_0(D) \) satisfying the Neumann boundary condition, \( \nabla P_t f \) is bounded on \([0, t] \times D\) for all \( t > 0 \).

**Proof.** We first observe that it suffices to prove (2.15). Indeed, if (2.15) holds, then for \( f \in C^2_0(D) \) satisfying the Neumann boundary condition,

\[ P_t f^2 - (P_t f)^2 = f^2 + \int_0^t (P_s Lf^2)ds - \left( f + \int_0^t (P_s Lf)ds \right)^2 \leq C(t + t^2), \quad t \geq 0 \]

holds for some constant \( C > 0 \). Combining this with (3.2), we conclude that \( \nabla P_t f \) is bounded on \([0, t] \times D\) for all \( t > 0 \).

Next, by the semigroup property and Jensen’s inequality, we only need to prove (2.15) for \( t \in (0, 1] \). Moreover, by an approximation argument, for the proof of (2.15) we may and do assume that \( f \in C^2_0(D) \) satisfying the Neumann boundary condition. Finally, for fixed \( t > 0 \) and \( x_0 \in D \), by using \( f - P_t f(x_0) \) to replace \( f \), to prove (2.15) at point \( x_0 \) we may assume further that \( P_t f(x_0) = 0 \).
Now, let \( t \in (0, 1], x_0 \in D \), and \( f \in C^2_0(D) \) satisfy the Neumann boundary condition with \( P_t f(x_0) = 0 \). For \( n > 1 + r_0 + W(x_0) \), let

\[
h_s = \frac{1}{t} \int_0^s g_n(x_r)^{-2} 1_{\{r < \tau(t)\}} dr, \quad s \geq 0,
\]

where \((X_t, Y_t)\) solves the equation \((1.1)\) with \((X_0, Y_0) = x_0\). Then \( h_0 = 0 \). Moreover, if \( s \geq \tau(t) \), then

\[
h_s = h_{\tau(t)} = \frac{1}{t} \int_0^{\tau(t)} g_n(x_r)^{-2} dr \leq \frac{T \circ \tau(t)}{t} = 1,
\]

where the last step follows since \( \tau(t) < \tau_n \) according to Lemma \(2.2\) so that \( T \circ \tau(t) = t \) by the definitions of \( T \) and \( \tau \). By (ii), \( \|P\| \geq -\sigma \), and \( \tau(t) \leq t \wedge \tau_n \), we can apply Theorem \(4.2\) below for \( D_0 = \{ (x, y) \in D : W(x) \leq n \} \) and

\[
\|Q_s\| \leq e^{K(s \wedge \tau_n) + \int_0^{s \wedge \tau_n} \sigma(x, y) dt}, \quad s \geq 0.
\]

By the Cauchy-Schwartz inequality, the definition of \( h_s \), Lemmas \(2.1, 2.2\) and \( \tau(t) \leq t \), we obtain

\[
\begin{align*}
\mathbb{E} \left( \int_0^t |h'(s)|^2 \|Q_s\|^2 ds \right)^2 &\leq \frac{1}{t^3} \mathbb{E} \int_0^{\tau(t)} g_n(x_s)^{-8} e^{4Ks + 4 \int_0^{s \wedge \tau_n} \sigma(x, y) dt} ds \\
&\leq \frac{e^{4Kt}}{t^3} \left( \mathbb{E} \int_0^{\tau(t)} g_n(x_s)^{-16} ds \right)^{\frac{1}{2}} \left( \mathbb{E} \int_0^{\tau(t)} e^{8 \int_0^t \sigma(x, y) dt} ds \right)^{\frac{1}{2}} \\
&\leq \frac{e^{c_1(t+1)}}{t^2} \left( \mathbb{E} \int_0^{\tau(t)} g_n(x_s)^{-14} ds \right)^{\frac{1}{2}} \leq \frac{e^{c_2(t+1)}}{t^2 g_n(x_0)^{\frac{1}{2}}},
\end{align*}
\]

for some constants \( c_1, c_2 > 0 \) independent of \( n \). Therefore, by Theorem \(4.2\) below,

\[
|\nabla P_t f|^2(x_0) \leq \frac{1}{2} \left( P_t f^2(x_0) \right) \mathbb{E} \int_0^t |h'(s)|^2 \|Q_s\|^2 ds \leq \frac{C}{t g_n(x_0)^{\frac{1}{2}}} P_t f^2(x_0), \quad t \in (0, 1]
\]

holds for some constant \( C > 0 \) and all \( n > 1 + r_0 + W(x_0) \). Then the proof is finished by letting \( n \to \infty \).

\section*{3 Proofs of Theorem 1.1 and Corollary 1.2}

\textbf{Proof of Theorem 1.1.} By an approximation argument, we may and do assume that \( f \in C^2_0(D) \) satisfying the Neumann boundary condition. In this case, \( \nabla P_t f \) is bounded on \([0, t] \times D\) according to Lemma \(2.3\).

(a) By (ii), \( \|P\| \geq -\sigma \), and Theorem \(4.1\) below, we have

\[
|\nabla P_t f| \leq \mathbb{E} \{ |\nabla f|(X_t, Y_t)e^{Kt + \int_0^t \sigma(X_s, Y_s) ds} \} \leq e^{Kt} (P_t |\nabla f|)^\frac{1}{p} \left( \mathbb{E} e^{\int_0^t \sigma(X_s, Y_s) dt} \right)^{\frac{p-1}{p}}.
\]
Then the gradient estimate in (1) follows from Lemma 2.1.

(b) Let $p \in (1, 2]$ and $v \in \mathbb{R}^{d+1}$ with $|v| = 1$. By (ii), $(\nabla_v Z, v) \leq K|v|^2$ holds for some constant $K > 0$ and all $v \in \mathbb{R}^{d+1}$. Combining this with $\mathbb{I} \geq -\sigma$ and using Theorem 1.1 below, for any $h \in C^1([0, t])$ with $h_0 = 0$ and $h_t = 1$, we have

$$\left|\nabla_v Pf \right|^2 \leq \frac{1}{2} (P_t f)^\frac{q}{p} \left(\mathbb{E}|M_t|^q\right)^{\frac{q}{p}}, \quad q := \frac{p}{p - 1} \geq 2,$$

where

$$M_t := \int_0^t \langle v, h_s Q_s dB_s \rangle$$

for some adapted process $Q_s$ satisfying

$$\|Q_s\| \leq e^{Ks + f_0^s \sigma(X, Y)dt}, \quad s \geq 0.$$

Noting that $d|M_t|^2 = 2M_t dM_t + d\langle M \rangle_t$, for any $\varepsilon > 0$ we have

$$\begin{align*}
d(M_t^2 + \varepsilon)^\frac{q}{2} &= dN_t + \frac{q}{2}(M_t^2 + \varepsilon)^{\frac{q-1}{2}}d\langle M \rangle_t + \frac{q}{2}(\frac{q}{2} - 1)(M_t^2 + \varepsilon)^{\frac{q-2}{2}}4M_t^2 d\langle M \rangle_t \\
&\leq dN_t + \frac{q(q-1)}{2}(M_t^2 + \varepsilon)^{\frac{q-2}{2}}\|h_t Q_t\|^2 dt,
\end{align*}$$

where $dN_t := qM_t(M_t^2 + \varepsilon)^{\frac{q-2}{2}}dM_t$ is a martingale due to Lemma 2.1 and (3.2). Moreover, letting $\eta_t = \mathbb{E}(M_t^2 + \varepsilon)^{\frac{q}{2}}$, and combining this with Lemma 2.1 we obtain

$$\eta_t' \leq \frac{q(q-1)}{2}\mathbb{E}\{(M_t^2 + \varepsilon)^{\frac{q-2}{2}}\|h_t^2 Q_t\|^2\} \leq \frac{q(q-1)}{2}\|h_t^2\|^\frac{q-2}{q}\left(\mathbb{E}||Q_t|^q\right)^{\frac{q}{q}}$$

$$\leq \frac{q(q-1)}{2}\|h_t^2\|^{\frac{q-2}{q}}e^{2Kt}\left(\mathbb{E}e^{q\int_0^t \sigma(X, Y_s)ds}\right)^{\frac{q}{q}}$$

$$\leq \frac{q(q-1)}{2}\|h_t^2\|^{\frac{q-2}{q}}e^{cqt}$$

for some constant $c > 0$. Therefore,

$$\eta_t \leq \left(\varepsilon^\frac{q}{2} + (q - 1)e^c \int_0^t |h_s|^2 e^{cq\sigma} ds \right)^{\frac{q}{2}}.$$

Letting $\varepsilon \to 0$ and taking

$$h_0 = 0, \quad h_s' = \frac{\exp[-cq s]}{\int_0^s \exp[-cq s]ds}, \quad s \in [0, t],$$

we arrive at

$$\mathbb{E}|M_t|^q \leq \left(\frac{cq(q-1)e^c}{1 - \exp[-cqt]}\right)^{\frac{q}{2}}.$$

Substituting this into (3.1), we prove (2). \qed
Proof of Corollary 1.2. By Theorem 1.1(1) with \( p = 2 \), we have

\[
|\nabla P_t f|^2 \leq (P_t|\nabla f|^2)e^{c+ct}, \quad t \geq 0, f \in C^1_b(D)
\]

for some constant \( c > 0 \). By an approximation argument, in (1) and (2) we may and do assume that \( f \in C^2_b(D) \) satisfying the Neumann boundary condition, which is constant outside a bounded set.

(a) The desired Poincaré inequality follows from (3.5) and the following simple calculations due to Bakry-Emery (cf. [1]):

\[
P_t f^2 - (P_t f)^2 = - \int_0^t \frac{d}{ds} P_{t-s}(P_s f)^2 ds = \int_0^t P_{t-s} |\nabla P_s f|^2 ds
\]

\[
\leq P_t |\nabla f|^2 \int_0^t e^{c+cs} ds = \frac{e^c(e^{ct}-1)}{c} P_t |\nabla f|^2.
\]

(b) The proof of (2) can be modified from that of Theorem 2.1 in [9]. More precisely, let \( x, y \in D \) and \( t > 0 \) be fixed. By the definition of \( \rho_D(x, y) \), for any \( \varepsilon > 0 \), there exists a \( C^1 \)-curve \( \gamma : [0, 1] \to D \) such that

\[
\gamma(0) = x, \quad \gamma(1) = y, \quad |\gamma'| \leq \rho_D(x, y) + \varepsilon.
\]

Let

\[
h_0 = 0, \quad h'_s = \frac{ce^{-cs}}{1-e^{-ct}}, \quad s \in [0, t].
\]

If \( f \in C^2_b(D) \) is positive, constant outside a compact set, and satisfies the Neumann boundary condition, then

\[
P_t \log f(x) - \log P_t f(y) \leq \int_0^t \frac{d}{ds} (P_s \log P_{t-s} f)(\gamma(h_s)) ds
\]

\[
= \int_0^t \{ h'_s \langle \gamma'(s), \nabla P_s \log P_{t-s} f \rangle - P_s |\nabla \log P_{t-s} f|^2 \} (\gamma(h_s)) ds
\]

\[
\leq \int_0^t \{ h'_s (\rho_D(x, y) + \varepsilon) |\nabla P_s \log P_{t-s} f| - e^{-c\varepsilon} |\nabla P_s \log P_{t-s} f|^2 \} (\gamma(h_s)) ds
\]

\[
\leq \frac{(\rho_D(x, y) + \varepsilon)^2}{4} \int_0^t |h'_s|^2 e^{c+cs} ds = \frac{ce^c(\rho_D(x, y) + \varepsilon)^2}{1-e^{-ct}}.
\]

Then the desired log-Harnack inequality follows by letting \( \varepsilon \to 0 \).

(c) Applying [15, Lemma 3.1(4)-(5)] for \( P = P_t \) and \( \Phi(s) = e^s \), the desired entropy inequality in (3) as well as the heat kernel estimate in (5) follow from (2). Moreover, the entropy-cost inequality in (4) follows from (2) and [9, Corollary 1.2(3)].
4 Derivative formulas for $P_t$

In this section, we introduce derivative formulas of $P_t$ on a $C^2$-domain $D$ in $\mathbb{R}^d$ for $d \geq 2$, where $P_t$ is the Neumann semigroup generated by $L := \Delta + Z$ on $D$ for some $C^1$-vector field $Z$. Let $K \in C(D)$ such that

\begin{equation}
\langle \nabla_v Z(x), v \rangle \leq K(x)|v|^2, \quad x \in D, v \in \mathbb{R}^d.
\end{equation}

Consider the following stochastic differential equations:

\begin{equation}
dX_t = \sqrt{2} dB_t + Z(X_t) dt + N(X_t) dl_t,
\end{equation}

where $B_t$ is the $d$-dimensional Brownian motion, $N$ is the inward unit normal vector field of $\partial D$, and $l_t$ is the local time of the solution on $\partial D$. We assume that for any $x \in D$, the solution $(X^x_t, l^x_t)_{t \geq 0}$ to this equation starting at $x$ is non-explosive. Then the associated Neumann semigroup is formulated as

$$P_t f(x) = \mathbb{E} f(X^x_t), \quad t \geq 0, x \in D, f \in \mathcal{B}(D).$$

Moreover, let $\sigma \in C(\partial D)$ such that

\begin{equation}
I(v, v) := -\langle \nabla_v N(x), v \rangle \geq -\sigma(x)|v|^2, \quad x \in \partial D, v \in T_x \partial D.
\end{equation}

To state the derivative formulas, we introduce the class

$$\mathcal{C}_N(D) := \{ f \in C^2(D), Nf|_{\partial D} = 0, Lf \in \mathcal{B}(D) \}.$$

By the Kolmogorov equations, we have (see e.g. [14, Theorem 3.1.3])

\begin{equation}
\frac{d}{dt} P_t f = P_t L f = LP_t f, \quad t \geq 0, f \in \mathcal{C}_N(D).
\end{equation}

The following global derivative formula is essentially taken from [14, Theorem 3.2.1]. This type of derivative formula was proved by Bismut [2] and Elworthy-Li [4] on manifolds without boundary.

**Theorem 4.1.** Let $t > 0$ and $x \in D$ be fixed. If

\begin{equation}
\sup_{s \in [0, t]} \mathbb{E} \int_0^s \mathbb{E} f(X^x_r) dr + \int_0^s \sigma(X^x_r) dt \int_0^s h^x_s Q_s dB_s < \infty,
\end{equation}

then there exists an adapted $\mathbb{R}^d \otimes \mathbb{R}^d$-valued process $(Q_s)_{s \in [0, t]}$ with

\begin{equation}
Q_0 = I, \quad \|Q_s\| \leq e^{\int_0^s \mathbb{E} f(X^x_r) dr + \int_0^s \sigma(X^x_r) dt}, \quad s \in [0, t],
\end{equation}

such that for any $f \in \mathcal{C}_N(D)$ with bounded $\nabla P f$ on $[0, t] \times D$,

\begin{equation}
\nabla P_t f(x) = \mathbb{E} \{ Q_t \nabla f(X^x_t) \} = \frac{1}{\sqrt{2}} \mathbb{E} \left\{ f(X^x_t) \int_{0}^{t} h^x_s Q_s dB_s \right\}
\end{equation}

holds for any $h \in C^1([0, t])$ with $h_0 = 0$ and $h_t = 1$. 

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Proof. The construction of $Q_s$ as well as the first equality in (4.7) are essentially due to \[7\]. Once $Q_s$ is constructed, the second equality in (4.7) can be proved as in \[7\].

(a) For any $z \in \partial D$, let $P_\partial z$ be the projection onto the tangent space $T_z \partial D$ of $\partial D$ at point $z$. We have

$$P_\partial z a = a - \langle a, N(z) \rangle N(z), \quad a \in \mathbb{R}^d.$$  

Next, let $\mathbb{I}_z \in \mathbb{R}^d \otimes \mathbb{R}^d$ such that

$$\langle \mathbb{I}_z a, b \rangle = \mathbb{I}_\partial (P_\partial z a, P_\partial z b), \quad a, b \in \mathbb{R}^d.$$  

Moreover, for any $n \geq 1$, let $(Q_s^{(n)})_{s \geq 0}$ solve the following equation on $\mathbb{R}^d \otimes \mathbb{R}^d$:

$$dQ_s^{(n)} = (\nabla Z(X_s^x))Q_s^{(n)} ds - \mathbb{I}_s^{X_s^x} Q_s^{(n)} dw_s - (n + \sigma(X_s^x)^+)((Q_s^{(n)})^* N(X_s^x)) \otimes N(X_s^x) dl_s^x, \quad Q_0^{(n)} = I,$$

where for any $v_1, v_2 \in \mathbb{R}^d$, $v_1 \otimes v_2 \in \mathbb{R}^d \otimes \mathbb{R}^d$ is defined by

$$(v_1 \otimes v_2)a = \langle v_1, a \rangle v_2, \quad a \in \mathbb{R}^d.$$  

Then for any $a \in \mathbb{R}^d$, it follows from (4.11), (4.13) and (4.8) that

$$d|Q_s^{(n)}|^2 = 2\langle \nabla Q_s^{(n)}, a \rangle Q_s^{(n)} ds - 2\langle P_\partial Q_s^{(n)}, a \rangle d\|Q_s^{(n)}\|^2 - 2(n + \sigma(X_s^x)^+)\langle Q_s^{(n)}, N(X_s^x) \rangle dl_s^x$$  

$$\leq 2|Q_s^{(n)}|^2 \{\sigma(X_s^x) dl_s^x + K(X_s^x) ds\} - 2n \langle Q_s^{(n)}, N(X_s^x) \rangle dl_s^x.$$  

In particular,

$$\|Q_s^{(n)}\|^2 \leq e^{2f_0^s K(X)^{dr+2}f_0^s \sigma(X^x)} ds < \infty, \quad s \geq 0, n \geq 1.$$  

By (4.5) and (4.10), we obtain

$$\sup_{s \in [0,t]} \mathbb{E} \sup_{n \geq 1} \|Q_s^{(n)}\| < \infty.$$  

So, that the sequence $(Q_s^{(n)})_{n \geq 1}$ is uniformly integrable in $L^1([0,t] \times \Omega \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d; ds \times \mathbb{P})$, and $(Q_t^{(n)})_{n \geq 1}$ is uniformly integrable in $L^1(\Omega \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d; \mathbb{P})$. Therefore, there exists a subsequence $n_k \uparrow \infty$ and a progressively measurable process $(Q_s)_{s \in [0,t]}$ satisfying (4.6) such that for any bounded measurable function $\xi : [0,t] \rightarrow \mathbb{R}^d$ and any bounded $d$-dimensional random variable $\eta$,

$$\lim_{k \rightarrow \infty} \mathbb{E} \int_0^t \langle (Q_s^{(n_k)} - Q_s), \xi_s \rangle ds = \lim_{k \rightarrow \infty} \mathbb{E} \langle Q_t^{(n_k)} - Q_t, \eta \rangle = 0, \quad a \in \mathbb{R}^d.$$  

Moreover, for any $m \geq 1$ and $\tau_m := \inf\{t \geq 0 : |X_t^x| \geq m\}$, it follows from (4.9) and (4.10) that

$$\lim_{n \rightarrow \infty} \mathbb{E} \int_0^{t \wedge \tau_m} \langle Q_s^{(n)}, N(X_s^x) \rangle dl_s^x$$  

$$\leq \lim_{n \rightarrow \infty} \frac{|a|^2}{n} \left(1 + \mathbb{E} \int_0^{t \wedge \tau_m} \|Q_s^{(n)}\|^2 \{K(|X_s^x|) ds + |\sigma|(X_s^x) dl_s^x\}\right) = 0,$$  

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where in the last step we have used (4.10), the boundedness of \( K \) and \( \sigma \) on the compact set \( D_m := \{ z \in D : |z| \leq m \} \) (where we take \( \sigma = 0 \) outside \( \partial D \)), and

\begin{equation}
(4.13) \quad \mathbb{E} e^{\lambda t} \mathbb{1}_{t \wedge \tau_m} < \infty, \quad x \in D, t \geq 0, \lambda > 0, m \in \mathbb{N}
\end{equation}

according to the proof of [11, Theorem 6.1]. In fact, as in Lemma 2.1(2), we have the stronger conclusion that \( \mathbb{E} e^{\lambda t} \mathbb{1}_{|X_t| \leq m} d\tau_s < \infty \).

(b) By (4.2), (4.3), (4.8) and that \( P_{t-s} f \) satisfies the Neumann boundary condition, Itô’s formula yields

\begin{equation}
(4.14) \quad d(\nabla Q_{t-s}^{(n)} P_{t-s} f)(X_s^x) = \sqrt{2} \langle \nabla (\nabla A_{t-s}^{(n)} P_{t-s} f)(X_s^x), dB_s \rangle + \{ \langle \nabla (\nabla Q_{t-s}^{(n)} P_{t-s} f), N \rangle (X_s^x) - \| P_{t-s} Q_{t-s}^{(n)} a, \nabla P_{t-s} f)(X_s^x) \rangle \} d\tau_s.
\end{equation}

Since \( P_{t-s} f \) satisfies the Neumann boundary condition, for any \( z \in \partial D \) and \( v \in T_z \partial D \) we have

\[ 0 = \langle v, \nabla (\nabla P_{t-s} f)(z) \rangle = \text{Hess}_{P_{t-s} f}(v, N)(z) - \| v, \nabla P_{t-s} f(z) \| . \]

Then whenever \( X_s^x \in \partial D \),

\[ \langle \nabla (\nabla Q_{t-s}^{(n)} P_{t-s} f), N \rangle (X_s^x) = \text{Hess}_{P_{t-s} f}(N, Q_{t-s}^{(n)} a) = \text{Hess}_{P_{t-s} f}(N, N)(X_s^x) \langle Q_{t-s}^{(n)} a, N(X_s^x) \rangle + \| P_{t-s} Q_{t-s}^{(n)} a, \nabla P_{t-s} f)(X_s^x) \|. \]

Combining this with (4.14), we obtain

\begin{equation}
(4.15) \quad d(\nabla Q_{t-s}^{(n)} P_{t-s} f)(X_s^x) = \sqrt{2} \langle \nabla (\nabla Q_{t-s}^{(n)} P_{t-s} f)(X_s^x), dB_s \rangle + \text{Hess}_{P_{t-s} f}(N, N)(X_s^x) \langle Q_{t-s}^{(n)} a, N(X_s^x) \rangle d\tau_s.
\end{equation}

Since \( P f \in C_b^2([0, t] \times D_m) \) due to the compactness of \( D_m \), there exists a constant \( C_m > 0 \) such that

\begin{equation}
(4.16) \quad \lim_{k \to \infty} \mathbb{E} \int_0^{t \wedge \tau_m} \left| \text{Hess}_{P_{t-s} f}(N, N)(X_s^x) \langle Q_{t-s}^{(n)} a, N(X_s^x) \rangle \right| d\tau_s
\end{equation}

\[ \leq C_m (\mathbb{E} \int_0^{t \wedge \tau_m} \langle Q_{t-s}^{(n)} a, N(X_s^x) \rangle^2 d\tau_s)^{\frac{1}{2}} = 0,
\]

where the last step follows from (4.13) and (4.12). Moreover, since \( \nabla P f \) is bounded on \([0, t] \times D\), it follows from (4.5), (4.10) and (4.11) that

\begin{equation}
(4.17) \quad \lim_{m \to \infty} \lim_{k \to \infty} \mathbb{E} \left| \langle \nabla P_{t-s} f(X_s^x), Q_{t-s}^{(n)} a \rangle - \mathbb{E} \langle \nabla f(X_s^x), Q_t a \rangle \right|
\end{equation}

\[ \leq \lim_{k \to \infty} \sup \mathbb{E} \left| \langle \nabla f(X_s^x), (Q_t^{(n)} - Q_t) a \rangle \right|
\]

\[ + 2 \sup_{[0, t] \times D} |\nabla P f| \lim_{m \to \infty} \mathbb{E} \left\{ 1_{\{ \tau_m < t \}} e^{\int_0^{\tau_m} K(X_s^x) ds + \int_0^{\tau_m} \sigma(X_s^x) d\tau_s} \right\} = 0.
\]
Combining (4.15), (4.16) and (4.17), we arrive at
\[
(\nabla_a P_t f)(x) = \lim_{m \to \infty} \lim_{k \to \infty} \mathbb{E}\langle \nabla P_{t-\tau_m} f(X_{t\wedge \tau_m}^x), Q_m^{(nk)} a \rangle \\
- \lim_{m \to \infty} \lim_{k \to \infty} \mathbb{E} \int_0^{t \wedge \tau_m} \text{Hess}_P_{t-r} f(N, N) \langle Q_r^{(nk)} a, N(X_r^x) \rangle dr \\
= \mathbb{E}\langle \nabla f(X_t^x), Q_t a \rangle.
\]
So, the first equality in (4.7) holds.
(c) By (4.4) and Itô’s formula we have
\[
dP_{t-s} f(X_s^x) = \sqrt{2} \langle \nabla P_{t-s} f(X_s^x), dB_s \rangle.
\]
Then
\[
f(X_t^x) = P_t f(x) + \sqrt{2} \int_0^t \langle \nabla P_{t-s} f(X_s^x), dB_s \rangle,
\]
so that by (4.11),
\[
\frac{1}{\sqrt{2}} \mathbb{E} \left( f(X_t^x) \int_0^t h_s' \langle Q_s a, dB_s \rangle \right) = \mathbb{E} \int_0^t h_s' \langle Q_s a, \nabla P_{t-s} f(X_s^x) \rangle ds \\
= \lim_{k \to \infty} \mathbb{E} \int_0^t h_s' \langle Q_s^{(nk)} a, \nabla P_{t-s} f(X_s^x) \rangle ds.
\]
Similarly to (4.17), we have
\[
\lim_{k \to \infty} \mathbb{E} \int_0^t h_s' \langle Q_s^{(nk)} a, \nabla P_{t-s} f(X_s^x) \rangle ds \\
= \lim_{m \to \infty} \lim_{k \to \infty} \int_0^t h_s' \mathbb{E}\langle Q_s^{(nk)} a, \nabla P_{t-s \wedge \tau_m} f(X_{s \wedge \tau_m}^x) \rangle ds.
\]
Finally, by (4.15) and (4.16),
\[
\lim_{k \to \infty} \mathbb{E}\langle Q_s^{(nk)} a, \nabla P_{t-s \wedge \tau_m} f(X_{s \wedge \tau_m}^x) \rangle \\
= (\nabla_a P_t f)(x) + \lim_{k \to \infty} \mathbb{E} \int_0^{s \wedge \tau_m} \text{Hess}_P_{t-r} f(N, N) \langle Q_r^{(nk)} a, N(X_r^x) \rangle dr \\
= (\nabla_a P_t f)(x)
\]
holds uniformly in \(s \in [0, t]\). Combining this with (1.18) and (1.19), we obtain
\[
\frac{1}{\sqrt{2}} \mathbb{E} \left( f(X_t^x) \int_0^t h_s' \langle Q_s a, dB_s \rangle \right) = \int_0^t h_s' (\nabla_a P_t f)(x) ds = \nabla_a P_t f(x).
\]
To verify the boundedness of $\nabla P_f$ on $[0, t] \times D$ required in Theorem 4.1, one may use the following local version of derivative formula, which is essentially due to [14] Lemma 3.2.2. This type of derivative formula goes back to [7] for manifolds without boundary.

For a compact subset $B$ of $D$, we let $\tau_B^x = \inf\{t \geq 0 : X_t^x \notin B\}, \ x \in B$.

**Theorem 4.2.** Let $x \in D$, and let $B$ be a compact subset of $D$ such that $\text{dist}(x, D \setminus B) > 0$. Then there exists an adapted process $(Q_s)_{s \in [0, t]}$ on $\mathbb{R}^d \times \mathbb{R}^d$ with $Q_0 = I$ and

$$\|Q_s\| \leq e^{\int_0^{s \wedge \tau_B^x} K(X_s^x) \, dt + \int_0^{s \wedge \tau_B^x} \sigma(X_s^x) \, dt}, \ s \in [0, t],$$

such that for any adapted process $(h_s)_{s \in [0, t]}$ with $h_0 = 0$, $h_s = 1$ for $s \geq t \wedge \tau_B^x$, and

$$\mathbb{E} \int_0^t |h'_s|^2 \|Q_s\|^2 \, ds < \infty,$$

there holds

$$\nabla P_tf(x) = \frac{1}{\sqrt{2}} \mathbb{E} \left( f(X_t^x) \int_0^t h'_s Q_s^* \, dB_s \right), \ f \in \mathcal{C}_N(D).$$

**Proof.** Let $Q_s^{(n)}$ solve (4.8). By (4.10) and the exponential integrability of $l_{t \wedge \tau_B^x}$ due to [14] Theorem 6.1, we have

$$\sup_{n \geq 1} \mathbb{E} \int_0^t \|Q_{s \wedge \tau_B^x}^{(n)}\|^2 \, ds < \infty.$$  

Then there exists a subsequence $n_k \uparrow \infty$ and a progressively measurable process $(Q_s)_{s \in [0, t]}$ such that

$$\lim_{k \to \infty} \mathbb{E} \int_0^t (Q_{s \wedge \tau_B^x} - Q_s) \xi_s \, ds = 0, \ \xi_s \in L^2([0, t] \times \Omega; ds \times \mathbb{P}).$$

Next, by (4.16) for $\tau_B^x$ in place of $\tau_m^x$, and using (4.15), we have

$$\lim_{k \to \infty} \mathbb{E} \int_0^t (1 - h_s) d\langle \nabla P_{t-s} f(X_s), Q_s^{(n_k)} a \rangle = 0.$$  

Combining this with (4.23), $h'_s = 0$ for $s \geq t \wedge \tau_B^x$, and noting that

$$d(P_{t-s} f)(X_s^x) = \sqrt{2} \langle \nabla P_{t-s} f(X_s^x), dB_s \rangle, \ s \in [0, t],$$

we obtain

$$\frac{1}{\sqrt{2}} \mathbb{E} \left( f(X_t^x) \int_0^t \langle h'_s Q_s a, dB_s \rangle \right) = \mathbb{E} \int_0^t \langle h'_s Q_s a, \nabla P_{t-s} f(X_s^x) \rangle \, ds$$

$$= \lim_{k \to \infty} \mathbb{E} \int_0^t (h_s - 1)' \langle Q_s^{(n_k)} a, \nabla P_{t-s} f(X_s^x) \rangle \, ds$$

$$= \lim_{k \to \infty} \mathbb{E} \left( \langle \nabla P_{t-s} f(X_s^x), Q_s^{(n_k)} a \rangle (h_s - 1) \right)_{t} - \int_0^t (1 - h_s) d\langle \nabla P_{t-s} f(X_s^x), Q_s^{(n_k)} a \rangle$$

$$= \langle \nabla P_t f(x), a \rangle.$$
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