A CHARACTER OF THE GRADIENT ESTIMATE FOR DIFFUSION SEMIGROUPS

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Abstract. Let \( P_t \) be the semigroup of the diffusion process generated by
\[
L := \sum_{i,j} a_{ij} \partial_i \partial_j + \sum_i b_i \partial_i
\]
on \( \mathbb{R}^d \). It is proved that there exists \( c \in \mathbb{R} \) and an \( \mathbb{R}^d \)-valued function \( b = (b_i) \) such that
\[
| \nabla P_t f | \leq e^{ct} P_t | \nabla f |, \quad t \geq 0, \quad f \in C^1_0(\mathbb{R}^d)
\]
holds for all \( t > 0 \) and all \( f \in C^1_0(\mathbb{R}^d) \) if and only if \( a = (a_{ij}) \) satisfies the formula
\[
\partial_k a_{ij} + \partial_j a_{ik} + \partial_i a_{kj} = 0 \quad \text{for all } i, j, k.
\]

1. Introduction

Consider the second-order differential operator on \( \mathbb{R}^d \):
\[
L = L_{a,b} := \sum_{i,j=1}^d a_{ij} \partial_i \partial_j + \sum_{i=1}^d b_i \partial_i,
\]
where \( a = \sigma \sigma^* \) with \( \sigma \) a matrix-valued \( C^1 \)-function such that \( a \) is non-degenerate, and \( b \) an \( \mathbb{R}^d \)-valued \( C^1 \)-function. Assume that the \( L \)-diffusion process is non-explosive and let \( P_t \) denote its semigroup. The main purpose of the paper is to search for explicit criteria for the following gradient estimate of \( P_t \):
\[
| \nabla P_t f | \leq e^{ct} P_t | \nabla f |, \quad t \geq 0, \quad f \in C^1_0(\mathbb{R}^d),
\]
where \( c \in \mathbb{R} \) is a constant, and \( \nabla \) and \( | \cdot | \) are, respectively, the Euclidean gradient operator and the Euclidean norm.

The gradient estimates of diffusion semigroups have played an important role in the study of functional inequalities and heat kernels. For instance, (1.1) has been related to (at least for \( a \equiv I \)) the log-Sobolev inequality, the dimension-free Harnack inequality and heat kernel upper bounds (see e.g. \cite{2, 6, 7, 8, 5}). Indeed, (1.2) with negative \( c \) can imply the log-Sobolev inequality even if \( a \) is not constant (cf. \cite{4}).

To search for the exact and simple feature of (1.1), we make use of the following equivalent condition following the line of Bakry \cite{1}:
\[
(\nabla f, \nabla L f) \leq | \nabla f | L | \nabla f | + c | \nabla f |^2, \quad f \in C^\infty(\mathbb{R}^d),
\]

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where we set $|\nabla f|L|\nabla f| = 0$ when $|\nabla f| = 0$. Starting from this equivalence, we obtain with some efforts the following result which implies that the formula (1.3) below is the character of (1.1).

**Theorem 1.1.** (1) (1.7) implies
\begin{equation}
\partial_k a_{ij} + \partial_i a_{kj} + \partial_j a_{ki} = 0, \quad 1 \leq i, j, k \leq d.
\end{equation}

(2) If (1.6) holds, then for any $c \in \mathbb{R}$ there exists $b$ such that (1.1) holds for the diffusion semigroup generated by $L_{a,b}$. More precisely, (1.7) follows from (1.5) and
\begin{equation}
c \geq \sup \left\{ \frac{1}{2\lambda(a)(x)} \sum_{i,j=1}^{d} |\partial X a_{ij}|^2(x) + \langle \partial X b, X \rangle(x) : x, X \in \mathbb{R}^d, |X| = 1 \right\}.
\end{equation}

When $a \equiv I$, according to Bakry [1], (1.3) is equivalent to
\begin{equation}
|\nabla P_t f|^2 \leq e^{2ct} t |\nabla f|^2, \quad t \geq 0, f \in C^1_0(\mathbb{R}^d).
\end{equation}

It is easy to see from [1] that (1.5) is always equivalent to
\begin{equation}
\langle \nabla f, \nabla L f \rangle \leq \frac{1}{2} L|\nabla f|^2 + c|\nabla f|^2, \quad f \in C^\infty(\mathbb{R}^d).
\end{equation}

But by combining the following result with Theorem 1.1 we see that (1.1) is not equivalent to (1.5) in general, since it is easy to find an example such that (1.7) holds but (1.3) does not hold (e.g. $d = 1, a(x) = (1 + x^2)^{1/2}, b = 0$).

**Proposition 1.2.** Let $\lambda(a)(x)$ denote the minimal eigenvalue of $a(x)$ for each $x$. (1.3) holds provided
\begin{equation}
c \geq \sup \left\{ \frac{1}{4\lambda(a)(x)} \sum_{i,j=1}^{d} |\partial X a_{ij}|^2(x) + \langle \partial X b, X \rangle(x) : x, X \in \mathbb{R}^d, |X| = 1 \right\}.
\end{equation}

Moreover, to see that (1.7) is somehow a reasonable condition for (1.5) to hold, we present the following estimate of $|\partial X a_{ij}|^2$ in terms of $b$ and $c$.

**Proposition 1.3.** If (1.5) holds, then $\langle \partial X b, X \rangle \leq c|X|^2$ for all $X$, and
\begin{equation}
\sum_{i,j=1}^{d} (\partial X a_{ij})^2 \leq 4\lambda(a)(c - \langle \partial X b, X \rangle), \quad |X| = 1,
\end{equation}

where at each point $\lambda(a)$ denotes the maximal eigenvalue of $a$.

**Remark 1.1.** In general, (1.1) holds provided (see the proof of Theorem 4.13 in [3])
\begin{equation}
\text{Tr} \left\{ (\sigma(x) - \sigma(y))(\sigma(x)^* - \sigma(y)^*) \right\} + \langle b(x) - b(y), x - y \rangle \leq c|x - y|^2, \quad x, y \in \mathbb{R}^d.
\end{equation}

Recently, Da Prato and Goldys claimed in [4] that (1.9) also implies (1.1) provided $a \geq \varepsilon I$ for some $\varepsilon > 0$. This assertion, however, is unfortunately wrong: there are a lot of counter-examples according to Theorem 1.1. Indeed, there is an obvious gap in their proof, i.e. in the proof of Proposition 2.8 in [4]: what they obtained is an upper bound of the second moment, rather than the uniform norm as they claimed, of the derivative process; thus, what they could prove there is (1.6) rather than (1.1).
Lemma 2.1. \([1.1]\) is equivalent to \([1.2]\), while \([1.3]\) is equivalent to \([1.0]\).

Proof of Theorem 1.1 (1). We shall only prove \([1.3]\) at the point 0, since at other points the proof also works by shifting our test functions. We consider three cases respectively: \(i = j = k\); \(i \neq j\) but \(k \in \{i, j\}\); and different \(i, j, k\).

(a) For any \(i\) one has \(\partial_i a_{ii} = 0\). Let \(f(x) = \cos x_i\). By \([1.2]\), we have

\[
\partial_i a_{ii}(x) \leq (c - \partial_i b_i(x)) \tan x_i, \quad x_i > 0.
\]

Letting \(x \to 0\) with \(x_i > 0\), we obtain \(\partial_i a_{ii}(0) \leq 0\). Similarly, for \(x_i < 0\) one has \(\partial_i a_{ii}(x) \geq (c - \partial_i b_i(x))\tan x_i\), and hence \(\partial_i a_{ii}(0) \geq 0\).

(b) For \(i \neq j\), it holds that \(2\partial_i a_{ij} + \partial_j a_{ii} = 0\). For \(\varepsilon > 0\), let \(f(x) = (\varepsilon x_j + x_i)^2\). For \(x_i, x_j > 0\) we have

\[
|\nabla f(x)| = 2(\varepsilon x_j + x_i)\sqrt{1 + \varepsilon^2}, \quad |\nabla f|L|\nabla f| = 4(1 + \varepsilon^2)(\varepsilon x_j + x_i)(\varepsilon b_j + b_i).
\]

Moreover, since \(\partial_i a_{ii} = \partial_j a_{jj} = 0\), we have

\[
\langle \nabla f, \nabla L f \rangle = 4(\varepsilon x_j + x_i)(\varepsilon \partial_j + \partial_i)[a_{ii} + \varepsilon^2 a_{jj} + 2\varepsilon a_{ij} + (\varepsilon x_j + x_i)(\varepsilon b_j + b_i)]
\]

\[
= 4(\varepsilon x_j + x_i)(\varepsilon \partial_j a_{ii} + 2\varepsilon^2 \partial_j a_{ij} + \varepsilon^2 \partial_i a_{jj} + 2\varepsilon \partial_i a_{ij})
\]

\[
+ \varepsilon x_j + x_i)(\varepsilon b_j + b_i)(1 + \varepsilon^2) + 4(\varepsilon x_j + x_i)^2(\varepsilon \partial_j + \partial_i)(\varepsilon b_j + b_i).
\]

Therefore, by \([1.2]\),

\[
2\partial_i a_{ij} + \partial_j a_{ii} \leq \frac{\varepsilon x_j + x_i}{\varepsilon} [c(1 + \varepsilon^2) - (\varepsilon \partial_j + \partial_i)(\varepsilon b_j + b_i)] - \varepsilon(2\partial_j a_{ij} + \partial_i a_{jj}).
\]

Letting \(x \to 0\) with \(x_i, x_j > 0\), we obtain

\[
(2\partial_j a_{ij} + \partial_i a_{jj})(0) \leq -\varepsilon(2\partial_j a_{ij} + \partial_i a_{jj})(0).
\]

Thus, letting \(\varepsilon \downarrow 0\), we arrive at \((2\partial_j a_{ij} + \partial_i a_{jj})(0) \leq 0\). Similarly, working with \(x_i, x_j < 0\) we obtain the inverse inequality.

(c) For any different \(i, j, k\), one has \(\partial_k a_{ij} + \partial_i a_{kj} + \partial_j a_{ik} = 0\). Let \(f(x) = (x_k + x_i + x_j)^2\). For \(x_i, x_j, x_k > 0\) we have

\[
|\nabla f(x)| = 2\sqrt{3}(x_k + x_i + x_j) = 2\sqrt{3}g(x), \quad |\nabla f|L|\nabla f| = 12g(x)(b_k + b_i + b_j)(x).
\]

Moreover, by (a) and (b) in this proof we have

\[
\langle \nabla f, \nabla L f \rangle
\]

\[
= 4g \cdot (\partial_k + \partial_i + \partial_j)[a_{ii} + a_{jj} + a_{kk} + 2a_{ij} + 2a_{ki} + 2a_{kj} + g \cdot (b_k + b_i + b_j)]
\]

\[
= 4g^2 \cdot (\partial_k + \partial_i + \partial_j)(b_k + b_i + b_j) + 12g \cdot (b_k + b_i + b_j)
\]

\[
+ 8g \cdot (\partial_k a_{ij} + \partial_i a_{kj} + \partial_j a_{ik}).
\]

Therefore, for \(x_i, x_j, x_k > 0\) it follows from \([1.2]\) that

\[
2(\partial_k a_{ij} + \partial_j a_{ik} + \partial_i a_{jk}) \leq 3cg - g \cdot (\partial_k + \partial_i + \partial_j)(b_k + b_i + b_j).
\]

Letting \(x \to 0\) we obtain \((\partial_k a_{ij} + \partial_j a_{ik} + \partial_i a_{jk})(0) \leq 0\). Similarly, we obtain the inverse inequality by considering \(x_i, x_j, x_k < 0\). \(\square\)
Proof of Theorem 1.1 (2). We first prove that (1.4) and (1.3) imply (1.2). For \( f \in C_0^\infty(\mathbb{R}^d) \) we have
\[
\langle a \nabla |\nabla f |, \nabla |\nabla f | \rangle = \frac{1}{|\nabla f|^2} \sum_{i,j=1}^d a_{ij} \langle \nabla f_i, \nabla f'_j \rangle \langle \nabla f, \nabla f_j \rangle
\]
at points with \( |\nabla f | > 0 \). Moreover, we have
\[
\frac{1}{2} L|\nabla f|^2 = \sum_{i,j=1}^d a_{ij} \left[ (\nabla f'_i, \nabla f_j) + \langle \nabla f, \nabla f''_j \rangle \right] + \sum_{i=1}^d b_i \langle \nabla f, \nabla f'_i \rangle,
\]
where \( f'_j := \partial_j f \) and \( f''_{ij} := \partial_i \partial_j f, 1 \leq i, j \leq d \). Combining (2.1) with (2.2) and (2.3) we obtain
\[
I_1 := \langle \nabla f, \nabla Lf \rangle = \langle \nabla f, \nabla |\nabla f | \rangle - \frac{1}{2} L|\nabla f|^2 + \langle a \nabla |\nabla f |, |\nabla f | \rangle = \sum_{i,j=1}^d \left\{ \langle \nabla f, \nabla a_{ij} \rangle f''_{ij} - a_{ij} \left( \langle \nabla f_i, \nabla f'_j \rangle - \frac{\langle \nabla f, \nabla f'_i \rangle \langle \nabla f, \nabla f_j \rangle}{|\nabla f|^2} \right) \right\} + \langle \partial \nabla f b, \nabla f \rangle
\]
where \( P \) denotes the projection to the vector space \( \{ X : \langle X, \nabla f \rangle = 0 \} \). To prove (1.5) we need to estimate
\[
I_2 := \sum_{i,j=1}^d \langle \nabla f, \nabla a_{ij} \rangle f''_{ij} = \sum_{i,j,k=1}^d f'_k \partial_k a_{ij} f''_{ij}
\]
in terms of \( \sum_{i,j=1}^d |P(\nabla f'_i)|^2 \). To this end, let us look at a fixed point \( x_0 \) with \( |\nabla f |(x_0) > 0 \). Since \( I_1 \) involves \( a \) only via \( a_{ij}(x_0) \) and \( \nabla a_{ij}(x_0) \), we may assume that \( a_{ij} \) is linear for all \( i, j \). Indeed, replacing \( a_{ij}(x) \) by \( a_{ij}(x_0) + \sum_k x_k \partial_k a_{ij}(x_0) \), the value of \( I_1 \) at \( x_0 \) does not change and (1.3) remains true.

Now, for each \( j \) let \( X^j \) be an \( \mathbb{R}^d \)-valued function with \( X^j := \sum_{k=1}^d f'_k \partial_k a_{ij} \), \( 1 \leq i \leq d \). We have
\[
I_2 = \sum_{j=1}^d \langle \nabla f'_j, X^j \rangle = \sum_{j=1}^d \langle P(X^j), P(\nabla f'_j) \rangle + \frac{1}{|\nabla f|^2} \sum_{j=1}^d \langle \nabla f'_j, \nabla f \rangle \langle \nabla f, X^j \rangle.
\]
Since by (1.3) one has
\[
\sum_{j=1}^d \langle X^j, \nabla f \rangle f'_j = \sum_{i,j,k=1}^d f'_k \partial_k a_{ij} = 0
\]
it follows that
\[
0 = \sum_{j=1}^d \langle \nabla f, \nabla (\langle X^j, \nabla f \rangle f'_j) \rangle = \sum_{j=1}^d \left[ \langle \nabla f'_j, \nabla f \rangle \langle X^j, \nabla f \rangle + f'_j |\nabla f | \langle X^j, \nabla f \rangle \right].
\]
Noting that we have assumed that $a_{ij}$ is linear for each $i, j$, we obtain

$$I_3 := \sum_{j=1}^{d} \langle \nabla f_j, \nabla f \rangle \langle \nabla f, X^j \rangle = - \sum_{j,k=1}^{d} f_j f_k \partial_k \left( \sum_{i=1}^{d} f_i X_i^j \right)$$

$$= - \sum_{i,j,k,l=1}^{d} f_j f_k \left[ f_i f_k \partial_i a_{ij} + f_l f_k \partial_l a_{ij} \right].$$

Combining this with (2.4) we obtain

$$I_3 = - \sum_{i,j,k,l=1}^{d} f_j f_k \left[ f_i f_k \partial_i a_{ij} - f_l f_k \partial_l a_{ij} - f_l f_k \partial_j a_{il} \right] = \sum_{i,j,k,l=1}^{d} f_j f_k \partial_i a_{ij}.$$ 

For fixed $k$, let $Y^k$ be the $\mathbb{R}^d$-valued function with $Y^k_i := f_k \sum_{j=1}^{d} f_j \partial_j a_{il}$. By (2.6) we have

$$\langle Y^k, \nabla f \rangle = f_k \sum_{i,j,l=1}^{d} f_j f_k \partial_j a_{il} = 0.$$ 

Then

$$I_3 = \sum_{k=1}^{d} \langle Y^k, \nabla f^k \rangle = \sum_{k=1}^{d} \langle Y^k, P(\nabla f^k) \rangle.$$ 

Combining this with (2.4) and (2.5) we obtain

$$I_1 = \sum_{j=1}^{d} \left( \langle P(X^j), P(\nabla f^j) \rangle + \frac{1}{|\nabla f|^2} \langle Y^j, P(\nabla f^j) \rangle \right)$$

$$- \sum_{i,j=1}^{d} a_{ij} \langle P(\nabla f^j), P(\nabla f^j) \rangle + \langle \partial_\nabla f b, \nabla f \rangle$$

$$\leq |\nabla f| \left\{ \sum_{j=1}^{d} \left| P(\nabla f^j) \right|^2 \right\}^{1/2} \left\{ \frac{2}{|\nabla f|^2} \sum_{j=1}^{d} \left| P(X^j) \right|^2 + \frac{2}{|\nabla f|^6} \sum_{j=1}^{d} \left| Y^j \right|^2 \right\}^{1/2}$$

$$- \lambda(a) \sum_{j=1}^{d} \left| P(\nabla f^j) \right|^2 + \langle \partial_\nabla f b, \nabla f \rangle$$

$$\leq \frac{|\nabla f|^2}{2 \lambda(a)} \sum_{j=1}^{d} \left( \frac{\left| P(X^j) \right|^2}{|\nabla f|^2} + \frac{|Y^j|^2}{|\nabla f|^6} \right) + \langle \partial_\nabla f b, \nabla f \rangle.$$ 

Since

$$\sum_{j=1}^{d} \left| X^j \right|^2 = \sum_{i,j=1}^{d} \left( \sum_{k=1}^{d} f_k \partial_k a_{ij} \right)^2 = \sum_{i,j=1}^{d} \left( \partial_\nabla f a_{ij} \right)^2$$

by (2.7), (1.2) follows from

$$\sum_{j=1}^{d} \left( \left| P(X^j) \right|^2 + \frac{|Y^j|^2}{|\nabla f|^4} \right) = \sum_{j=1}^{d} |X^j|^2.$$
or equivalently
\[
(2.8) \quad |\nabla f|^2 \sum_{j=1}^{d} \langle X^j, \nabla f \rangle^2 = \sum_{j=1}^{d} |Y^j|^2.
\]

By the definitions of $X^j$ and $Y^k$, we have
\[
\sum_{k=1}^{d} |Y^k|^2 = |\nabla f|^2 \sum_{i=1}^{d} \left( \sum_{j,l=1}^{d} f_j^i f_l^i \partial_j a_{il} \right)^2 = |\nabla f|^2 \sum_{i,j=1}^{d} \left( \sum_{i,l=1}^{d} f_j^i f_l^i \partial_j a_{ij} \right)^2
\]
\[
= |\nabla f|^2 \left( \sum_{j=1}^{d} \left( \sum_{i,l=1}^{d} f_j^i \partial_j a_{ij} \right) \right)^2 = |\nabla f|^2 \sum_{j=1}^{d} (X^j, \nabla f)^2.
\]
Thus (2.8) and hence (1.2) holds.

Now, assume that (1.3) holds and let $c \in \mathbb{R}$ be fixed. Let $F \in C^2([0, \infty))$ be such that $F' \geq 0$ and
\[
F(|x|^2) \geq \frac{1}{2\lambda(a)(x)} \sum_{i,j=1}^{d} |\nabla a_{ij}(x)|^2, \quad x \in \mathbb{R}^d.
\]
Indeed, letting $\gamma \in C^2[0, \infty)$ with
\[
\gamma(r) \geq \sup_{|x|^2=r} \frac{1}{2\lambda(a)(x)} \sum_{i,j=1}^{d} |\nabla a_{ij}(x)|^2,
\]
we may take $F(r) = \gamma(0) + \int_{0}^{r} \sqrt{1+\gamma'(s)^2} ds$. Let
\[
V(x) = -\frac{1}{2} \int_{0}^{|x|^2} F(r)dr + \frac{1}{2} c|x|^2, \quad b(x) = \nabla V(x).
\]
We have
\[
\langle \partial_X b, X \rangle(x) = \operatorname{Hess}_V(X, X)(x) \leq \frac{1}{2}(c - F(|x|^2))\operatorname{Hess}_{|x|^2}(X, X)(x) = c - F(|x|^2).
\]
Therefore, (1.4) holds and hence one has (1.1). \qed

**Proof of Proposition 1.2.** By Lemma 2.1, it suffices to show that each of (1.7) implies (1.6). By (2.2) and (2.3) we have
\[
\langle \nabla f, \nabla L f \rangle - \frac{1}{2} |\nabla f|^2 = \sum_{i,j=1}^{d} \langle \nabla f, \nabla a_{ij} \rangle f_j^i - \sum_{i,j=1}^{d} a_{ij} \langle \nabla f_i^j, \nabla f_j^i \rangle + \langle \partial_{\nabla f} b, \nabla f \rangle
\]
\[
\leq \sum_{i,j=1}^{d} \langle \nabla f, \nabla a_{ij} \rangle f_j^i - \lambda(a) \sum_{i,j=1}^{d} (f_j^i)^2 + \langle \partial_{\nabla f} b, \nabla f \rangle
\]
\[
\leq \frac{1}{4\lambda(a)} \sum_{i,j=1}^{d} |\partial_{\nabla f} a_{ij}|^2 + \langle \partial_{\nabla f} b, \nabla f \rangle.
\]
Thus (1.7) implies (1.6) and hence (1.5) by Lemma 2.1. \qed
Proof of Proposition 1.3. The estimate of $\langle \partial_X b, X \rangle$ follows from (1.6) with $f(x) = \sum_{i,j} X_i x_i$. Now, for fixed $X, x \in \mathbb{R}^d$ with $|X| = 1$, let

$$f(y) = 2\lambda(a)(x)\langle X, y \rangle + \frac{1}{2} \sum_{i,j=1}^d (\partial_X a_{ij}(x))(y_i - x_i)(y_j - x_j).$$

It follows from (1.6), (2.2) and (2.3) that

$$h(0) = 0 \quad \text{and} \quad h(t) = 2 \lambda(a)(x) \langle X, x \rangle \quad \text{for} \quad t > 0.$$

Then, using (1.2) and (1.6), we obtain

$$h(t) = 2 \lambda(a)(x) \langle X, x \rangle \quad \text{for} \quad t > 0.$$
Therefore,
\[
Eh_\delta(\|\nabla P_{\tau_n - s}^f\|)(x_{s\wedge \tau_n}) - Eh_\delta(\|\nabla P_{\tau_n - s'}^f\|)(x_{s'\wedge \tau_n}) \\
\geq -cE \int_{s'\wedge \tau_n}^{s\wedge \tau_n} (h_\delta(\|\nabla P_{\tau_n-u}^f\|)(x_u) du, \quad 0 \leq s' < s \leq t.
\]
Let \(\phi_n(s) := E|\nabla P_{\tau_n - s}^f|(x_{s\wedge \tau_n})\). By letting \(\delta \downarrow 0\) in the above inequality, we obtain
\[
(3.1) \quad \phi_n(s) - \phi_n(s') \geq -cE \int_{s'\wedge \tau_n}^{s\wedge \tau_n} |\nabla P_{\tau_n-u}^f|(x_u) du \geq -c + \int_{s'}^{s} \phi_n(u) du, \quad t \geq s > s' \geq 0.
\]
Thus \(\phi_n(t) \geq e^{-ct}\phi_n(0)\). Since \(|\nabla f|\) is bounded, by Fatou’s lemma and the dominated convergence theorem we obtain
\[
|\nabla P_t f| = E \liminf_{n \to \infty} |\nabla P_{\tau_n}^f| \leq \liminf_{n \to \infty} \phi_n(0) \leq e^{-ct} \liminf_{n \to \infty} \phi_n(t) = e^{-ct} P_t|\nabla f|.
\]
Therefore, we are able to use the dominated convergence theorem by letting \(n \to \infty\) in the first inequality of (3.1) to obtain
\[
E|\nabla P_{t-s} f|(x_s) - E|\nabla P_{t-s'} f|(x_{s'}) \geq -c \int_{s'}^{s} E|\nabla P_{t-u} f|(x_u) du.
\]
This implies (1.1).

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