

Derivatives of Feynman-Kac semigroups

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Abstract

We prove Bismut-type formulae for the first and second derivatives of a Feynman-Kac semigroup on a complete Riemannian manifold. We derive local estimates and give bounds on the logarithmic derivatives of the integral kernel. Stationary solutions are also considered. The arguments are based on local martingales, although the assumptions are purely geometric.

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1 Introduction

Suppose M is a complete Riemannian manifold of dimension n with Levi-Civita connection ∇ . Denote by Δ the Laplace-Beltrami operator, suppose Z is a smooth vector field and set $L := \frac{1}{2}\Delta + Z$. Any elliptic diffusion operator on a smooth manifold induces, via its principle symbol, a Riemannian metric with respect to which it takes this form. Denote by x_t a diffusion on M starting at $x_0 \in M$ with generator L and explosion time $\zeta(x_0)$. The explosion time is the random time at which the process leaves all compact subsets of M . Suppose $V : [0, \infty) \times M \rightarrow \mathbb{R}$ is a smooth function which is bounded below and denote by $P_t^V f$ the associated Feynman-Kac semigroup, acting on bounded measurable functions f . For $T > 0$ fixed, $P_t^V f$ is smooth and bounded on $(0, T] \times M$, satisfies the parabolic equation

$$\partial_t \phi_t = (L - V_t) \phi_t \tag{1}$$

on $(0, T] \times M$ with $\phi_0 = f$ and for

$$\mathbb{V}_t := e^{-\int_0^t V_{T-s}(x_s) ds} \tag{2}$$

is represented probabilistically by the Feynman-Kac formula

$$P_T^V f(x_0) = \mathbb{E} [\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}}]. \tag{3}$$

In the self-adjoint case, equation (1) corresponds (via Wick rotation) to the Schrödinger equation for a single non-relativistic particle moving in an electric field in curved space. In this sense, the derivative $dP_T^V f$ corresponds to the momentum of the particle and $LP_T^V f$ the kinetic energy.

In this article, we prove probabilistic formulae and estimates for $dP_T^V f$, $LP_T^V f$ and $\nabla dP_T^V f$. In doing so, we extend results in [18] (by including V) and in [1] (by including Z and V). In each case, we allow for unbounded and time-dependent V . Our approach

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is more concise than that of [1], since we avoid the extrinsic argument in favour of the differential Bianchi identity. Our results imply new Bismut-type formulae for the derivatives of the heat kernel in the *forward* variable (see, for example, Corollary 2.3). Our formula for $dP_T^V f$ is given by Theorem 2.2. For $v \in T_{x_0}M$ it states

$$(dP_T^V f)(v) = -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right]$$

where $//_t$ and W_t are the usual parallel and damped parallel transports, respectively, and B_t the martingale part of the antidevelopment of x_t to $T_{x_0}M$. The process k_t is chosen so that it vanishes once x_t exits a regular domain (an open connected subset with compact closure and smooth boundary). Imposing this condition on k_t obviates the need for any assumptions on Ric_Z . Conversely, if we assume Ric_Z is bounded below then we can choose $k_t = (T-t)/T$ and our formula for $dP_t^V f$ reduces to that of [5, Theorem 5.2]. Formulae in [5] are derived from the assumption that one can differentiate under the expectation, and thus require global assumptions. Our approach, on the other hand, follows that of [18] and [1] in using local martingales to obtain local formula for which no assumptions are needed.

Our formula for $LP_T^V f$ is given by Theorem 2.6. It states

$$\begin{aligned} & L(P_T^V f)(x_0) \\ = & \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle \right] \\ & + \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right] \end{aligned}$$

where the processes k and l are assumed to vanish outside of a regular domain. A formula for ΔP_T (acting on differential forms) was previously given in [6], for the case of a compact manifold with $Z = 0$ and $V = 0$.

Our formula for $\nabla dP_T^V f$ is given by Theorem 2.8. For $v, w \in T_{x_0}M$ it states

$$\begin{aligned} & (\nabla dP_T^V f)(v, w) \\ = & -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\ & - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\ & + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle + dV_{T-s}(W_s(l_s w)) ds \right) \right. \\ & \quad \left. \cdot \left(\int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right) \right] \end{aligned}$$

where W'_t solves a covariant Itô equation determined by the curvature tensor and its derivative. This extends [1, Theorem 2.1] while avoiding the use of a stochastic differential equation.

The formulae mentioned above are derived in Section 2. Solutions to the time independent equation

$$(L - V)\phi = -E\phi$$

with $E \in \mathbb{R}$ are subject to a similar analysis, as outlined in Section 3. In Section 4 we derive local estimates, using the formulae of Section 2 and local assumptions on curvature and the derivative of the potential function. We do so by choosing the processes k and l appropriately, as in [18] and [1], and applying the Cauchy-Schwarz inequality. These local estimates are given by Theorems 4.1, 4.3 and 4.5; global estimates are then given as corollaries. The global estimates are derived under appropriate global assumptions and imply the boundedness of $dP_t^V f$, $LP_t^V f$ and $\nabla dP_t^V f$ on $[\epsilon, T] \times M$. These bounds lead to the non-local formulae of Section 5, in which the processes k and l are chosen deterministically. For the case in which Z is a gradient, estimates on the logarithmic derivatives of the integral kernel can then be derived, using Jensen's inequality. They are given in Section 6 and extend those of [8] and [17].

2 Local Formulae

For the remainder of this article, we fix $T > 0$ and set $f_t := P_{T-t}^V f$.

2.1 Gradient

Denote by $\text{Ric}_Z^\sharp := \text{Ric}^\sharp - 2\nabla Z$ the Bakry-Emery tensor (see [3]). Then the damped parallel transport $W_t : T_{x_0}M \rightarrow T_{x_t}M$ is the solution, along the paths of x_t , to the covariant ordinary differential equation

$$DW_t = -\frac{1}{2}\text{Ric}_Z^\sharp W_t \quad (4)$$

with $W_0 = \text{id}_{T_{x_0}M}$. Suppose D is a regular domain in M with $x_0 \in D$ and denote by τ the first exit time of x_t from D .

Lemma 2.1. *Suppose $v \in T_{x_0}M$ and that k is a bounded adapted process with paths in the Cameron-Martin space $L^{1,2}([0, T]; \text{Aut}(T_{x_0}M))$ such that $k_t = 0$ for $t \geq T - \epsilon$. Then*

$$\mathbb{V}_t df_t(W_t(k_t v)) - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{k}_s v), / /_s dB_s \rangle - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(k_s v)) ds \quad (5)$$

is a local martingale on $[0, \tau \wedge T)$.

Proof. Setting $N_t(v) := df_t(W_t(v))$ we see by Itô's formula and the relations

$$\begin{aligned} d\Delta f &= \text{tr} \nabla^2 df - df(\text{Ric}^\sharp) \\ dZf &= \nabla_Z df + df(\nabla Z) \\ dV_t f &= f dV_t + V_t df \end{aligned}$$

(the first one is the Weitzenböck formula) that

$$\begin{aligned} dN_t(v) &\stackrel{m}{=} df_t(DW_t(v))dt + (\partial_t df_t)(W_t(v))dt + \left(\frac{1}{2} \text{tr} \nabla^2 + \nabla_Z \right) (df_t)(W_t(v))dt \\ &= V_{T-t} N_t(v)dt + f_t(x_t) dV_{T-t}(W_t(v))dt \end{aligned}$$

where $\stackrel{m}{=}$ denotes equality modulo the differential of a local martingale. Recalling the definition of \mathbb{V}_t given by equation (2), it follows that

$$d(\mathbb{V}_t N_t(k_t v)) \stackrel{m}{=} \mathbb{V}_t N_t(\dot{k}_t v)dt + \mathbb{V}_t f_t(x_t) dV_{T-t}(W_t(k_t v))dt$$

so that

$$\mathbb{V}_t N_t(k_t v) - \int_0^t \mathbb{V}_s df_s(W_s(\dot{k}_s v))ds - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(k_s v))ds$$

is a local martingale. By the formula

$$\mathbb{V}_t f_t(x_t) = f_0(x_0) + \int_0^t \mathbb{V}_s df_s(//_s dB_s)$$

and integration by parts we see that

$$\int_0^t \mathbb{V}_s df_s(W_s(\dot{k}_s v)) ds - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle$$

is also a local martingale and so the lemma is proved. \square

Theorem 2.2. *Suppose $x_0 \in D$ with $v \in T_{x_0}M$, $f \in \mathcal{B}_b$, V bounded below and $T > 0$. Suppose k is a bounded adapted process with paths belonging to the Cameron-Martin space $L^{1,2}([0, T]; \text{Aut}(T_{x_0}M))$, such that $k_0 = 1$, $k_t = 0$ for $t \geq \tau \wedge T$ and $\int_0^{\tau \wedge T} |\dot{k}_s|^2 ds \in L^1$. Then*

$$(dP_T^V f)(v) = -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right]. \quad (6)$$

Proof. As in the proof of [18, Theorem 2.3], the process k_t can be modified to k_t^ϵ so that $k_t^\epsilon = k_t$ for $t \leq \tau \wedge (T - 2\epsilon)$ and $k_t^\epsilon = 0$ for $t \geq \tau \wedge (T - \epsilon)$, cutting off appropriately in between. Since $(df_t)_x$ is smooth and therefore bounded for $(t, x) \in [0, T - \epsilon] \times D$, it follows from Lemma 2.1 and the strong Markov property that formula (6) holds with k_t^ϵ in place of k_t . The result follows by taking $\epsilon \downarrow 0$. \square

Denoting by $p_T^Z(x, y)$ the transition density of the diffusion with generator L , using Theorem 2.2 we can easily obtain the following Bismut formula, for the derivative of $p_T^Z(x, y)$ the in the forward variable y .

Corollary 2.3. *Suppose $x_0 \in D$ with $\text{div } Z$ bounded below and k as in Theorem 2.2. Then*

$$d \log p_T^Z(y, \cdot)_{x_0} = - \frac{\mathbb{E} \left[e^{-\int_0^T \text{div } Z(x_s) ds} \int_0^T \langle W_s \dot{k}_s, //_s dB_s \rangle + d(\text{div } Z)(W_s k_s) ds \mid x_T = y \right]}{\mathbb{E} \left[e^{-\int_0^T \text{div } Z(x_s) ds} \mid x_T = y \right]}$$

where here x_t is a diffusion on M with generator $\frac{1}{2}\Delta - Z$ starting at x_0 .

Proof. According to the Fokker-Planck equation, we have

$$p_T^Z(x, y) = p_T^{-Z, -\text{div } Z}(y, x)$$

where $p_T^{-Z, -\text{div } Z}(y, x)$ denotes the minimal integral kernel for the semigroup generated by the operator $L^* = \frac{1}{2}\Delta - Z - \text{div } Z$. The result is therefore obtained simply by conditioning in Theorem 2.2, having replaced Z with $-Z$ and V with $\text{div } Z$. \square

2.2 Generator

Now suppose D_1 and D_2 are regular domains with $x_0 \in D_1$ and $\overline{D_1} \subset D_2$. Denote by σ and τ the first exit times of x_t from D_1 and D_2 , respectively.

Lemma 2.4. *Suppose $x_0 \in D_1$ and $0 < S < T$ and that k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, T]; \mathbb{R})$ such that $k_s = 0$ for*

$s \geq \sigma \wedge S$, $l_s = 1$ for $s \leq \sigma \wedge S$ and $l_s = 0$ for $s \geq \tau \wedge (T - \epsilon)$. Then

$$\begin{aligned} & \mathbb{V}_t(Lf_t)(x_t)k_t - \frac{1}{2}\mathbb{V}_t df_t \left(W_t l_t \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \right) \\ & + \frac{1}{2}\mathbb{V}_t f_t(x_t) \int_0^t \langle W_s \dot{l}_s, //_s dB_s \rangle \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \frac{1}{2} \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s l_s) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \mathbb{V}_t f_t(x_t) \int_0^t \langle \dot{k}_s Z - k_s \nabla V_{T-s}, //_s dB_s \rangle \\ & - \int_0^t \mathbb{V}_s f_s k_s LV_{T-s} ds \end{aligned}$$

is a local martingale on $[0, \tau \wedge T)$.

Proof. Defining

$$n_t := (Lf_t)(x_t)$$

we have, by Itô's formula, that

$$\begin{aligned} dn_t &= d(Lf_t)_{x_t} //_t dB_t + \partial_t(Lf_t)(x_t)dt + L(Lf_t)(x_t)dt \\ &= d(Lf_t)_{x_t} //_t dB_t + L(V_{T-t}f_t)dt \\ &= d(Lf_t)_{x_t} //_t dB_t + (LV_{T-t})f_t dt + V_{T-t}n_t dt + \langle df_t, dV_{T-t} \rangle dt. \end{aligned}$$

It follows that

$$d(\mathbb{V}_t n_t k_t) \stackrel{m}{=} \mathbb{V}_t n_t \dot{k}_t + k_t \mathbb{V}_t (f_t LV_{T-t} + \langle df_t, dV_{T-t} \rangle) dt$$

and so

$$\mathbb{V}_t(Lf_t)(x_t)k_t - \int_0^t \mathbb{V}_s(Lf_s)(x_s) \dot{k}_s ds - \int_0^t \mathbb{V}_s k_s (f_s LV_{T-s} + \langle df_s, dV_{T-s} \rangle) ds$$

is a local martingale, with

$$-(Lf_t)(x_t) \dot{k}_t dt = \left(\frac{1}{2} d^* d - Z \right) f_t(x_t) \dot{k}_t dt = \left(\frac{1}{2} d^*(df_t) - (df_t)(Z) \right) \dot{k}_t dt.$$

By the Weitzenböck formula

$$d(\langle df_t, W_t \rangle) = (\nabla //_{/t} dB_t df_t)(W_t) - V_{T-t}(df_t)(W_t) dt + f_t(x_t) dV_{T-t}(W_t) dt$$

from which it follows that

$$d(\mathbb{V}_t \langle df_t, W_t \rangle) = \mathbb{V}_t (\nabla //_{/t} dB_t df_t)(W_t) + \mathbb{V}_t f_t(x_t) dV_{T-t}(W_t) dt.$$

Consequently, for an orthonormal basis $\{e_i\}_{i=1}^n$ of $T_{x_0}M$, by integration by parts we have

$$\begin{aligned} \mathbb{V}_t d^*(df_t) \dot{k}_t dt &= - \sum_{i=1}^n \mathbb{V}_t (\nabla //_{/t} e_i df_t) (//_t e_i) \dot{k}_t dt \\ &\stackrel{m}{=} - \mathbb{V}_t (\nabla //_{/t} dB_t df_t)(W_t) \dot{k}_t W_t^{-1} //_t dB_t \\ &= - d(\mathbb{V}_t df_t(W_t) \int_0^t \dot{k}_s W_s^{-1} //_s dB_s) \\ &\quad + d \left(\int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \right). \end{aligned}$$

Furthermore

$$\int_0^t \mathbb{V}_s df_s(Z) \dot{k}_s ds - \mathbb{V}_t f_t(x_t) \int_0^t \langle \dot{k}_s Z, //_s dB_s \rangle$$

is a local martingale and therefore

$$\begin{aligned} & \int_0^t \mathbb{V}_s(Lf_s)(x_s) \dot{k}_s ds \\ & - \frac{1}{2} \mathbb{V}_t df_t(W_t) \int_0^t \dot{k}_s W_s^{-1} //_s dB_s + \frac{1}{2} \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \mathbb{V}_t f_t(x_t) \int_0^t \langle \dot{k}_s Z, //_s dB_s \rangle \end{aligned}$$

is also a local martingale. By the assumptions on k and l it follows from Lemma 2.1 that

$$\begin{aligned} O_t^1 &= \mathbb{V}_t df_t(W_t((l_t - 1))) - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{l}_s), //_s dB_s \rangle \\ & \quad - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s((l_s - 1))) ds, \\ O_t^2 &= \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \end{aligned}$$

are two local martingales. So the product $O_t^1 O_t^2$ is also a local martingale, since $O^1 = 0$ on $[0, \sigma \wedge S]$ with O^2 constant on $[\sigma \wedge S, \tau \wedge (T - \epsilon)]$. Consequently

$$\begin{aligned} & - \mathbb{V}_t df_t \left(W_t \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \right) + \mathbb{V}_t df_t \left(W_t l_t \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \right) \\ & - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s \dot{l}_s, //_s dB_s \rangle \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s((l_s - 1))) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \end{aligned}$$

is a local martingale and therefore so is

$$\begin{aligned} & \mathbb{V}_t(Lf_t)(x_t) k_t - \frac{1}{2} \mathbb{V}_t df_t \left(W_t l_t \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \right) \\ & + \frac{1}{2} \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s \dot{l}_s, //_s dB_s \rangle \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \frac{1}{2} \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s l_s) ds \int_0^t \dot{k}_s W_s^{-1} //_s dB_s \\ & + \mathbb{V}_t f_t(x_t) \int_0^t \langle \dot{k}_s Z, //_s dB_s \rangle \\ & - \int_0^t \mathbb{V}_s k_s (f_s LV_{T-s} + \langle df_s, dV_{T-s} \rangle) ds. \end{aligned}$$

Since

$$\int_0^t \mathbb{V}_s df_s(\nabla V_{T-s}) k_s ds - \mathbb{V}_t f_t(x_t) \int_0^t \langle k_s \nabla V_{T-s}, //_s dB_s \rangle$$

is a local martingale, the result follows. \square

Lemma 2.5. Suppose $x_0 \in D_1$, $f \in \mathcal{B}_b$, V bounded below and $0 < S < T$. Suppose k is a bounded adapted process with paths in the Cameron-Martin space $L^{1,2}([0, T]; \mathbb{R})$ such that $k_s = 0$ for $s \geq \sigma \wedge S$, $k_0 = 1$ and $\int_0^{\sigma \wedge S} |\dot{k}_s|^2 ds \in L^1$. Then

$$V_T(x_0)P_T^V f(x_0) = \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T (k_s \dot{V}_{T-s}(x_s) - \dot{k}_s V_{T-s}(x_s)) ds \right].$$

Proof. By Itô's formula, we have

$$d(\mathbb{V}_t V_{T-t} f_t k_t) \stackrel{m}{=} -k_t \mathbb{V}_t \dot{V}_{T-t} f_t + \dot{k}_t \mathbb{V}_t V_{T-t} f_t$$

which implies

$$\mathbb{V}_t V_{T-t} f_t k_t - \int_0^t (\dot{k}_s \mathbb{V}_s V_{T-s} f_s - k_s \mathbb{V}_s \dot{V}_{T-s} f_s) ds$$

is a local martingale on $[0, \tau \wedge T)$. The assumptions on f and V imply it is a martingale on $[0, \tau \wedge T]$, so result follows by taking expectations and applying the strong Markov property. \square

Theorem 2.6. Suppose $x_0 \in D_1$, $f \in \mathcal{B}_b$, V bounded below and $0 < S < T$. Suppose k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, T]; \mathbb{R})$ such that $k_s = 0$ for $s \geq \sigma \wedge S$, $k_0 = 1$, $l_s = 1$ for $s \leq \sigma \wedge S$, $l_s = 0$ for $s \geq \tau \wedge T$, $\int_0^{\sigma \wedge S} |\dot{k}_s|^2 ds \in L^1$ and $\int_{\sigma \wedge S}^{\tau \wedge T} |\dot{l}_s|^2 ds \in L^1$. Then

$$\begin{aligned} L(P_T^V f)(x_0) &= \\ &\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle \right] \\ &+ \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right]. \end{aligned}$$

Proof. Modifying the process l_t to l_t^ϵ as in the proof of Theorem 2.2, it follows from Lemma 2.4, the strong Markov property, the boundedness of $P_t^V f$ on $[0, T] \times \bar{D}_2$ and the boundedness of $dP_t^V f$ and $LP_t^V f$ on $[\epsilon, T] \times \bar{D}_2$ that the formula

$$\begin{aligned} &L(P_T^V f)(x_0) \\ &= \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle - \int_0^T k_s (dV_{T-s} //_s dB_s + LV_{T-s} ds) \right) \right] \\ &+ \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right] \end{aligned}$$

holds with l_t^ϵ in place of l_t . The formula also holds as stated, in terms of l_t , by taking $\epsilon \downarrow 0$. Applying the Itô formula yields

$$\int_0^T k_s (dV_{T-s} //_s dB_s + LV_{T-s} ds) = -V_T(x_0) + \int_0^T (k_s \dot{V}_{T-s}(x_s) - \dot{k}_s V_{T-s}(x_s)) ds$$

and therefore

$$\begin{aligned}
& (L - V_T(x_0))(P_T^V f)(x_0) = \\
& \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle - \int_0^T (k_s \dot{V}_{T-s}(x_s) - \dot{k}_s V_{T-s}(x_s)) ds \right) \right] \\
& + \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right].
\end{aligned}$$

The result follows from this by Lemma 2.5. \square

2.3 Hessian

For each $w \in T_{x_0}M$ define an operator-valued process $W'_t(\cdot, w) : T_{x_t}M \rightarrow T_{x_t}M$ by

$$\begin{aligned}
W'_s(\cdot, w) &:= W_s \int_0^s W_r^{-1} R(//_r dB_r, W_r(\cdot)) W_r(w) \\
&\quad - \frac{1}{2} W_s \int_0^s W_r^{-1} (\nabla \text{Ric}_Z^\# + d^*R - 2R(Z))(W_r(\cdot), W_r(w)) dr.
\end{aligned}$$

Here the operator $R(Z)$ is defined by $R(Z)(v_1, v_2) := R(Z, v_1)v_2$ and the operator d^*R is defined by $d^*R(v_1)v_2 := -\text{tr} \nabla \cdot R(\cdot, v_1)v_2$ and satisfies

$$\langle d^*R(v_1)v_2, v_3 \rangle = \langle (\nabla_{v_3} \text{Ric}^\#)(v_1), v_2 \rangle - \langle (\nabla_{v_2} \text{Ric}^\#)(v_3), v_1 \rangle$$

for all $v_1, v_2, v_3 \in T_x M$ and $x \in M$. The process $W'_t(\cdot, w)$ is the solution to the covariant Itô equation

$$\begin{aligned}
DW'_t(\cdot, w) &= R(//_t dB_t, W_t(\cdot)) W_t(w) \\
&\quad - \frac{1}{2} \left(d^*R - 2R(Z) + \nabla \text{Ric}_Z^\# \right) (W_t(\cdot), W_t(w)) dt \\
&\quad - \frac{1}{2} \text{Ric}_Z^\#(W'_t(\cdot, w)) dt
\end{aligned}$$

with $W'_0(\cdot, w) = 0$. As in the previous section, suppose D_1 and D_2 are regular domains with $x_0 \in D_1$ and $\bar{D}_1 \subset D_2$. Denote by σ and τ the first exit times of x_t from D_1 and D_2 , respectively.

Lemma 2.7. *Suppose $v, w \in T_{x_0}M$, $0 < S < T$ and that k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, T]; \text{Aut}(T_{x_0}M))$ such that $k_s = 0$ for $s \geq \sigma \wedge S$, $l_s = 1$ for $s \leq \sigma \wedge T$ and $l_s = 0$ for $s \geq \tau \wedge (T - \epsilon)$. Then*

$$\begin{aligned}
& \mathbb{V}_t(\nabla df_t)(W_t(k_t v), W_t(w)) + \mathbb{V}_t(df_t)(W'_t(k_t v, w)) - \mathbb{V}_t f_t(x_t) \int_0^t \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \\
& - \int_0^t \mathbb{V}_s f_s(x_s) ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \\
& + \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{l}_s w), //_s dB_s \rangle \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \\
& - \mathbb{V}_t df_t(W_t(l_t w)) \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \\
& + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s((l_s - 1)w)) ds \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle
\end{aligned}$$

$$\begin{aligned}
& + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(w)) \int_0^s \langle W_r(\dot{k}_r v), //_{/r} dB_r \rangle ds \\
& - 2 \int_0^t \mathbb{V}_s(df_s \odot dV_{T-s})(W_s(k_s v), W_s(w)) ds
\end{aligned} \tag{2}$$

is a local martingale on $[0, \tau \wedge T)$.

Proof. Setting

$$N'_t(v, w) := (\nabla df_t)(W_t(v), W_t(w)) + (df_t)(W'_t(v, w))$$

and

$$R_x^{\sharp, \sharp}(v_1, v_2) := R_x(\cdot, v_1, v_2, \cdot)^{\sharp} \in T_x M \otimes T_x M$$

we see by Itô's formula and the relations

$$\begin{aligned}
d\Delta f &= \text{tr } \nabla^2 df - df(\text{Ric}^{\sharp}) \\
dZf &= \nabla_Z df + df(\nabla Z) \\
dVf &= f dV + V df \\
\nabla d(\Delta f) &= \text{tr } \nabla^2(\nabla df) - 2(\nabla df)(\text{Ric}^{\sharp} \odot \text{id} - R^{\sharp, \sharp}) - df(d^* R + \nabla \text{Ric}^{\sharp}) \\
\nabla d(Zf) &= \nabla_Z(\nabla df) + 2(\nabla df)(\nabla Z \odot \text{id}) + df(\nabla \nabla Z + R(Z)) \\
\nabla d(V_t f) &= f \nabla dV_t + 2df \odot dV_t + V_t \nabla df
\end{aligned}$$

(the fourth one is a consequence of the differential Bianchi identity; see [4, p. 219], and the fifth one a consequence of the Ricci identity) that

$$\begin{aligned}
& dN'_t(v, w) \\
&= (\nabla //_{/t} dB_t \nabla df_t)(W_t(v), W_t(w)) + (\nabla df_t) \left(\frac{D}{dt} W_t(v), W_t(w) \right) dt \\
&+ (\nabla df_t) \left(W_t(v), \frac{D}{dt} W_t(w) \right) dt \\
&+ \partial_t(\nabla df_t)(W_t(v), W_t(w)) dt + \left(\frac{1}{2} \text{tr } \nabla^2 + \nabla_Z \right) (\nabla df_t)(W_t(v), W_t(w)) dt \\
&+ (\nabla //_{/t} dB_t df_t)(W'_t(v, w)) + (df_t)(DW'_t(v, w)) + \langle d(df_t), DW'_t(v, w) \rangle \\
&+ \partial_t(df_t)(W'_t(v, w)) dt + \left(\frac{1}{2} \text{tr } \nabla^2 + \nabla_Z \right) (df_t)(W'_t(v, w)) dt \\
&\stackrel{m}{=} f_t(x_t)(\nabla dV_{T-t})(W_t(v), W_t(w)) dt + f_t(x_t)(dV_{T-t})(W'_t(v, w)) dt \\
&+ 2(df_t \odot dV_{T-t})(W_t(v), W_t(w)) dt + V_{T-t} N'_t(v, w) dt
\end{aligned}$$

for which we calculated

$$[d(df), DW'(v, w)]_t = (\nabla df_t)(R^{\sharp, \sharp}(W_t(v), W_t(w))) dt.$$

It follows that

$$\begin{aligned}
d(\mathbb{V}_t N'_t(k_t v, w)) &\stackrel{m}{=} \mathbb{V}_t f_t(x_t) ((\nabla dV_{T-t})(W_t(k_t v), W_t(w)) + (dV_{T-t})(W'_t(k_t v, w))) dt \\
&+ \mathbb{V}_t N'_t(\dot{k}_t v, w) dt + 2\mathbb{V}_t(df_t \odot dV_{T-t})(W_t(k_t v), W_t(w)) dt
\end{aligned}$$

so that

$$\begin{aligned}
\mathbb{V}_t N'_t(k_t v, w) &- \int_0^t \mathbb{V}_s(\nabla df_s)(W_s(k_s v), W_s(w)) ds - \int_0^t \mathbb{V}_s(df_s)(W'_s(k_s v, w)) ds \\
&- 2 \int_0^t \mathbb{V}_s(df_s \odot dV_{T-s})(W_s(k_s v), W_s(w)) ds \\
&- \int_0^t \mathbb{V}_s f_s(x_s) ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds
\end{aligned}$$

is a local martingale. By the formula

$$\mathbb{V}_t f_t(x_t) = f_0(x_0) + \int_0^t \mathbb{V}_s df_s(//_s dB_s)$$

and integration by parts we see that

$$\int_0^t \mathbb{V}_s(df_s)(W'_s(\dot{k}_s v, w)) ds - \mathbb{V}_t f_t(x_t) \int_0^t \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle$$

is a local martingale. Similarly, by the formula

$$\mathbb{V}_t df_t(W_t) = df_0 + \int_0^t \mathbb{V}_s(\nabla df_s)(//_s dB_s, W_s) + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s) ds$$

and integration by parts we see that

$$\begin{aligned} & \int_0^t \mathbb{V}_s(\nabla df_s)(W_s(\dot{k}_s v), W_s(w)) ds - \mathbb{V}_t df_t(W_t(w)) \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \\ & + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(w)) \int_0^s \langle W_r(\dot{k}_r v), //_r dB_r \rangle ds \end{aligned}$$

is yet another local martingale. Therefore

$$\begin{aligned} & \mathbb{V}_t(\nabla df_t)(W_t(\dot{k}_t v), W_t(w)) + \mathbb{V}_t(df_t)(W'_t(\dot{k}_t v, w)) \\ & - \int_0^t \mathbb{V}_s f_s(x_s) ((\nabla dV_{T-s})(W_s(\dot{k}_s v), W_s(w)) + (dV_{T-s})(\dot{k}_s W'_s(v, w))) ds \\ & - \mathbb{V}_t f_t(x_t) \int_0^t \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle - 2 \int_0^t \mathbb{V}_s(df_s \odot dV_{T-s})(W_s(\dot{k}_s v), W_s(w)) ds \\ & + \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s(w)) \int_0^s \langle W_r(\dot{k}_r v), //_r dB_r \rangle ds \\ & - \mathbb{V}_t df_t(W_t(w)) \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \end{aligned}$$

is a local martingale. By Lemma 2.1 it follows that

$$\begin{aligned} O_t^1 &= \mathbb{V}_t df_t(W_t((l_t - 1)w)) - \mathbb{V}_t f_t(x_t) \int_0^t \langle W_s(\dot{l}_s w), //_s dB_s \rangle \\ & \quad - \int_0^t \mathbb{V}_s f_s(x_s) dV_{T-s}(W_s((l_s - 1)w)) ds, \\ O_t^2 &= \int_0^t \langle W_s(\dot{k}_s v), //_s dB_s \rangle \end{aligned}$$

are two local martingales. So the product $O_t^1 O_t^2$ is also a local martingale, since $O^1 = 0$ on $[0, \sigma \wedge S]$ with O^2 constant on $[\sigma \wedge S, \tau \wedge (T - \epsilon))$. Applying this fact to the previous equation completes the proof. \square

Theorem 2.8. *Suppose $x_0 \in D_1$ with $v, w \in T_{x_0}M$, $f \in \mathcal{B}_b$, V bounded below and $0 < S < T$. Assume k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, T]; \text{Aut}(T_{x_0}M))$ such that $k_s = 0$ for $s \geq \sigma \wedge S$, $k_0 = 1$, $l_s = 1$ for*

$s \leq \sigma \wedge S$, $l_s = 0$ for $s \geq \tau \wedge T$, $\int_0^{\sigma \wedge S} |\dot{k}_s|^2 ds \in L^1$ and $\int_{\sigma \wedge S}^{\tau \wedge T} |\dot{l}_s|^2 ds \in L^1$. Then

$$\begin{aligned}
& (\nabla dP_T^V f)(v, w) \\
&= -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\
&\quad - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\
&\quad + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \left(\int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle + dV_{T-s}(W_s(l_s w)) ds \right) \right. \\
&\quad \quad \left. \cdot \left(\int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right) \right].
\end{aligned}$$

Proof. Modifying the process l_t to l_t^ϵ as in the proof of Theorem 2.2, it follows from Lemma 2.7, the strong Markov property, the boundedness of $P_t^V f$ on $[0, T] \times \bar{D}_2$ and the boundedness of $dP_t^V f$ and $\nabla dP_t^V f$ on $[\epsilon, T] \times \bar{D}_2$ that the formula

$$\begin{aligned}
& (\nabla dP_T^V f)(v, w) \\
&= -\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\
&\quad + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
&\quad - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\
&\quad + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-s}(W_s(l_s w)) ds \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
&\quad - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^s dV(W_r(w)) dr \right) \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
&\quad - \mathbb{E} \left[\int_0^T \mathbb{V}_s df_s(W_s(k_s v)) dV_{T-s}(W_s(w)) ds \right] \\
&\quad - \mathbb{E} \left[\int_0^T \mathbb{V}_s df_s(W_s(w)) dV_{T-s}(W_s(k_s v)) ds \right]
\end{aligned}$$

holds with l_t^ϵ in place of l_t , and therefore in terms of l_t by taking $\epsilon \downarrow 0$. Paying close attention to the assumptions on l and k , it follows from this, by Theorem 2.2 and the strong Markov property, that

$$\begin{aligned}
& -\mathbb{E} \left[\int_0^T \mathbb{V}_s df_s(W_s(w)) dV_{T-s}(W_s(k_s v)) ds \right] \\
&= +\mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \int_r^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle dV_{T-r}(W_r(k_r v)) dr \right] \\
&\quad - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^r dV_{T-u}(W_u(w)) du \right) dV_{T-r}(W_r(k_r v)) dr \right]
\end{aligned}$$

$$\begin{aligned}
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-r}(W_r(k_r v)) dr \int_0^T dV_{T-s}(W_s(l_s w)) ds \right] \\
= & + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle \int_0^T dV_{T-r}(W_r(k_r v)) dr \right] \\
& - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^r dV_{T-u}(W_u(w)) du \right) dV_{T-r}(W_r(k_r v)) dr \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-r}(W_r(k_r v)) dr \int_0^T dV_{T-s}(W_s(l_s w)) ds \right]
\end{aligned}$$

from which it follows that

$$\begin{aligned}
& (\nabla dP_T^V f)(v, w) \\
= & - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s(\dot{l}_s w), //_s dB_s \rangle \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
& - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(\dot{k}_s v, w))) ds \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-s}(W_s(l_s w)) ds \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \langle W_s \dot{l}_s w, //_s dB_s \rangle \int_0^T dV_{T-r}(W_r(k_r v)) dr \right] \\
& + \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T dV_{T-r}(W_r(k_r v)) dr \int_0^T dV_{T-s}(W_s(l_s w)) ds \right] \\
& - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^s dV_{T-r}(W_r(w)) dr \right) \langle W_s(\dot{k}_s v), //_s dB_s \rangle \right] \\
& - \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_0^s dV_{T-r}(W_r(w)) dr \right) dV_{T-s}(W_s(k_s v)) ds \right] \\
& - \mathbb{E} \left[\int_0^T \mathbb{V}_s df_s(W_s(k_s v)) dV_{T-s}(W_s(w)) ds \right].
\end{aligned}$$

Finally, by the stochastic Fubini theorem [20, Theorem 2.2] we have

$$\begin{aligned}
& \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \int_0^s dV_{T-r}(W_r(w)) dr (\langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s k_s v)) ds \right] \\
= & \mathbb{E} \left[\mathbb{V}_T f(x_T) \mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T \left(\int_s^T \langle W_r(\dot{k}_r v), //_r dB_r \rangle + dV_{T-r}(W_r k_r v) dr \right) dV_{T-s}(W_s(w)) ds \right]
\end{aligned}$$

which cancels the final three terms in the previous equation, by the strong Markov property, Theorem 2.2 and the assumptions on k . \square

For the case $Z = 0$ and $V = 0$, Theorem 2.8 reduces to [1, Theorem 2.1].

Remark 2.9. We have assumed that V is bounded below and smooth. However, so long as V is bounded below and continuous with $V_t \in C^1$ for each $t \in [0, T]$ and $P^V f \in$

$C^{1,3}([\epsilon, T] \times M)$ then the results of Subsection 2.1 evidently remain valid. Similarly, the results of Subsection 2.2 evidently remain valid if V is bounded below, C^1 with $V_t \in C^2$ for each $t \in [0, T]$ and $P^V f \in C^{1,4}([\epsilon, T] \times M)$. Similarly, the results of Subsection 2.3 evidently remain valid if V is bounded below and continuous with $V_t \in C^2$ for each $t \in [0, T]$ and $P^V f \in C^{1,4}([\epsilon, T] \times M)$.

3 Stationary Solutions

Now suppose $\phi \in C^2(D) \cap C(\overline{D})$ solves the eigenvalue equation

$$(L - V)\phi = -E\phi$$

on the regular domain D , for some $E \in \mathbb{R}$ and a function $V \in C^2$ which does not depend on time and which is bounded below. Denoting by τ the first exit time from D of the diffusion x_t with generator L and assuming $x_0 \in D$, one has, in analogy to the Feynman-Kac formula (3), the formula

$$\phi(x_0) = \mathbb{E} \left[\mathbb{V}_\tau \phi(x_\tau) e^{E\tau} \right].$$

Furthermore, the methods of the previous section can easily be adapted to find formulae for the derivatives of ϕ . In particular, one simply sets $f_t = \phi$, replaces V_{T-t} with $V - E$ and the calculations carry over almost verbatim (although there is no application of the strong Markov property; in this case the local martingale property is enough). In particular, for the derivative $d\phi$, supposing k is a bounded adapted process with paths in the Cameron-Martin space $L^{1,2}([0, \infty), \text{Aut}(T_{x_0}M))$ with $k_0 = 1$, $k_t = 0$ for $t \geq \tau$ and $\int_0^\tau |\dot{k}_s|^2 ds \in L^1$, one obtains

$$(d\phi)(v) = -\mathbb{E} \left[\mathbb{V}_\tau \phi(x_\tau) e^{E\tau} \int_0^\tau \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV(W_s(k_s v)) ds \right]$$

for each $v \in T_{x_0}M$. When $V = 0$ and $E = 0$ this formulae reduces to the one given in [18]. Similarly, denoting by D_1 a regular domain with $x_0 \in D_1$ and $\overline{D_1} \subset D$ and by σ the first exit time of x_t from D_1 , supposing k, l are bounded adapted processes with paths in the Cameron-Martin space $L^{1,2}([0, \infty); \text{Aut}(T_{x_0}M))$ such that $k_s = 0$ for $s \geq \sigma$, $k_0 = 1$, $l_s = 1$ for $s \leq \sigma$, $l_s = 0$ for $s \geq \tau$, $\int_0^\sigma |\dot{k}_s|^2 ds \in L^1$ and $\int_\sigma^\tau |\dot{l}_s|^2 ds \in L^1$, for the Hessian of ϕ one obtains

$$\begin{aligned} & (\nabla d\phi)(v, w) \\ &= -\mathbb{E} \left[\mathbb{V}_\sigma \phi(x_\sigma) e^{E\sigma} \int_0^\sigma \langle W'_s(\dot{k}_s v, w), //_s dB_s \rangle \right] \\ & \quad - \mathbb{E} \left[\mathbb{V}_\sigma \phi(x_\sigma) e^{E\sigma} \int_0^\sigma ((\nabla dV)(W_s(k_s v), W_s(w)) + (dV)(W'_s(k_s v, w))) ds \right] \\ & \quad + \mathbb{E} \left[\mathbb{V}_\tau \phi(x_\tau) e^{E\tau} \left(\int_0^\tau \langle W_s(\dot{l}_s w), //_s dB_s \rangle + dV(W_s(l_s w)) ds \right) \right. \\ & \quad \quad \left. \cdot \left(\int_0^\sigma \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV(W_s(k_s v)) ds \right) \right] \end{aligned}$$

for all $v, w \in T_{x_0}M$.

4 Local and Global Estimates

4.1 Gradient

Theorem 4.1. *Suppose D_0, D are regular domains with $x_0 \in \overline{D_0} \subset D$, V bounded below and $T > 0$. Set*

$$\begin{aligned}\underline{\kappa}_D &:= \inf\{\text{Ric}_Z(v, v) : v \in T_y M, y \in D, |v| = 1\}; \\ v_D &:= \sup\{|(dV_t)_y(v)| : v \in T_y M, y \in D, |v| = 1, t \in [0, T]\}.\end{aligned}$$

Then there exists a positive constant

$$C \equiv C(n, T, \inf V, \underline{\kappa}_D, v_D, d(\partial D_0, \partial D))$$

such that

$$|dP_t^V f_{x_0}| \leq \frac{C}{\sqrt{t}} |f|_\infty \quad (13)$$

for all $0 < t \leq T$, $x_0 \in D_0$ and $f \in \mathcal{B}_b$.

Proof. According to [1], the process k_t appearing in Theorem 2.2 can be chosen so that $|k_s| \leq c(T)$ for all $s \in [0, T]$, almost surely, with

$$\mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \leq \frac{\tilde{C}}{\sqrt{1 - e^{-\tilde{C}^2 T}}}$$

for a positive constant \tilde{C} which depends continuously on $\underline{\kappa}$, n and $d(\partial D_0, \partial D)$. The details of this can be found in [19]. By Theorem 2.2 and the Cauchy-Schwarz inequality, using equation (4) and the parameter $\underline{\kappa}_D$ to control the size of the damped parallel transport, we have

$$\begin{aligned}|dP_T^V f| &\leq |f|_\infty e^{-\inf V} \left(\mathbb{E} \left[\mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T |W_s|^2 |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \right. \\ &\quad \left. + \mathbb{E} \left[\mathbf{1}_{\{T < \zeta(x_0)\}} \int_0^T |dV_{T-s}| |W_s| |k_s| ds \right] \right) \\ &\leq |f|_\infty e^{(-\inf V - \frac{1}{2}(\underline{\kappa}_D \wedge 0))T} \left(\mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} + v_D \mathbb{E} \left[\int_0^T |k_s| ds \right] \right)\end{aligned}$$

so the estimate (13) follows by substituting the bounds on k and \dot{k} . \square

Note that in the above theorem, the dependence of the constant C on $d(D_0, D)$ is such that if one tries to shrink D onto D_0 , so as to reduce the information needed about Ric_Z and dV , then the constant blows up at rate $1/d(D_0, D)$. There is therefore a trade-off between the size of the domain and the size of the constant. This behaviour is unavoidable and also occurs with respect to the domains D_0, D_1 and D_2 which appear in Theorems 4.3 and 4.5 below.

Corollary 4.2. *Suppose Ric_Z is bounded below with $|dV|$ bounded and V bounded below. Then for all $T > 0$ there exists a positive constant $C \equiv C(n, T)$ such that*

$$|dP_t^V f_x| \leq \frac{C}{\sqrt{t}} |f|_\infty$$

for all $0 < t \leq T$, $x \in M$ and $f \in \mathcal{B}_b$.

Proof. As explained in the proof of Theorem 4.1, the dependence on D_0 of the constant appearing there is via the quantity $d(\partial D_0, \partial D)$. If M is compact then the injectivity radius $\text{inj}(M)$ is positive and we can choose $D_0 = B_{\text{inj}(M)/4}(x_0)$ and $D = B_{\text{inj}(M)/2}(x_0)$, in which case $d(\partial D_0, \partial D) = \text{inj}(M)/4$. Conversely, if M is non-compact then for each $x_0 \in M$ there exist D_0, D with $x_0 \in \overline{D_0} \subset D$ and $d(\partial D_0, \partial D) = 1$. Consequently, the result follows from Theorem 4.1. \square

4.2 Generator

Theorem 4.3. *Suppose D_0, D_1 and D_2 are regular domains with $x_0 \in \overline{D_0} \subset D_1, \overline{D_1} \subset D_2, V$ bounded below and $T > 0$. Set*

$$\begin{aligned}\kappa_{D_2} &:= \sup\{|\text{Ric}_Z(v, v)| : v \in T_y M, y \in D_2, |v| = 1\}; \\ v_{D_2} &:= \sup\{|(dV_t)_y(v)| : v \in T_y M, y \in D_2, |v| = 1, t \in [0, T]\}; \\ z_{D_1} &:= \sup\{|Z|_y : y \in D_1\}.\end{aligned}$$

Then there exists a positive constant

$$C \equiv C(n, T, \inf V, \kappa_{D_2}, v_{D_2}, z_{D_1}, d(\partial D_0, \partial D_1), d(\partial D_0, \partial D_2))$$

such that

$$|LP_t^V f_{x_0}| \leq \frac{C}{t} |f|_\infty$$

for all $0 < t \leq T, x_0 \in D_0$ and $f \in \mathcal{B}_b$.

Proof. According to [1], the processes k_t and l_t appearing in Theorem 2.6 can be chosen so that

$$\begin{aligned}|k_s| &\leq c_1(n, \kappa_{D_1}, T, d(\partial D_0, \partial D_1)), \\ |l_s| &\leq c_2(n, \kappa_{D_2}, T, d(\partial D_0, \partial D_2))\end{aligned}$$

for all $s \in [0, T]$, almost surely, with

$$\mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \leq \frac{\tilde{C}_1}{\sqrt{1 - e^{-\tilde{C}_1^2 T}}}, \quad \mathbb{E} \left[\int_0^T |\dot{l}_s|^2 ds \right]^{\frac{1}{2}} \leq \frac{\tilde{C}_2}{\sqrt{1 - e^{-\tilde{C}_2^2 T}}}$$

for positive constants \tilde{C}_1 and \tilde{C}_2 which depend continuously on κ, n and on $d(\partial D_0, \partial D_1)$ and $d(\partial D_0, \partial D_2)$, respectively. By Theorem 2.6 and the Cauchy-Schwarz inequality we have

$$\begin{aligned}& |L(P_T^V f)(x_0)| \\ & \leq e^{-\inf V} |f|_\infty z_{D_1} \mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \\ & \quad + \frac{1}{2} |f|_\infty e^{T(\kappa_{D_2} - \inf V)} \mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} \left(\mathbb{E} \left[\int_0^T |\dot{l}_s|^2 ds \right]^{\frac{1}{2}} + v_{D_2} \mathbb{E} \left[\left(\int_0^T |l_s| ds \right)^2 \right]^{\frac{1}{2}} \right)\end{aligned}$$

so the result follows by substituting the bounds on k, \dot{k}, l and \dot{l} . \square

Corollary 4.4. *Suppose $|\text{Ric}_Z|, |dV|, |Z|$, are bounded with V bounded below. Then there exists a positive constant $C \equiv C(n, T)$ such that*

$$|LP_t^V f_x| \leq \frac{C}{t} |f|_\infty$$

for all $0 < t \leq T, x \in M$ and $f \in \mathcal{B}_b$.

Proof. The result follows from Theorem 4.3, since as in Corollary 4.2 any dependence of the constant on D_0, D_1 and D_2 can be eliminated. \square

4.3 Hessian

Theorem 4.5. *Suppose D_0, D_1 and D_2 are regular domains with $x_0 \in \overline{D_0} \subset D_1, \overline{D_1} \subset D_2, V$ bounded below and $T > 0$. Set*

$$\begin{aligned}\kappa_{D_2} &:= \sup\{|\text{Ric}_Z(v, v)| : v \in T_y M, y \in D_2, |v| = 1\}; \\ v_{D_2} &:= \sup\{|(dV_t)_y(v)| : v \in T_y M, y \in D_2, |v| = 1, t \in [0, T]\}; \\ v'_{D_1} &:= \sup\{|(\nabla dV_t)_y(v, v)| : v \in T_y M, y \in D_1, |v| = 1, t \in [0, T]\}; \\ \rho_{D_1} &:= \sup\{|R(w, v)v| : v, w \in T_y M, y \in D_1, |v| = |w| = 1\}; \\ \rho'_{D_1} &:= \sup\{|(\nabla \text{Ric}_Z^\sharp + d^*R - 2R(Z))(v, v)| : v \in T_y M, y \in D_1, |v| = 1\}.\end{aligned}$$

Then there exists a positive constant

$$C \equiv C(n, T, \inf V, \kappa_{D_2}, v_{D_2}, v'_{D_1}, \rho_{D_1}, \rho'_{D_1}, d(\partial D_0, \partial D_1), d(\partial D_0, \partial D_2))$$

such that

$$|\nabla dP_t^V f_{x_0}| \leq \frac{C}{t} |f|_\infty$$

for all $0 < t \leq T, x_0 \in D_0$ and $f \in \mathcal{B}_b$.

Proof. Recalling the defining equation for $W'_s(v, w)$ and choosing the processes k_t and l_t as in the proof of Theorem 4.3, it follows for the process k_t that

$$\begin{aligned}\mathbb{E} \left[\left(\int_0^T \langle \dot{k}_s W_s \int_0^s W_r^{-1} R(//_r dB_r, W_r) W_r, //_s dB_s \rangle \right)^2 \right]^{\frac{1}{2}} &\leq \frac{\tilde{C}_3 e^{\kappa_{D_1} T}}{\sqrt{1 - e^{-\tilde{C}_3^2 T}}}, \\ \mathbb{E} \left[\left(\int_0^T \langle \dot{k}_s W_s \int_0^s W_r^{-1} (\nabla \text{Ric}_Z^\sharp + d^*R)(W_r, W_r) dr, //_s dB_s \rangle \right)^2 \right]^{\frac{1}{2}} &\leq \frac{\tilde{C}_4 e^{\kappa_{D_1} T}}{\sqrt{1 - e^{-\tilde{C}_4^2 T}}}\end{aligned}$$

for positive constants \tilde{C}_3 and \tilde{C}_4 which depend continuously on $\kappa_{D_1}, \rho_{D_1}, \rho'_{D_1}, n$ and on $d(\partial D_0, \partial D_1)$ and $d(\partial D_0, \partial D_2)$, respectively. The details of this, including explicit bounds on these constants (and on those appearing in Theorems 4.1 and 4.3) are found in [14, Section 4.2], with appropriate bounds for the radial part of the diffusion being given as in the proof of [21, Corollary 2.1.2]. By Theorem 2.8 and the Cauchy-Schwarz inequality we have

$$\begin{aligned}&|\nabla dP_T^V f| \\ &\leq |f|_\infty e^{T(\kappa_{D_2} - \inf V)} \left(\frac{\tilde{C}_3}{\sqrt{1 - e^{-\tilde{C}_3^2 T}}} + \frac{1}{2} \frac{\tilde{C}_4}{\sqrt{1 - e^{-\tilde{C}_4^2 T}}} \right) \\ &\quad + |f|_\infty e^{T(\kappa_{D_2} - \inf V)} \left(v'_{D_1} \mathbb{E} \left[\left(\int_0^T |k_s| ds \right)^2 \right]^{\frac{1}{2}} + v_{D_2} c_1^2(\rho_{D_1} \vee \frac{1}{2} \rho'_{D_1}) \frac{T^2}{\sqrt{2}} \right) \\ &\quad + |f|_\infty e^{T(\kappa_{D_2} - \inf V)} \left(\mathbb{E} \left[\int_0^T |i_s|^2 ds \right]^{\frac{1}{2}} + v_{D_2} \mathbb{E} \left[\left(\int_0^T |l_s| ds \right)^2 \right]^{\frac{1}{2}} \right) \\ &\quad \cdot \left(\mathbb{E} \left[\int_0^T |\dot{k}_s|^2 ds \right]^{\frac{1}{2}} + v_{D_2} \mathbb{E} \left[\left(\int_0^T |k_s| ds \right)^2 \right]^{\frac{1}{2}} \right)\end{aligned}$$

so the result follows by substituting the bounds on k, \dot{k}, l and \dot{l} . \square

Corollary 4.6. *Suppose $|\text{Ric}_Z|, |dV|, |\nabla dV|, |\nabla \text{Ric}_Z^\sharp + d^*R - 2R(Z)|, |R|$ are bounded with V bounded below. Then there exists a positive constant $C \equiv C(n, T)$ such that*

$$|\nabla dP_t^V f_x| \leq \frac{C}{t} |f|_\infty$$

for all $0 < t \leq T, x \in M$ and $f \in \mathcal{B}_b$.

Proof. The result follows from Theorem 4.5, since as in Corollaries 4.2 and 4.4 any dependence of the constant on D_0, D_1 and D_2 can be eliminated. \square

5 Non-local Formulae

If Ric_Z is bounded below then, by [21, Corollary 2.1.2], the diffusion x_t is non-explosive, which is to say $\zeta(x_0) = \infty$, almost surely. While the formulae in this section require non-explosion and global bounds on the various curvature operators, they are expressed in terms of explicit and deterministic processes k and l .

Theorem 5.1. *Suppose $x_0 \in M$ with $v \in T_{x_0}M, f \in \mathcal{B}_b, V$ bounded below and $T > 0$. Set*

$$k_s = \frac{T-s}{T}.$$

Suppose Ric_Z is bounded below with $|dV|$ bounded and V bounded below. Then

$$(dP_T^V f)(v) = -\mathbb{E} \left[\mathbb{V}_T f(x_T) \int_0^T \langle W_s(\dot{k}_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right].$$

Proof. It follows from Corollary 4.2 that $|dP_t^V|$ is bounded on $[\epsilon, T] \times M$. Therefore, using

$$k_s^\epsilon = \frac{T-\epsilon-s}{T-\epsilon} \vee 0$$

the local martingale (5) is a true martingale. Taking expectations and eliminating ϵ with dominated convergence yields the above formula. \square

Theorem 5.1 is precisely [5, Theorem 5.2], which was also obtained in [11] by a slightly different method.

Theorem 5.2. *Suppose $x_0 \in M, f \in \mathcal{B}_b, V$ bounded below and $T > 0$. Set*

$$k_s = \frac{T-2s}{T} \vee 0, \quad l_s = 1 \wedge \frac{2(T-s)}{T}.$$

Suppose $|\text{Ric}_Z|, |dV|$ and $|Z|$ are bounded with V bounded below. Then

$$\begin{aligned} & L(P_T^V f)(x_0) \\ &= \mathbb{E} \left[\mathbb{V}_T f(x_T) \int_0^T \langle \dot{k}_s Z, //_s dB_s \rangle \right] \\ & \quad + \frac{1}{2} \mathbb{E} \left[\mathbb{V}_T f(x_T) \left(\int_0^T \langle W_s \dot{l}_s, //_s dB_s \rangle + dV_{T-s}(W_s l_s) ds \right) \int_0^T \dot{k}_s W_s^{-1} //_s dB_s \right]. \end{aligned}$$

Proof. It follows from Corollary 4.4 that $|LP_t^V|$ is bounded on $[\epsilon, T] \times M$. Therefore, using k_s and

$$l_s^\epsilon = \left(1 \wedge \frac{T - \epsilon - s}{\frac{T}{2} - \epsilon} \right) \vee 0$$

the local martingale appearing in Lemma 2.4 is a true martingale. Taking expectations, using Lemma 2.5 as in the proof of Theorem 2.6 and eliminating ϵ with dominated convergence yields the above formula. \square

Theorem 5.3. *Suppose $x_0 \in M$ with $v, w \in T_{x_0}M$, $f \in \mathcal{B}_b$, V bounded below and $T > 0$. Define k_s and l_s as in Theorem 5.2. Suppose $|\text{Ric}_Z|$, $|dV|$, $|\nabla dV|$, $|\nabla \text{Ric}_Z^\sharp + d^*R - 2R(Z)|$ and $|R|$ are bounded with V bounded below. Then*

$$\begin{aligned} & (\nabla dP_T^V f)(v, w) \\ = & -\mathbb{E} \left[\mathbb{V}_T f(x_T) \int_0^T \langle W'_s(k_s v, w), //_s dB_s \rangle \right] \\ & - \mathbb{E} \left[\mathbb{V}_T f(x_T) \int_0^T ((\nabla dV_{T-s})(W_s(k_s v), W_s(w)) + (dV_{T-s})(W'_s(k_s v, w))) ds \right] \\ & + \mathbb{E} \left[\mathbb{V}_T f(x_T) \left(\int_0^T \langle W_s(l_s w), //_s dB_s \rangle + dV_{T-s}(W_s(l_s w)) ds \right) \right. \\ & \quad \left. \cdot \left(\int_0^T \langle W_s(k_s v), //_s dB_s \rangle + dV_{T-s}(W_s(k_s v)) ds \right) \right]. \end{aligned}$$

Proof. It follows from Corollary 4.6 that $|dP_t^V|$ and $|\nabla dP_t^V|$ are bounded on $[\epsilon, T] \times M$. Therefore, using l_s^ϵ defined as in the proof of Theorem 5.2, the local martingale appearing in Lemma 2.7 is a true martingale. Taking expectations, proceeding as in the proof of Theorem 2.8 and eliminating ϵ with dominated convergence yields the above formula. \square

For the case $V = 0$, Theorem 5.3 gives the filtered version of the second part of [5, Theorem 3.1], which was proved by differentiating under the expectation for $f \in BC^2$ and which, as observed in [14], contains a slight error, permuting the vectors v and w .

Remark 5.4. *Our gradient and Hessian formulae require $V \in C^1$ and $V \in C^2$, respectively (see Remark 2.9). More generally, it is desirable to consider possibly very singular potentials, such as those which appear in many quantum mechanical problems. See, for example, [7] and [15]. It was pointed out to the authors of [5] by G. Da Prato, and to the author of this article by X.-M. Li, that non-smooth potentials V can be dealt with using the variation of constants formula:*

$$P_T^V f = P_T f - \int_0^T P_{T-s}(V_s P_s^V f) ds \quad (14)$$

where P_T denotes the minimal semigroup associated to the operator L . So long as $P_T^V f$ is sufficiently regular, formulae and estimates $dP_T^V f$ can be obtained from formulae and estimates for $dP_T f$, simply by differentiating the above formula. In particular, this approach results in gradient estimates depending only on $\|V\|_\infty$ (like those in [15] for domains in \mathbb{R}^n). Our gradient estimate, Theorem 4.1, on the other hand, does not require that V is bounded (only bounded below). For the second derivatives one must take care in passing the derivatives through the integral in formula (14). For the case in which the potential is a bounded Hölder continuous function V which does not depend

on time, this can be achieved at each point $x_0 \in M$ by shifting V to $V(x_0) = 0$. The details of this for, the Hessian, are given in [10], where the approach taken is based on that of [5].

6 Kernel Estimates

Now suppose $Z = \nabla h$, for some $h \in C^2$, and consider the m -dimensional Bakry-Emery curvature tensor

$$\text{Ric}_{m,n} := \text{Ric}^\sharp - \nabla dh - \frac{\nabla h \otimes \nabla h}{m-n}$$

where $m \geq n$ is a constant (see [13]). Denoting by $p_t^h(x, y)$ the density of the diffusion with generator L , with respect to the weighted Riemannian measure $e^h dy$, it follows, as explained in the proof of [9, Theorem 1.4], that if $\text{Ric}_{m,n} \geq -\kappa$ for some $\kappa \geq 0$ then there exists a positive constant $C \equiv C(\kappa, m, T)$ such that

$$\log \left(\frac{p_{\frac{t}{2}}^h(x, z)}{p_t^h(x, y)} \right) \leq C \left(1 + \frac{d^2(x, y)}{t} \right)$$

for all $x, y, z \in M$ and $t \in (0, T]$. Assuming V is bounded, it follows that the same inequality holds for the integral kernel $p_t^{h,V}(x, y)$ of the semigroup $P_t^V f$, since

$$p_t^{h,V}(x, y) = p_t^h(x, y) \mathbb{E}[\mathbb{V}_t | x_0 = x, x_t = y]$$

by the Feynman-Kac formula. We can therefore derive from Theorems 5.1, 5.2 and 5.3 estimates on the logarithmic derivatives of $p_t^{h,V}(x, y)$ by using Jensen's inequality (as in [16, Lemma 6.45]). In particular, the assumptions of Theorem 5.1 with $Z = \nabla h$ plus boundedness of V and a lower bound on $\text{Ric}_{m,n}$ imply the existence of a constant $C_1(T)$ such that

$$|d \log p_t^{h,V}(\cdot, y)_x|^2 \leq C_1(T) \left(\frac{1}{t} + \frac{d^2(x, y)}{t^2} \right)$$

for all $x, y \in M$ and $t \in (0, T]$. The details of this (for the case $h = 0$) can be found in [11]. Similarly, the assumptions of Theorem 5.2 with $Z = \nabla h$ plus boundedness of V and a lower bound on $\text{Ric}_{m,n}$ imply for the Witten Laplacian $\Delta_h := \frac{1}{2}\Delta + \nabla h$ the existence of a constant $C_2(T)$ such that

$$|\Delta_h \log p_t^{h,V}(\cdot, y)(x)| \leq C_2(T) \left(\frac{1}{t} + \frac{d^2(x, y)}{t^2} \right)$$

for all $x, y \in M$ and $t \in (0, T]$. Finally, the assumptions of Theorem 5.3 with $Z = \nabla h$ plus boundedness of V and a lower bound on $\text{Ric}_{m,n}$ imply the existence of a constant $C_3(T)$ such that

$$|\nabla d \log p_t^{h,V}(\cdot, y)_x| \leq C_3(T) \left(\frac{1}{t} + \frac{d^2(x, y)}{t^2} \right)$$

for all $x, y \in M$ and $t \in (0, T]$.

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