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On-Diagonal Estimates on Schrödinger Semigroup Kernels and Reduced Heat Kernels

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Abstract: We prove various estimates for the kernels of semigroups generated by Schrödinger operators with magnetic field and potential of polynomial growth. We also investigate the reduced heat kernels.

1. Introduction

Let M be a connected and complete Riemannian manifold with Riemannian metric $\langle\cdot,\cdot\rangle$. By d we denote the Riemannian distance on M and by H we denote the operator

$$(H\psi,\psi) = \int_M dx\ \left(|grad\ \psi(x) + i\psi(x)Y|^2 + V(x)|\psi(x)|^2\right) \quad , \tag{1}$$

where dx is a Riemannian measure on M, $\psi \in C_c^\infty(M)$, Y is a real vector field such that $\langle Y, Y\rangle \in L^1_{\text{loc}}(M)$, $V: M \to \mathbb{R}$, $V \in L^1_{\text{loc}}(M)$ and $V \geq 0$. With some abuse of notation, we will also denote by H the Friedrichs extension of this operator. For any bounded Borel function $F: [0,\infty) \to \mathbb{C}$ we define the operator $F(H)$ by the spectral decomposition and we denote its kernel by $K_{F(H)}$, i.e.

$$F(H)(\psi)(x) = \int_M dy\, K_{F(H)}(x,y)\psi(y) \quad .$$

The operator H is called a Schrödinger operator with magnetic field. Various properties of such operators were studied in many papers, see e.g. [2, 9, 12, 14].

In the sequel we will always assume that the following Nash inequality holds:

$$\|\psi\|_{L^2} \leq \varepsilon\left(\|grad\ \psi\|^2_{L^2} + \gamma^2\|\psi\|^2_{L^2}\right)^{1/2} + c\,(\gamma\varepsilon)^{-k/2}\|\psi\|_{L^1} \tag{2}$$

for some $c > 0$, all $\varepsilon > 0$, all $\gamma \in (0, 1]$ and all $\psi \in C_c^\infty(M)$. Note that (2) is equivalent to the formula

$$\|\psi\|_{L^2}^{2+4/k} \le c' \left(\|grad\ \psi\|_{L^2}^2 + \|\psi\|_{L^2}^2\right) \|\psi\|_{L^1}^{4/k} \tag{3}$$

for some $c' > 0$ and all $\psi \in C_c^\infty(M)$. The form (2) of the Nash inequality comes from [7] Corollary 3.7 and [16] (2.22) IV.2. However, it is a variation of inequalities originally discovered by Nash [13]. The theory of Nash inequalities and their connections with Sobolev inequalities and L^∞ estimates for heat kernels corresponding to Laplace-Beltrami operators constitute a very broad subject; we refer the readers who are looking for a rationale of using the assumption (2) (or (3)) to [19, 4 and 16]. However, we want to point out that (2) holds in many interesting cases, for example for group invariant operators on Lie groups (see [16]) or for uniformly elliptic operators on $\mathbb{R}^n$.

The main aim of this paper is the study of on-diagonal bounds for heat kernels corresponding to the operator H under the following assumption of polynomial growth of the potential V:

$$V(x) \ge \sigma d(0, x)^\alpha, \tag{4}$$

where $\alpha > 0$ and $0 \in M$ is an arbitrary fixed point of M (see also [6, 4, §4.5]). We also obtain some off-diagonal estimates as a direct consequence of on-diagonal estimates. However, if points x and y are far apart we do not gain additional information, since in this case our estimates are weaker than known Gaussian bounds (see Theorem 4.1 [7] and Theorem 2 below). In this paper, similarly as in [18], we use the connection of heat and the wave equation which has a long history, see [11].

In the last section, to investigate the sharpness of our estimates, we compare them with the lower bounds for the kernel of the semigroup generated by the operator

$$-\Delta + |x|^\alpha = -\sum_{j=1}^{k} \partial^2/\partial x_j^2 + |x|^\alpha \quad . \tag{5}$$

The estimates for the heat kernel corresponding to the operator (5) were studied by Davies and Simon [6, 4, §4.5]. They obtained sharp estimates for large time and $\alpha > 2$. For a large time our results give the same kind of behaviour of the heat kernels as Davies and Simon's estimates. However, their approach gives also the precise values of the constants in the estimates (see Theorem 7 below). On the other hand, our estimates are stronger for small times and work also for $\alpha < 2$, whereas Davies and Simon's approach in this case gives only negative results.

We will apply our result to the kernels, which following ter Elst and Robinson [7] we call reduced heat kernels, and which can be described as follows. Let $\mathcal{U}$ be an irreducible unitary representation of a nilpotent Lie group G on $L^2(\mathbb{R}^k)$ and let $U = d\mathcal{U}$ denote the representation of the Lie algebra $\mathfrak{g}$ obtained by differentiation. If $b_1, \ldots, b_n$ is a basis of $\mathfrak{g}$ and we define the operator H by

$$H = -\sum_{j=1}^{n} U(b_j)^2 \quad , \tag{6}$$

then H generates a continuous semigroup S_t, holomorphic in the open right half-plane, with a kernel κ_t

$$(S_t\psi)(x) = \int_{\mathbb{R}^k} dy \kappa_t(x, y)\psi(y) \quad .$$

We will call κ_t a reduced heat kernel. In [7] ter Elst and Robinson proved that

$$|\kappa_t(x,y)| \le Ce^{-\lambda_1 t} \exp(-c(|x|^\alpha + |y|^\alpha)) \tag{7}$$

for $t > 1$ and some $\alpha > 0$, where λ_1 is the smallest eigenvalue of the operator H and $|x|$ denote Euclidean norm of x. Our result applied to the operator (6) yields that

$$|\kappa_t(x,y)| \le Ct^{-k/2} \exp(-ct(|x|^\alpha + |y|^\alpha)) \tag{8}$$

for $t < 1$ and some $\alpha > 0$. Note that our estimates are sufficiently strong to verify the well known fact that S_t is of trace class. We also give an alternative proof of (7). We do it by showing that the large time estimate (7) is a direct consequence of the small time estimate (8).

2. Preliminaries

In what follows we will use the following version of the finite speed propagation property of solutions of the wave equation for the operator H.

Theorem 1. *Suppose that the operator H is defined by (1) and that $V \ge 0$. Then for $C_t(\lambda) = \cos t\sqrt{\lambda}$ the following holds:*

$$\operatorname{supp} K_{C_t(H)} \subset \{(x,y) \in M^2 : \ d(x,y) \le t\} \ .$$

Proof. By virtue of Theorem 4.1 [17] for any vector field Y such that $\langle Y, Y\rangle \in L^1_{\text{loc}}(M)$ and any function $V\colon M \to \mathbb{R}$, $V \in L^1_{\text{loc}}(M)$ there exist sequences of smooth vector fields Y_n and smooth positive functions V_n such that $H_n = H(Y_n, V_n)$ converges to $H = H(Y, V)$ in the strong resolvent sense. Hence by [15, Theorem VIII.20] $C_t(H_n)$ converges to $C_t(H)$ in the strong operator topology. Therefore it is enough to prove Theorem 1 for a smooth vector field Y and a smooth function V. Now the proof of Theorem 1 relies on the following lemma.

Lemma 1. *Suppose that a function $\Phi \in C^\infty(M \times \mathbb{R})$ solves the wave equation, i.e.*

$$\partial_t^2 \Phi(x,t) = -H\Phi(x,t). \tag{9}$$

Then for every $y \in M$ there exists a constant $c_y > 0$, such that the function

$$P(t) = \int_{B(c_y - t, y)} \langle grad\,\Phi + i\Phi Y, grad\,\Phi + i\Phi Y\rangle + V|\Phi|^2 + |\partial_t \Phi|^2 \, dx,$$

is nonincreasing for $0 < t < c_y$, where $B(r,y) = \{x : \ d(x,y) \le r\}$.

Proof. To prove Lemma 1 it is enough to show that

$$\partial_t P(t) = \partial_t \int_{B(c_y - t, y)} \langle grad\,\Phi + i\Phi Y, grad\,\Phi + i\Phi Y\rangle + V|\Phi|^2 + |\partial_t \Phi|^2 \, dx \le 0.$$

We choose c_y so small that the geodesic exponential map is a diffeomorphism for $x \in B(c_y, y)$. Next we note that in that domain any vector tangent to a geodesic is a normal vector to the sphere, so

$$\partial_t \int\limits_{B(t,y)} \phi \, dx = \int\limits_{\partial B(t,y)} \phi \, d\sigma,$$

where $d\sigma$ is surface measure on ∂B. Hence

$$\partial_t P(t) = 2\mathrm{Re}\Bigg[\int\limits_{B(c_y-t,y)} \langle grad\,\Phi + i\Phi Y, grad\,\partial_t\Phi + i\partial_t\Phi Y\rangle + V\Phi\partial_t\overline{\Phi} + \partial_t^2\Phi\partial_t\overline{\Phi}\,dx \Bigg] - \int\limits_{\partial B(c_y-t,y)} \langle grad\,\Phi + i\Phi Y, grad\,\Phi + i\Phi Y\rangle + V|\Phi|^2 + |\partial_t\Phi|^2\,d\sigma. \tag{10}$$

Now put $X_t = grad\ \Phi + i\Phi Y$. By the definition of gradient

$$\langle X_t, grad\ \partial_t\Phi\rangle = X_t\partial_t\overline{\Phi}. \tag{11}$$

On the other hand for any $\phi \in C^\infty(M)$,

$$div\,\phi X = \phi\ div\,X + X\phi, \tag{12}$$

so

$$\begin{aligned}
&\langle grad\,\Phi + i\Phi Y, grad\,\partial_t\Phi + i\partial_t\Phi Y\rangle + V\Phi\partial_t\overline{\Phi} + \partial_t^2\Phi\partial_t\overline{\Phi} \\
&= X_t\partial_t\overline{\Phi} + \langle grad\,\Phi + i\Phi Y, iY\rangle\partial_t\overline{\Phi} + V\Phi\partial_t\overline{\Phi} + \partial_t^2\Phi\partial_t\overline{\Phi} \\
&= div\,(\partial_t\overline{\Phi}X_t) - \partial_t\overline{\Phi}div\ X_t + \langle grad\,\Phi + i\Phi Y, iY\rangle\partial_t\overline{\Phi} \\
&\quad + V\Phi\partial_t\overline{\Phi} + \partial_t^2\Phi\partial_t\overline{\Phi} \\
&= div\,(\partial_t\overline{\Phi}grad\,\Phi) + (H + \partial_t^2)\Phi\partial_t\overline{\Phi} \\
&= div\,(\partial_t\overline{\Phi}grad\,\Phi).
\end{aligned} \tag{13}$$

In virtue of (10) and (13),

$$\partial_t P(t) = 2\mathrm{Re}\Bigg[\int\limits_{B(c_y-t,y)} div\,(\partial_t\overline{\Phi}X_t)\,dx \Bigg] - \int\limits_{\partial B(c_y-t,y)} \langle grad\,\Phi + i\Phi Y, grad\,\Phi + i\Phi Y\rangle + V|\Phi|^2 + |\partial_t\Phi|^2 d\sigma.$$

We denote by **n** a normal vector to the surface $\partial B(c_y - t, y)$. Then

$$2\mathrm{Re}\Bigg[\int\limits_{B(c_y-t,y)} div\,(\partial_t\overline{\Phi}X_t)\,dx \Bigg] = 2\mathrm{Re}\Bigg[\int\limits_{\partial B(c_y-t,y)} \langle \partial_t\overline{\Phi}X_t, \mathbf{n}\rangle\,d\sigma \Bigg] \le \int\limits_{\partial B(c_y-t,y)} \langle X_t, X_t\rangle + |\partial_t\Phi|^2 + V|\Phi|^2\,d\sigma.$$

This proves Lemma 1. (See also [8, §5, pp. 209–215]).

Using Lemma 1 we can easily obtain Theorem 1. First we note that if $\phi, \psi \in C_c^\infty(M)$, and $\Psi : M \times \mathbb{R} \mapsto \mathbb{C}$ is defined by

$$\Psi(x,t) = C_t(\sqrt{H})(\phi)(x) + S_t(\sqrt{H})(\psi)(x), \tag{14}$$

where $C_t(\lambda) = \cos t\lambda$ and $S_t(\lambda) = \frac{\sin t\lambda}{\lambda}$, then

$$\partial_t^2 \Psi(x,t) = -H\Psi(x,t)$$

and

$$\Psi(x,0) = \phi(x),$$
$$\partial_t \Psi(x,0) = \psi(x).$$

In virtue of Lemma 1 if $c_x > t$,

$$\text{supp } K_{C_t(\sqrt{H})}(x,\cdot) = \text{supp } K_{C_t(\sqrt{H})}(\cdot,x) \subset B(t,x), \tag{15}$$

$$\text{supp } K_{S_t(\sqrt{H})}(x,\cdot) = \text{supp } K_{S_t(\sqrt{H})}(\cdot,x) \subset B(t,x). \tag{16}$$

However operators $S_t(\sqrt{H})$ and $C_t(\sqrt{H})$ as functions of t are continuous in the strong operator topology. Therefore for a given point $x \in M$ the set of all t such that (15) and (16) holds is closed. Hence either (15) and (16) are true for all t or we can choose the biggest number t_1 such that for all $0 \le t \le t_1$, (15) and (16) hold. By the completeness of the Riemannian metric the ball $B(t_1+1,x)$ is compact, so there exists $c > 0$ such that for any $y \in B(t_1+1,x)$ we have $c_y > c$, where c_y is the constant from Lemma 1. By virtue of Lemma 1 if functions $\phi, \psi \in C_c^\infty(M)$ satisfy

$$dist\{x, \text{supp } \phi \cup \text{supp } \psi\} > t_1 + t_2 \tag{17}$$

for $t_2 \le c$, then

$$(\text{supp } \Psi(t_2,\cdot) \cup \text{supp } \partial_t\Psi(t_2,\cdot)) \cap B(t_1,x) = \emptyset.$$

However

$$\Psi(t_1+t_2,x) = C_{t_1}(\sqrt{L})\Psi(t_2,\cdot)(x) + S_{t_1}\partial_t\Psi(t_2,\cdot)(x).$$

Hence (15) and (16) hold for all $t \le t_1 + c$ which contradicts the definition of t_1. This proves Theorem 1.

In the sequel we will also need the following Gaussian estimates for the heat kernel corresponding to H.

Theorem 2. *Suppose that* (2) *holds and $k_t(x,y)$ is the heat kernel corresponding to the operator H, i.e., $k_t(x,y) = K_{\exp(-tH)}(x,y)$. Then*

$$|k_t(x,y)| \le C(1 \wedge t)^{-k/2} \exp\left(-\frac{d^2(x,y)}{4(1+\epsilon)t}\right)$$

with a constant C independ cutof the function $V \ge 0$.

Proof. Assume that $Y = 0$ and $V = 0$. Then by Corollary 2.4.7. of [4], (see also [7, §4.2a]).

$$|K_{\exp(-tH(0,0))}(x,y)| \le Ct^{-k/2}$$

for $t \le 1$. However $H(0,0)$ is positive definite so $\| \exp(-tH(0,0))\|_{L^2\to L^2} \le 1$ and for $t \ge 1$,

$$\begin{aligned} K_{\exp(-tH(0,0))}(x,y) &\le \| \exp(-tH(0,0))\|_{L^1\to L^\infty} \\ \le \| \exp(-tH(0,0)/2))\|^2_{L^2\to L^\infty} &\le \| \exp(-H(0,0)/2))\|^2_{L^2\to L^\infty} \\ = \sup_{x\in M} \|K_{\exp(-H(0,0)/2))}(x,\cdot)\|^2_{L^2} &= \sup_{x,y\in M} K_{\exp(-H(0,0))}(x,y) \le C. \end{aligned}$$

Thus

$$K_{\exp(-tH(0,0))}(x,y) \le C(1 \wedge t)^{-k/2}$$

and Theorem 2 follows by Theorem 1 of [18] or [5]. We obtain Theorem 2 for any $V \ge 0$ and Y in virtue of the following theorem (we put $A = H(0,0)$ and $B = H(Y,V)$, see also Theorem 2.3 [17]).

Theorem 3. (Theorem 4.2, p. 270 [1]) *Let* $(T(t))_{t\ge 0}$ *be a positive semigroup with generator* A *and* $(S(t))_{t\ge 0}$ *a semigroup with generator* B*. The following assertions are equivalent:*
(i) $|S(t)\psi| \le T(t)|\psi|$.
(ii) Re $(\text{sign}\, \psi B\psi, \phi) \le (|\psi|, A'\phi)$ *for all* $\psi \in D(B)$ *and* $\phi \in D(A')$ *and* $\phi \ge 0$.

Remark 1. It is also possible to derive the finite speed propagation property of the wave equation, i.e. Theorem 1, from Gaussian estimates given by Theorem 2 (see Theorem 3 of [18]).

3. Abstract Theorem

The main result of this paper is the following theorem

Theorem 4. *Let* $k_t(x,y)$ *be the heat kernel corresponding to the operator* H*. Suppose that, the Nash inequality* (2) *is satisfied and that* (4) *holds. Then*

$$|k_t(x,x)| \le C(1\wedge t)^{-k/2} \left(\exp\left(-c_1 t d(x,0)^\alpha\right) + \exp\left(-c_2 t^{-1} d(x,0)^2\right)\right) \quad .$$

Proof. For $s > 0$ we define a function v_s by the formula

$$v_s(x) = \sigma \max\{s^\alpha - d(x,0)^\alpha, 0\}$$

and an operator H_s by

$$H_s\psi(x) = H\psi(x) + v_s(x)\psi(x) \quad ,$$

i.e. $H_s = H(Y, V_s)$, where $V_s = V + v_s$. Next, if we put $s = d(x,0)/2$ in Lemma 2 and Lemma 3 below we obtain Theorem 4 just by the triangle inequality.

Lemma 2. *For any $x, y \in \mathbb{R}^k$ and $t > 0$*

$$|K_{\exp(-tH_s)}(x,y)| \le C(1 \wedge t)^{-k/2} e^{-\sigma\, ts^\alpha} \ .$$

Lemma 3. *For any $s, t > 0$ and $x \in M$,*

$$|K_{\exp(-tH_s)}(x,x) - k_t(x,x)| \le C_\varepsilon (1 \wedge t)^{-k/2} \exp\left(-\frac{d(x, B(s,0))^2}{t(4+\varepsilon)}\right),$$

for all $\varepsilon > 0$, where $B(s,0) = \{y \in \mathbb{R}^k \ ;\ d(y,0) \le s\}$.

Proof (of Lemma 2). Let $s > 0$. Then by (4)

$$V_s - \sigma s^\alpha \ge 0 \ .$$

Hence by Theorem 2 we have

$$\begin{aligned} &|K_{\exp(-tH(Y, V_s - \sigma s^\alpha))}(x,y)| = |K_{\exp(-t(H_s - \sigma s^\alpha))}(x,y)| \\ &\le C(1 \wedge t)^{-k/2} \exp\left(-\frac{d^2(x,y)}{4(1+\epsilon)t}\right) \le C(1 \wedge t)^{-k/2} \ . \end{aligned} \tag{18}$$

However,

$$K_{\exp(-t(H_s - \sigma s^\alpha))}(x,y) = K_{\exp(-tH_s)}(x,y) e^{\sigma\, ts^\alpha}$$

and Lemma 2 follows from (18).

Proof (of Lemma 3). Let the function $(\,\cdot\,)_+ \colon \mathbb{R} \to \mathbb{R}$ be defined by

$$(x)_+ = \begin{cases} x & \text{if } x \ge 0 \\ 0 & \text{if } x < 0 \end{cases} \ .$$

Then, for $\beta > -1$,

$$\exp(-x^2) = \frac{\Gamma(\beta+1)}{2} \int_0^\infty dr\, (r^2 - x^2)_+^\beta\, r\, e^{-r^2} \quad .$$

Hence

$$\frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right) = \frac{\Gamma(\beta+1)}{2\sqrt{\pi}} \left(\frac{1}{4t}\right)^{\beta+3/2} \int_0^\infty dr\, (r^2 - x^2)_+^\beta\, r\, e^{-\frac{r^2}{4t}} \quad .$$

Taking the Fourier transform on both sides yields

$$\exp(-t\lambda^2) = \frac{\Gamma(\beta+1)}{2} \left(\frac{1}{4t}\right)^{\beta+3/2} \int_0^\infty dr\, F_r^\beta(\lambda) r e^{-\frac{r^2}{4t}} \quad , \tag{19}$$

where F_r^β is the Fourier transform of $x \in \mathbb{R} \to \pi^{-1/2}(r^2 - x^2)_+^\beta$. By (19)

$$\exp(-tL) = \frac{\Gamma(\beta+1)}{2} \left(\frac{1}{4t}\right)^{\beta+3/2} \int_0^\infty dr\, F_r^\beta(\sqrt{L}) r e^{-\frac{r^2}{4t}} \quad , \tag{20}$$

where L is any positive self-adjoint operator. Next for $L = H$ or $L = H_s$ we have

$$\text{supp } K_{(F_r^\beta)(\sqrt{L})}(x,\cdot) \subset B(r,x) \quad . \tag{21}$$

Indeed, if f is an even function then by the Fourier inversion formula

$$f(\lambda) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\, \hat{f}(t)\cos(t\lambda) \tag{22}$$

and in virtue of (22),

$$f(\sqrt{L}) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dt\, \hat{f}(t) C_t(\sqrt{L}) \quad . \tag{23}$$

Thus by (23)

$$F_r^\beta(\sqrt{L}) = \frac{2}{\sqrt{\pi}}\int_0^{\infty} dt\,(r^2-t^2)_+^\beta\, C_t(\sqrt{L}) \quad , \tag{24}$$

and (21) follows by Theorem 1 and (24). Note that $H_s = H$ on $\mathbb{R}^k - B(s,0)$, so by (21)

$$K_{F_r^\beta(\sqrt{H_s})}(x,\cdot) = K_{F_r^\beta(\sqrt{H})}(x,\cdot) \tag{25}$$

for $r \le d(x,B(s,0))$.

Now assume that for $L = H$, or $L = H_s$, and $\beta > k-1$,

$$|K_{F_r^\beta(\sqrt{L})}(x,y)| \le C(r^{2\beta-k+1} + r^{2\beta+1}) \quad . \tag{26}$$

Then by (20) and (25),

$$\begin{aligned} &|K_{\exp(-tH_s)}(x,x) - K_{\exp(-tH)}(x,x)| \qquad (27)\\ &\le \frac{\Gamma(\beta)}{2}\left(\frac{1}{4t}\right)^{\beta+3/2}\int_0^\infty dr\,|K_{F_r^\beta(\sqrt{H_s})}(x,y) - K_{F_r^\beta(\sqrt{H})}(x,y)|\, r\, e^{-\frac{r^2}{4t}}\\ &= \frac{\Gamma(\beta)}{2}\left(\frac{1}{4t}\right)^{\beta+3/2}\int_{d(x,B(s,0))}^\infty dr\,|K_{F_r^\beta(\sqrt{H_s})}(x,x) - K_{F_r^\beta(\sqrt{H})}(x,x)|\, r\, e^{-\frac{r^2}{4t}} \quad . \end{aligned}$$

Finally by (26) for $L = H$, or $L = H_s$,

$$\begin{aligned} &\left(\frac{1}{4t}\right)^{\beta+3/2}\int_{d(x,B(s,0))}^\infty dr\,|K_{F_r^\beta(\sqrt{L})}(x,y)|\, r\, e^{-\frac{r^2}{4t}}\\ &\qquad \le C\left(\frac{1}{4t}\right)^{\beta+3/2}\int_{d(x,B(s,0))}^\infty dr\,(r^{2\beta-k+1} + r^{2\beta+1})\, r\, e^{-\frac{r^2}{4t}}\\ &\qquad = C(4t)^{-k/2}\int_{\frac{d(x,B(s,0))}{\sqrt{4t}}}^\infty dr\, r^{2\beta-k+1}\, r\, e^{-r^2}\\ &\qquad\quad + C\int_{\frac{d(x,B(s,0))}{\sqrt{4t}}}^\infty dr\, r^{2\beta+1}\, r\, e^{-r^2} \end{aligned} \tag{28}$$

and we obtain Lemma 3 from the elementary inequality

$$\int_a^\infty dr\, r^b\, r\, e^{-r^2} \le C_b\,(1+a)^b \exp(-a^2) \le C_{b,\varepsilon}\, \exp(-a^2/(1+\varepsilon)) \quad .$$

Proof (of (26)). As above we put $L = H$ or $L = H_s$. By p_t we denote

$$p_t(x,y) = K_{\exp(-tL)}(x,y).$$

It follows easily from spectral theory that if L is a self-adjoint, positive-definite operator, $p_1(x,\cdot) \in L^2$ and we define a measure μ_x by the formula

$$\int_0^\infty F(\lambda) d\mu_x(\lambda) = \int_0^\infty (e^{-\lambda^2})^{-2} F(\lambda) 2\lambda d(E(\lambda^2) p_1(x,\cdot), p_1(x,\cdot)) \quad ,$$

then

$$\|K_{F(\sqrt{L})(x,\cdot)}\|^2_{L^2(dx)} = \int_0^\infty |F(\lambda)|^2 \, d\mu_x(\lambda) \quad . \tag{29}$$

On the other hand, by Theorem 2 for $L = H$ or $L = H_s$,

$$\|p_t(x,\cdot)\|^2_{L^2(dx)} = p_{2t}(x,x) \le C(1 \wedge t)^{-\frac{k}{2}} \quad .$$

Hence

$$\begin{aligned}
\mu_x([0,r)) &\le e \int_0^r d\mu_x(\lambda) \, e^{\lambda^2 r^{-2}} \\
&\le e \int_0^\infty d\mu_x(\lambda) \, e^{\lambda^2 r^{-2}} \\
&= e \, \|p_{\frac{1}{r^2}}(x,\cdot)\|^2_{L^2} \le C' \, (1 + r^k) \quad .
\end{aligned} \tag{30}$$

Now, for a function F, we put $G_1 = |F|\text{sign}F$ and $G_2 = |F|$. Then

$$\begin{aligned}
|K_{F(\sqrt{L})}(x_1,x_2)| &= \Big| \int_M dy \, K_{G_1(\sqrt{L})}(x_1,y) K_{G_2(\sqrt{L})}(y,x_2) \Big| \\
&\le \|K_{G_1(\sqrt{L})}(x_1,\cdot)\|_{L^2} \|K_{G_2(\sqrt{L})}(x_1,\cdot)\|_{L^2} \\
&= \Big(\int_0^\infty d\mu_{x_1}(\lambda) \, |G_1(\lambda)|^2 \Big)^{1/2} \Big(\int_0^\infty d\mu_{x_2}(\lambda) \, |G_2(\lambda)|^2 \Big)^{1/2} \\
&= \Big(\int_0^\infty d\mu_{x_1}(\lambda) \, |F(\lambda)| \Big)^{1/2} \Big(\int_0^\infty d\mu_{x_2}(\lambda) \, |F(\lambda)| \Big)^{1/2} \quad ,
\end{aligned}$$

i.e.,

$$|K_{F(\sqrt{L})}(x_1,x_2)| \le \Big(\int_0^\infty d\mu_{x_1}(\lambda) \, |F(\lambda)| \Big)^{1/2} \Big(\int_0^\infty d\mu_{x_2}(\lambda) \, |F(\lambda)| \Big)^{1/2} \quad . \tag{31}$$

It is not difficult, however, to verify that for some constant C_β independent of λ and r,

$$|F_r^\beta(\lambda)| \le C_\beta \frac{r^{2\beta+1}}{1 + |r\lambda|^{\beta+1}}, \tag{32}$$

so by (30)

$$\begin{aligned}
\int_0^\infty d\mu_x(\lambda)\,|F_r^\beta(\lambda)| &\leq C_\beta \int_0^\infty d\mu_x(\lambda)\,\frac{r^{2\beta+1}}{1+|r\lambda|^{\beta+1}} \\
&= -C_\beta \int_0^\infty d\mu_x(\lambda) \int_\lambda^\infty ds\,\Big(\frac{d}{ds}\Big(\frac{r^{2\beta+1}}{1+(rs)^{\beta+1}}\Big)\Big) \\
&= -C_\beta \int_0^\infty ds\,\mu_x([0,s))\Big(\frac{d}{ds}\Big(\frac{r^{2\beta+1}}{1+(rs)^{\beta+1}}\Big)\Big) \\
&\leq -C_\beta \int_0^\infty ds\,\Big(\frac{d}{ds}\Big(\frac{r^{2\beta+1}}{1+(rs)^{\beta+1}}\Big)\Big)\,C'(1+s^k) \\
&= r^{2\beta-k+1}C'C_\beta(\beta+1)\int_0^\infty ds\,\frac{s^\beta s^k}{(1+s^{\beta+1})^2} \\
&\qquad + r^{2\beta+1}C'C_\beta\,(\beta+1)\int_0^\infty ds\,\frac{s^\beta}{(1+s^{\beta+1})^2} \quad ,
\end{aligned}$$

which in virtue of (31) proves (26).

Remark 2. 1. The particular form of the operator H seems to play very little role in the proof of Theorem 4 and one could ask whether Theorem 4 could be stated in more general way, for example for a generator of a semigroup with finite speed propagation property of the solution of the wave equation. However, if we consider differential operators with constant coefficients on $\mathbb{R}^n$ then in virtue of the Paley-Wiener theorem, Theorem 1 holds only for operators of the form (1). We do not know how to precisely state and prove a generalisation of the above observation to the case of differential operators with variable coefficients, but we conjecture that any extension of Theorem 1 is contained in Remark 2.2 below.

2. It is possible to prove a version of Theorem 4 for operators of the following form:

$$(H\psi,\psi) = -\int_M \sum_{j=1}^n |(X_j + iY_j(x))\psi(x)|^2 + |\psi(x)|^2 V(x) \quad , \tag{33}$$

where we assume that the vector fields X_j satisfy Hörmander's condition. We can prove Theorem 1 for the operator in (33) using Theorem 3 of [18]. However, we have to replace the Riemannian distance with the sub-Riemannian distance corresponding to the vector fields X_j (see §III.4 of [19] or §IV.4b of [16]). The proof of Theorem 4 in this case is the same.

3. It follows from the proof that for any $0 < s < 1$ and $\varepsilon > 0$ we can put $c_1 = \sigma\, s^\alpha$ and $c_2 = (1-s)^2/(4+\varepsilon)$ as constants in Theorem 4.

4. Large Time Lstimates

In virtue of Theorem 4 we can easily obtain large time estimates on the semigroup kernels.

Theorem 5. *If H satisfies the hypotheses of Theorem 4 and k_t is the corresponding heat kernel, then*

$$|k_t(x,x)| \leq \begin{cases} Ct^{-k/2}\exp(-ctd(0,x)^\alpha) & \text{if } t \leq (1+d(0,x))^{1-\alpha/2} \\ Ce^{-t\lambda_1}\exp(-cd(0,x)^{1+\alpha/2}) & \text{if } t > (1+d(0,x))^{1-\alpha/2} \end{cases} , \tag{34}$$

where λ_1 is the smallest eigenvalue of H.

Proof. For $t \le (1 + d(0,x))^{1-\alpha/2}$ and some constants $C, c > 0$,

$$C \exp\left(-c\, t d(x,0)^{\alpha}\right) \ge \exp\left(-c_2 d(x,0)^2 t^{-1}\right) \ ,$$

where c_2 is a constant from Theorem 4. Hence estimates (34) follow from Theorem 4. To prove Theorem 5 for $t > (1 + d(0,x))^{1-\alpha/2}$ we note first that

$$\|e^{-tH}\|_{L^2 \mapsto L^2} = e^{-t\lambda_1}$$

and

$$e^{-tH} k_s(x,\cdot) = k_{s+t}(x,\cdot) \ .$$

Next

$$\begin{aligned}
k_t(x,x) &= \|k_{t/2}(x,\cdot)\|^2_{L^2} \\
&= \|e^{\left(-t/2+2^{-1}(1+d(x,0))^{1-\alpha/2}\right)H} k_{2^{-1}(1+d(x,0))^{1-\alpha/2}}(x,\cdot)\|^2_{L^2} \\
&\le e^{\left(-t+(1+d(x,0))^{1-\alpha/2}\right)\lambda_1} \|k_{2^{-1}(1+d(x,0))^{1-\alpha/2}}(x,\cdot)\|^2_{L^2} \\
&= e^{\left(-t+(1+d(x,0))^{1-\alpha/2}\right)\lambda_1} k_{(1+d(x,0))^{1-\alpha/2}}(x,x) \\
&\le C e^{-t\lambda_1} \left(1 \wedge (1 + d(x,0))^{1-\alpha/2}\right)^{-k/2} \\
&\times \left(\exp\left(- c_1 \frac{d(0,x)^{\alpha}}{(1 + d(0,x))^{\alpha/2-1}}\right) + \exp\left(- c_2 \frac{d(0,x)^2}{(1 + d(0,x))^{1-\alpha/2}}\right)\right) \\
&\times \left(\exp\left((1 + d(x,0))^{1-\alpha/2} \lambda_1\right)\right) \\
&\le C' e^{-t\lambda_1} \exp\left(- c' d(0,x)^{1+\alpha/2} + (1 + d(x,0))^{1-\alpha/2}\lambda_1\right) \\
&\le C'' e^{-t\lambda_1} \exp(-c'' d(0,x)^{1+\alpha/2}) \ .
\end{aligned}$$

Corollary 1. *Under the assumptions of Theorem 4,*

$$|k_t(x,y)| \le \begin{cases} C t^{-k/2} \exp\left(- ct(d(0,x)^{\alpha'} + d(0,y)^{\alpha'})\right) & \text{if } t \le 1 \\ C e^{-t\lambda_1} \exp\left(- c(d(0,x)^{\alpha''} + d(0,y)^{\alpha''})\right) & \text{if } t > 1 \ , \end{cases} \tag{35}$$

where λ_1 is the smallest eigenvalue of H and $\alpha' = 2 \wedge \alpha$ and $\alpha'' = \alpha \wedge (1 + \alpha/2)$.

Proof. In virtue of Theorem 5 and Theorem 4 there exist constants C', c' such that

$$|k_t(x,x)| \le \begin{cases} C' t^{-k/2} \exp(-c' t d(0,x)^{\alpha'}) & \text{if } t \le 1 \\ C' e^{-t\lambda_1} \exp(-c'(d(0,x)^{\alpha''}) & \text{if } t > 1 \ . \end{cases} \tag{36}$$

However

$$\begin{aligned}
|k_t(x,y)| &= |\int k_{t/2}(x,z) k_{t/2}(z,y)| \\
&\le \|k_{t/2}(x,\cdot)\|_{L^2} \|k_{t/2}(y,\cdot)\|_{L^2} = k_t(x,x)^{1/2} k_t(y,y)^{1/2}
\end{aligned}$$

and for $c = c'/2$ (35) follows from (36).

5. Reduced Heat Kernel

We will apply Theorem 4 to the reduced heat kernel on a nilpotent Lie group G, i.e. to the semigroup kernel corresponding to the operator H defined by (6). In the sequel we will assume that our unitary irreducible representation U is constructed in the same way as in Theorem 1.1, Theorem 1.8 and Lemma 1.10 of [14]. Any unitary irreducible representation is equivalent to some representation constructed in such a way. Alternatively we can assume that the representation U is the one considered in case 1 in the proof of Theorem 4.1.1 of [3]. Such a representation U acts on $\mathbb{R}^k$ and there exists a subalgebra $\mathfrak{g}'$ of codimension one in $\mathfrak{g}$ and vector $a_k \in \mathfrak{g}$ such that

$$U(a')(x_1,\ldots,x_k) = U'(Ad_{\exp x_k a_k} a')(x_1,\ldots,x_{k-1}) \tag{37}$$
$$= \sum_{j=1}^{r} \frac{x_k^j}{j!} U'(ad\, a_k)^j a')(x_1,\ldots,x_{k-1})$$

for all $a' \in \mathfrak{g}'$, where U' is an irreducible representation of the subalgebra $\mathfrak{g}'$ acting on $\mathbb{R}^{k-1}$. In addition by Theorem 1.12 and (1.29) of [14] (or see the proof of Theorem 4.1.1, case 1 of [3]) there exists $b \in \mathfrak{g}$ satisfying

$$U(b) = ix_k, \tag{38}$$

and by (1.29) of [14] there is $b' \in \mathfrak{g}$ such that

$$U(b') = i. \tag{39}$$

We can state a version of the condition (4) for the operator H defined by (6) in the following way.

Lemma 4. *If U is a representation described above, $b_1,\ldots,b_n$ is a linear basis of $\mathfrak{g}$, then there exist $\alpha > 0$ and $C > 0$ such that*

$$\sum_{j=1}^{n} |U(b_j)\psi(x)|^2 \geq C(1+|x|)^\alpha |\psi(x)|^2 \quad .$$

Proof. We will prove Lemma 4 by induction on the dimension of $\mathfrak{g}$. For dim $\mathfrak{g} = 1$, Lemma 4 is obvious. Next let b satisfy (38) and b' satisfy (39). We assume that the set b_j is a base for $\mathfrak{g}$, so there exist numbers ξ_j and η_j such that

$$b = \sum_{j=1}^{n} \xi_j b_j$$

and

$$b' = \sum_{j=1}^{n} \eta_j b_j \ .$$

Hence by Hölder's inequality

$$(1+x_k^2)|\psi(x)|^2 = |U(b)\psi(x)|^2 + |U(b')\psi(x)|^2 \tag{40}$$
$$= |\sum_{j=1}^{n} \xi_j U(b_j)|^2 + |\sum_{j=1}^{n} \eta_j U(b_j)|^2 \leq (\|b\|^2 + \|b'\|^2) \sum_{j=1}^{n} |U(b_j)\psi(x)|^2 \ ,$$

where $\|\cdot\|$ is the Euclidean norm on $\mathfrak{g}$ for which the vectors b_i form an orthonormal basis. By the induction hypothesis, if b'_j is a basis of $\mathfrak{g}'$, then

$$\sum_{j=1}^{n-1} |U'(b'_j)\psi(x)|^2 \geq C(1 + |(x_1, \ldots, x_{k-1})|)^{\alpha'} |\psi(x)|^2 \quad . \tag{41}$$

Next by (37),

$$\sum_{j=1}^{n-1} |U(b'_j)\psi(x)|^2 = \sum_{j=1}^{n-1} |U'(Ad_{\exp x_k a_k} b'_j)\psi(\cdot, x_k)|^2. \tag{42}$$

However $\mathfrak{g}$ is nilpotent so there exist polynomials $A_{mj}(x_k)$ such that

$$b'_m = \sum_{j=1}^{n-1} A_{mj}(x_k) Ad_{\exp x_k a_k} b'_j \quad .$$

Hence

$$\begin{aligned} |U'(b'_m)\psi(x)|^2 &\leq (\sum_{j=1}^{n-1} A_{mj}(x_k)^2)(\sum_{j=1}^{n-1} |U'(Ad_{\exp x_k a_k} b'_j)\psi(x)|^2) \\ &\leq C(1 + |x_k|)^r (\sum_{j=1}^{n} |U(b'_j)\psi(x)|^2) \quad . \end{aligned} \tag{43}$$

Thus by (41), (42) and (43)

$$\sum_{j=1}^{n} |U(b_j)\psi(x)|^2 \geq C \sum_{j=1}^{n-1} |U(b'_j)\psi(x)|^2 \tag{44}$$

$$\geq C_1(1 + |x_k|)^{-r} \sum_{j=1}^{n-1} |U'(b'_j)\psi(x)|^2 \geq C \frac{(1 + |(x_1, \ldots, x_{k-1})|)^{\alpha'} |\psi(x)|^2}{(1 + |x_k|)^r} \quad .$$

Finally, if $p, q > 1$ and $1/p + 1/q = 1$, in virtue of (44), (40) we have

$$\begin{aligned} \sum_{i=j}^{n} |U(b_j)\psi(x)|^2 \geq C &\left(\frac{(1 + |(x_1, \ldots, x_{k-1})|)^{\alpha'} |\psi(x)|^2}{(1 + |x_k|)^r} \right)^{1/p} \\ &\times ((1 + |x_k|)^2 |\psi(x)|^2)^{1/q} \geq C(1 + |x|)^{\alpha} \end{aligned}$$

for $\frac{\alpha'}{p} = \frac{2}{q} - \frac{r}{p} = \alpha$. This proves Lemma 4.

For any $a \in \mathfrak{g}$, $U(a)$ is a differential operator acting on $\mathbb{R}^k$ of the form

$$U(a) = \sum_{j=1}^{k} X_j^\circ(x, a) \frac{\partial}{\partial x_j} + iY(x, a) \quad ,$$

where $X_j^\circ(x, a) = X_j^\circ(x_1, \ldots, x_{j-1}, a)$ and $Y(x, a)$ are polynomials in $\mathbb{R}^k$ (see [7, 14 or 3]). We define $U^\circ(a)$ by

$$U^\circ(a) = \sum_{j=1}^{k} X_j^\circ(x,a)\frac{\partial}{\partial x_j} \quad .$$

Next we define the Riemannian metric $\langle \cdot\,,\cdot\rangle$ in such a way that

$$\langle grad\,\psi(x), grad\,\psi(x)\rangle = \sum_{j=1}^{n} |U^\circ(b_j)(x)\psi(x)|^2$$

for any $\psi \in C^\infty(\mathbb{R}^k)$. Finally we define a potential V and a vector field A by the formula

$$\langle grad\,\psi(x) + i\psi(x)A, grad\,\psi(x) + i\psi(x)A\rangle + V|\psi(x)|^2 = \sum_{j=1}^{n} |U(b_j)(x)\psi(x)|^2$$

for any $\psi \in C^\infty(R^k)$. In virtue of Lemma 4,

$$V(x) \geq C(1+|x|)^\alpha.$$

By $d(\cdot,\cdot)$ we denote the Riemannian distance corresponding to the metric $\langle\cdot\,,\cdot\rangle$. Using standard techniques we can easily prove that

Lemma 5. *There exist $\beta > 0$ and constants C, C' such that*

$$C|x|^\beta \leq d(x,0) \leq C'|x| \quad .$$

Finally, to apply Theorem 4 we need the following lemma

Lemma 6. *The system $U^\circ(b_1)(x),\dots,U^\circ(b_n)(x)$ satisfies the Nash inequality (condition (2)).*

Proof. For a weak Malcev basis $a_1,\dots,a_k$ satisfying an additional condition (3) [7], Lemma 6 is stated in Corollary 3.10 of [7]. But in virtue of Lemma 2.3 of [7] if $\tilde a_1,\dots,\tilde a_k$ is any other weak Malcev basis, then the representation $\tilde U$ corresponding to this basis is given by the formula

$$\tilde U = JUJ^\star,$$

where J is an isomorphism of $L^p(\mathbb{R}^k)$ for any $1 \leq p \leq \infty$. J maps the system $U^\circ(b_1)(x),\dots,U^\circ(b_n)(x)$ onto the system $\tilde U^\circ(b_1)(x),\dots,\tilde U^\circ(b_n)(x)$. Hence Corollary 3.10 of [7] is true for any weak Malcev basis. This proves Lemma 6.

In virtue of Corollary 1, Lemma 4, Lemma 5 and Lemma 6 we obtain the following theorem.

Theorem 6. *If κ_t is the reduced heat kernel then there exist constants $C, c, \alpha > 0$ such that*

$$|\kappa_t(x,y)| \leq \begin{cases} Ct^{-k/2}\exp(-ct(|x|^\alpha + |y|^\alpha)) & \text{for } t < 1 \\ Ce^{-t\lambda_1}\exp(-c(|x|^\alpha + |y|^\alpha)) & \text{for } t \geq 1 \end{cases} , \tag{45}$$

where λ_1 is the smallest eigenvalue of H.

6. Lower Bounds

In order to verify to what extent the estimates of Theorem 4 and Theorem 5 are sharp we prove some lower bounds for the heat kernel corresponding to the Schrödinger operator

$$-\Delta + |x|^\alpha = -\sum_{j=1}^{k} \partial^2/\partial x_j^2 + |x|^\alpha .$$

Proposition 1. *If k_t is a kernel of the semigroup generated by the operator $-\Delta + |x|^\alpha$, then there exist constants $c, C > 0$ such that for $t \le (1 + |x|)^{1-\alpha/2}$*

$$C^{-1} t^{-k/2} \exp(-ct|x|^\alpha) \ge k_t(x,x) \ge C t^{-k/2} \exp(-c^{-1} t|x|^\alpha) \tag{46}$$

and for $t \ge (1 + |x|)^{1-\alpha/2}$

$$C^{-1} e^{-t\lambda_1} \exp(-c|x|^{1+\alpha/2}) \ge k_t(x,x) \ge C e^{-t\lambda_1} \exp(-c^{-1}|x|^{1+\alpha/2}) . \tag{47}$$

Proof. If we put

$$V_s(y) = \min\{s^\alpha, |y|^\alpha\} \ ,$$

then in virtue of the Feynman–Kac formula,

$$K_{exp(t(\Delta - V_s))}(y, y') \ge K_{exp(t(\Delta - s^\alpha))}(y, y')$$

and

$$K_{exp(t(\Delta - V_s))}(y, y) \ge C t^{-k/2} \exp(-ts^\alpha). \tag{48}$$

In the same way as in Lemma 3 we can show that

$$|K_{\exp(t(\Delta - V_{|2x|})}(x,x) - k_t(x,x)| \le C_\varepsilon t^{-k/2} \exp\left(-\frac{|x|^2}{t(4+\varepsilon)}\right)$$

and by (48)

$$k_t(x,x) \ge C t^{-k/2} \exp(-t|2x|^\alpha) - C_\varepsilon t^{-k/2} \exp\left(-\frac{|x|^2}{t(4+\varepsilon)}\right) . \tag{49}$$

On the other hand, let $\lambda_1 < \lambda_2 \le \ldots$ denote the eigenvalues of the operator $H = -\Delta + |x|^\alpha$, repeated according to multiplicity, and let $\varphi_1, \varphi_2, \ldots$ be the corresponding orthonormal basis of eigenfunctions. By Proposition 1.4.3 [4] λ_1 has multiplicity one. Note that

$$k_t(x,x) = \sum_{i=1}^{\infty} e^{-t\lambda_i} |\varphi_i(x)|^2 \ge e^{-t\lambda_1} |\varphi_1(x)|^2 \ . \tag{50}$$

Next, by Corollary 4.5.7 of [4] for some constants C, c

$$\varphi_1(x) \ge C \exp(-c|x|^{1+\alpha/2}) \ . \tag{51}$$

and in virtue of of Theorem 4, (49) (50), (51) we obtain Proposition 1.

For $\alpha < 2$ and $t < 1$ we can obtain a more precise result. Namely, we can control the constant c in the estimate (46).

Proposition 2. *If k_t is the heat kernel corresponding to the operator $-\Delta + |x|^\alpha$ and $\alpha < 2$ then for any $\varepsilon > 0$ there exist constants C_ε and C'_εsuch that for $t \le 1$,*

$$C_\varepsilon t^{-k/2} \exp(-(1-\varepsilon)t|x|^\alpha) \ge k_t(x,x) \ge C'_\varepsilon t^{-k/2} \exp(-(1+\varepsilon)t|x|^\alpha).$$

Proof. It is not difficult to show (see Lemma 4.5.9 of [4]) that

Lemma 7. *If k_t is the heat kernel corresponding to the operator $H = -\Delta + |x|^\alpha$, then for some constants C and T and for all $t \le T$,*

$$k_t(x,x) \ge Ct^{-k/2} \exp(-t(|x|+1)^\alpha).$$

However, a careful examination of the constants in Theorem 4 (see the Remark 2.3 at the end of §3) shows that

$$k_t(x,x) \le Ct^{-k/2}\Big(\exp(-(1-\varepsilon)t|x|^\alpha) + \exp(-c_\varepsilon|x|^2)\Big)$$
$$\le C_\varepsilon t^{-k/2} \exp(-(1-\varepsilon)t|x|^\alpha).$$

Although according to Proposition 1 and Proposition 2 it seems that Theorem 4 and 5 are quite sharp, for $\alpha \ge 2$ and large t Davies and Simon have obtained a more precise result which gives exactly the value of the constant c in Proposition 1. In [6] it is proved that the Schrödinger operator generated by the operator $-\Delta+|x|^\alpha$ for $\alpha > 2$ is so called intrinsic ultracontractive (Theorem 6.3 of [6]) and by Theorem 4.2.5 and Corollary 4.5.8 of [4]

Theorem 7. *For any $\epsilon > 0$ there exists T such that for $t > T$,*

$$(1-\varepsilon)e^{-t\lambda_1}\varphi_1(x)\varphi_1(y) \le k_t(x,y) \le (1+\varepsilon)e^{-t\lambda_1}\varphi_1(x)\varphi_1(y),$$

where φ_1 is a ground state (eigenfunction corresponding to the smallest eigenvalue) of the operator $-\Delta + |x|^\alpha$ and

$$C'(1+|x|)^{(1-k)/2} \exp\left(-\frac{2}{2+\alpha}|x|^{1+\alpha/2}\right) \le \varphi_1(x)$$
$$\le C(1+|x|)^{(1-k)/2} \exp\left(-\frac{2}{2+\alpha}|x|^{1+\alpha/2}\right) .$$

For $\alpha < 2$ the Schrödinger semigroup is not intrinsically ultracontractive and this approach does not give any upper bound for the semigroup kernel.

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References

1. Arendt, W., Grabosch, A., Greiner, G., Groh, U., Lotz, H.P., Moustakas, U., Nagel, R., Neubrander, F., Schlotterbeck, U.: *One-parameter semigroups of positive operators*. Lecture Notes in Mathematics, **1184**. Berlin–Heidelberg–New York: Springer-Verlag, 1986
2. Avron, J., Herbst, I., Simon, B.: Schrödinger operators with magnetic fields, I General interactions. Duke Math. J. **45**, 847–84 (1978)
3. Corwin, L.J., Greenleaf, F.P.: *Representation of nilpotent Lie groups and their applications, Part 1: Basic theory and examples*. Cambridge: Cambridge Univ. Press, 1990

4. Davies, E.B.: *Heat kernels and spectral theory*. Cambridge: Cambridge Univ. Press, 1989
5. Davies, E.B., Pang, M.M.H.: Sharp Heat kernel bounds for some Laplace operators. Quar. J. Math. Oxford (2) 40, 281–290 (1989)
6. Davies, E.B., Simon, B.: Ultracontractivity and the heat kernel for Schrödinger operators and Dirichlet Laplacians. J. Funct. Anal. **59**, 335–95 (1984)
7. ter Elst, A.F.M., Robinson, D.W.: Reduced heat kernels on nilpotent Lie groups. Commun. Math. Phys. **173**, 475–511 (1995)
8. Folland, G. B.: Introduction to partial differential equations. Math. Notes, Princeton, NJ: Princeton Univ. Press, 1976
9. Helffer, B., Nourrigat, J.: Décroissance à l'infini des fonctions propres de l'opérateur de Schrödinger avec champ électromagnétique polynomial. J. Analyse Math. **58**, 263–75 (1992)
10. Hörmander, L.: *The analysis of linear partial differential operators 1*. Berlin–Heidelberg–New York: Springer-Verlag, 1983
11. Melrose, R.: *Propagation for the wave group of a positive subelliptic second order differential operator in Hyperbolic Equations and related topics*. Boston, Mass.: Academic Press 1989
12. Mohamed, A., Lévy-Bruhl, P., Nourrigat, J.: Etude spectrale d'opérateurs liés à des représentations de groupes nilpotents. J. Funct. Anal. **113**, 65–93 (1993)
13. Nash, J.: Continuity of solutions of parabolic and elliptic equations. Amer. J. Math. **81**, 931–954 (1958)
14. Nourrigat, J.: L^2 *inequalities and representations of nilpotent group*. Lectures notes C.I.M.P.A. School of Harmonic Analysis Wuhan (China), 1991
15. Reed, M., Simon, B.: *Methods of modern mathematical physics, I, Functional Analysis, self-adjointness,*. New York: Academic press, 1972
16. Robinson D.W.: *Elliptic operators and Lie groups*. Oxford: Oxford Univ. Press, 1991
17. Simon, B.: Maximal and Minimal Schrödinger forms. J. Operator Theory **1**, 37–47 (1979)
18. Sikora, A.: Sharp pointwise estimates on heat kernels. Quart. J. Math. Oxford (2) **47**, 371–382 (1996)
19. Varopoulos, N.Th., Saloff-Coste, L., Coulhon, T.: *Analysis and geometry on Groups*. Cambridge: Cambridge Univ. Press, 1992

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