Chapter 4

Ultracontractivity of Schrödinger semigroups

In this chapter we consider again a Schrödinger operator $H = -\Delta + V$ with a nonnegative potential $V \in L^1_{\text{loc}}(\mathbb{R}^N)$. If $V(x) = |x|^\alpha$, $\alpha > 2$, an estimate of the form $p(x, y, t) \le c(t)\psi(x)\psi(y)$ holds, where ψ is the ground state of H and $c(t)$ has an explicit behavior near 0 (see [13, Section 4.5]). We consider the Davies-Simon estimates and we obtain bounds on Schrödinger kernels using the similarity between Schrödinger and Kolmogorov operators. Even though this similarity is well-known, see [13, Section 4.7], we reverse the usual order, i.e. we deduce bounds on Schrödinger kernels from those for Kolmogorov's kernels rather than the converse and this allows us to improve the estimates obtained by Davies and Simon. It is also shown how the same technique works for other potentials, for example heat kernel bounds are obtained for $V(x) = \exp\{|x|^\alpha\}$, $\alpha > 0$.

4.1 Kernel estimates for a class of Kolmogorov operators

In this section we prove estimates of the form $p(x, y, t) \le c(t)\omega(x)\omega(y)$ for Kolmogorov operators of the form

$$A = \Delta - \nabla\phi \cdot \nabla$$

with $\phi \in C^2(\mathbb{R}^N)$. The operator A can be easily defined, through form methods, as a self-adjoint, nonpositive operator in $L^2(\mathbb{R}^N, \mu)$, where $d\mu$ is the measure with density $\exp\{-\phi\}$. If the function $|\nabla\phi|^2 - 2\Delta\phi$ is bounded from below in $\mathbb{R}^N$, then the operator A in $L^2(\mathbb{R}^N, \mu)$ is unitarily equivalent to the Schrödinger operator $-H$ with potential $V = \frac{1}{4}|\nabla\phi|^2 - \frac{1}{2}\Delta\phi$ in $L^2(\mathbb{R}^N)$ (with respect to the Lebesgue measure), see [26, Proposition 2.2]. In particular $A = -THT^{-1}$

where T is the multiplication operator $Tu = e^{\frac{\phi}{2}}u$. Moreover $e^{tA} = Te^{-tH}T^{-1}$ and consequently for all $x,\ y \in \mathbb{R}^N$ and $t > 0$

$$p_A(x, y, t) = e^{\frac{\phi(x)}{2}} p(x, y, t) e^{-\frac{\phi(y)}{2}} \tag{4.1}$$

where p_A and p are the heat kernels corresponding to the operators A and $-H$. This equality shows that the problems of finding estimates for p_A and p are equivalent and, in [13, Section 4.7], this fact is used to deduce bounds for p_A from deep estimates on p based on log-Sobolev inequalities leading to the intrinsic ultracontractivity of the Schrödinger semigroup. We reverse the approach and show bounds on p_A based on subsolution estimates. Then we deduce bounds on p. This method has the advantage to give more precise information on the function $c(t)$ quoted at the beginning of this section and allows us to improve some kernel estimates on Schrödinger operators, as shown in the next section.

As first step we prove L^1 bounds for some Lyapunov functions (or subsolutions) for A. For all $0 < c < 1$, let $W_c = e^{c\phi}$. It is easy to check that

$$AW_c = e^{c\phi}[c\Delta\phi + (c^2 - c)|\nabla\phi|^2].$$

Under suitable assumptions on ϕ, W_c is a Lyapunov function for A that is a C^2-function $W : \mathbb{R}^N \to [0, \infty)$ such that $\lim_{|x|\to\infty} W(x) = +\infty$ and $AW \leq \lambda W$ for some $\lambda > 0$.
We need some preliminary lemmas (see [30, Lemma 3.8, Lemma 3.9]).
Let W be a Lyapunov function. For $\alpha \geq 0$ set $W_\alpha = W \wedge \alpha$ and $u_\alpha(x, t) = T(t)W_\alpha(x)$.

Lemma 4.1.1. *With the notation above, the inequality*

$$\partial_t u_\alpha(x, t) \leq \int_{\{W\leq\alpha\}} p(x, y, t) AW(y)\, dy$$

holds for every $t \geq 0$ and $x \in \mathbb{R}^N$.

Proof. For every $\varepsilon > 0$ let $\psi_\alpha \in C^\infty(\mathbb{R})$ be such that $\psi_\varepsilon(t) = t$ for $t \leq \alpha$, ψ_ε is constant in $[\alpha + \varepsilon, \infty[$, $\psi_\varepsilon' \geq 0$, $\psi_\varepsilon'' \leq 0$. Observe that $\psi_\varepsilon(t) \to t \wedge \alpha$ and $\psi_\varepsilon'(t) \to \chi_{]-\infty,\alpha]}(t)$ pointwise as $\varepsilon \to 0$. Since the function $\psi_\varepsilon \circ V$ belongs to $D_{max}(A)$, we have

$$\partial_t T(t)(\psi_\varepsilon \circ W)(x) = \int_{\mathbb{R}^N} p(x, y, t) A(\psi_\varepsilon \circ W)(y)\, dy.$$

On the other hand, by the assumptions on ψ_ε,

$$\begin{aligned} A(\psi_\varepsilon \circ W)(x) &= \psi_\varepsilon'(W(x))AW(x) + \psi_\varepsilon''(W(x)) \sum_{i,j=1}^N a_{ij}(x) D_i W(x) D_j W(x) \\ &\leq \psi_\varepsilon'(W(x))AW(x) \end{aligned}$$

and then

$$\begin{aligned}\partial_t T(t)(\psi_\varepsilon \circ W)(x) &\le \int_{\mathbb{R}^N} p(x,y,t)\psi_\varepsilon'(W(y))AW(y)\,dy \qquad (4.2)\\ &= \int_{0\le W\le \alpha+\varepsilon} p(x,y,t)\psi_\varepsilon'(W(y))AW(y)\,dy.\end{aligned}$$

Observe that $\psi_\varepsilon \circ W \le \alpha + 1$ and $\psi_\varepsilon \circ W \to W_\alpha$ pointwise as $\varepsilon \to 0$. By Proposition 1.1.3 we deduce that $T(t)(\psi_\varepsilon \circ W) \to u_\alpha$ uniformly on compact sets of $]0,\infty[\times\mathbb{R}^N$, then by the interior Schauder estimates (see [17, Chapter 3, Section 2]) $\partial_t T(t)(\psi_\varepsilon \circ W) \to \partial_t u_\alpha$ pointwise as $\varepsilon \to 0$. Letting ε to zero in (4.2) we obtain the claim by dominated convergence. $\square$

The next result has been partially obtained in Chapter 2 in the more general case of Lyapunov functions depending also on the variable t.

Lemma 4.1.2. *Suppose that $AW \le \lambda W$ for some positive λ. Then for every $t > 0$, $x \in \mathbb{R}^N$ the functions W and $|AW|$ are integrable with respect to the measure $p(x,\cdot,t)$. If we set*

$$u(x,t) = \int_{\mathbb{R}^N} p(x,y,t)W(y)\,dy,$$

the function u belongs to $C^{1,2}(\mathbb{R}^N\times]0,\infty[) \cap C(\mathbb{R}^N \times [0,\infty[)$ and satisfies the inequalities $u(x,t) \le e^{\lambda t}W(x)$, $\partial_t u(x,t) \le \int_{\mathbb{R}^N} p(x,y,t)AW(y)\,dy$.

Proof. By Lemma 4.1.1 and by assumption we have

$$\partial_t u_\alpha(x,t) \le \int_{\{W\le\alpha\}} p(x,y,t)AW(y)\,dy \le \lambda u_\alpha(x,t). \qquad (4.3)$$

By Gronwall's lemma we deduce $u_\alpha(x,t) \le e^{\lambda t}W_\alpha(x)$. Letting α to infinity we obtain $u(x,t) \le e^{\lambda t}W(x)$ by monotone convergence. This implies that W is integrable with respect to the measure $p(x,\cdot,t)$. The inequality $0 \le u_\alpha \le u$ and the interior Schauder estimates show that (u_α) is relatively compact in $C^{1,2}(\mathbb{R}^N \times (0,\infty))$. Since $u_\alpha \to u$ pointwise as $\alpha \to \infty$ it follows that $u \in C^{1,2}(\mathbb{R}^N \times (0,\infty))$. Moreover the inequality $u_\alpha(x,t) \le u(x,t) \le e^{\lambda t}W(x)$ implies that $u(\cdot,t) \to W(\cdot)$ as $t \to 0$ uniformly on compact sets. Set $E = \{x \in \mathbb{R}^N : AW(x) \ge 0\}$, clearly

$$\int_E p(x,y,t)AW(y)\,dy \le \lambda \int_E p(x,y,t)W(y)\,dy \le \lambda u(x,t) < \infty. \qquad (4.4)$$

Letting α to infinity in (4.3) we obtain

$$\partial_t u(x,t) \le \liminf_{\alpha\to\infty} \int_{\{W\le\alpha\}} p(x,y,t)AW(y)\,dy.$$

The last inequality and (4.4) imply that

$$-\int_{\{AW\le 0\}} p(x,y,t)AW(y)\,dy < \infty,$$

then $|AW|$ is integrable with respect to the measure $p(x,\cdot,t)$ and so the above $\liminf$ is a limit and the claim follows. $\square$

Proposition 4.1.3. *Let $\phi \geq 0$ such that $\lim_{|x|\to\infty} \phi(x) = +\infty$ and let $0 < c < 1$. Suppose that for some $0 < \varepsilon < 1 - c$ there exists $C_\varepsilon > 0$ such that*

$$\Delta\phi \leq \varepsilon|\nabla\phi|^2 + C_\varepsilon \tag{4.5}$$

and suppose that

$$|\nabla\phi| \geq C_1\phi^\gamma - C_2 \tag{4.6}$$

for some positive constant C_1, C_2 and some $\gamma > \frac{1}{2}$. Then the function W_c defined above is a Lyapunov function. Moreover, setting

$$\xi_c(x,t) = \int_{\mathbb{R}^N} p_A(x,y,t)W_c(y)\,dy,$$

we have

$$\xi_c(x,t) \leq C_3 \exp\{C_4 t^{\frac{1}{1-2\gamma}}\} \tag{4.7}$$

for some positive constants C_3, C_4.

Proof. By (4.5) and (4.6) for $|x|$ large enough

$$\begin{aligned} AW_c &= e^{c\phi}[c\Delta\phi + (c^2 - c)|\nabla\phi|^2] \leq e^{c\phi}[(c\varepsilon + c^2 - c)|\nabla\phi|^2 + C_\varepsilon c] \\ &\leq e^{c\phi}(-C_1|\nabla\phi|^2 + C_2) \leq -e^{c\phi}(\widetilde{C}_1\phi^{2\gamma} - \widetilde{C}_2). \end{aligned}$$

This proves that, for $|x|$ large enough, AW_c is negative. By the regularity of W_c, for $|x|$ small $AW_c \leq \lambda \leq \lambda W_c$ for some positive λ. Therefore W_c is a Lyapunov function. Moreover, setting $g(s) = c_1 s(\log s)_+^{2\gamma} - c_2$ for suitable constants c_1 and c_2, we have

$$AW_c \leq -g(W_c)$$

for $|x|$ sufficiently large. Observe that the existence of a Lyapunov function for A implies the uniqueness for the solution of problem (1.1), hence $\mathbf{1} = T(t)\mathbf{1} = \int_{\mathbb{R}^N} p_A(x,y,t)\,dy$. Since g is convex, by Jensen's inequality

$$\int_{\mathbb{R}^N} p_A(x,y,t)g(W_c(y))\,dy \geq g(\xi_c(x,t)).$$

By Lemma 4.1.2 and the previous inequalities we have

$$\begin{aligned} \partial_t\xi_c(x,t) &\leq \int_{\mathbb{R}^N} p_A(x,y,t)AW_c(y)\,dy \leq -\int_{\mathbb{R}^N} p_A(x,y,t)g(W_c(y))\,dy \\ &\leq -g(\xi_c(x,t)) \end{aligned}$$

and then $\xi_c(x,t) \leq z(x,t)$ where z is the solution of the ordinary Cauchy problem

$$\begin{cases} z' = -g(z) \\ z(x,0) = W_c(x). \end{cases}$$

Let l be the greatest zero of g. Then $z(x,t) \le l$ if $W_c(x) \le l$. If $W_c(x) > l$, z is decreasing and satisfies

$$t = \int_{z(x,t)}^{W_c(x)} \frac{ds}{g(s)} \le \int_{z(x,t)}^{\infty} \frac{ds}{g(s)}.$$

Choosing suitable constants C_3 and C_4, we finally obtain

$$\xi_c(x,t) \le z(x,t) \le C_3 \exp\{C_4 t^{\frac{1}{1-2\gamma}}\}.$$

□

Now we are able to deduce bounds on the kernel p_A from the bound on the function ξ_{W_c} proved above.

Proposition 4.1.4. *Let ϕ as in the previous proposition and suppose moreover that*

$$\exp\{-\frac{\phi}{4}\} \in L^1(\mathbb{R}^N), \qquad |\nabla\phi| \le C\phi^\beta, \tag{4.8}$$

for some positive $C,\ \beta$. Then

$$p_A(x,y,t) \le C_1 \exp\left\{C_2 t^{\frac{1}{1-2\gamma}}\right\} \exp\{-\phi(y)\} \tag{4.9}$$

and

$$p(x,y,t) \le C_1 \exp\left\{C_2 t^{\frac{1}{1-2\gamma}}\right\} \exp\left\{-\frac{\phi(y)}{2}\right\} \exp\left\{-\frac{\phi(x)}{2}\right\} \tag{4.10}$$

for all $x,\ y \in \mathbb{R}^N$ and $0 < t \le 1$ and suitable $C_1, C_2 > 0$.

Proof. Let $\omega = W_{\frac{1}{2}}$ and $\frac{1}{2} < c < 1$. Then, if $k > N+2$, by the assumptions on ϕ it follows that

$$\begin{aligned}
&\omega \le W_c,\\
&|\nabla\omega| = \frac{1}{2}e^{\frac{\phi}{2}}|\nabla\phi| \le C\omega^{\frac{k-1}{k}}W_c^{\frac{1}{k}} = C\exp\left\{\frac{\phi}{2}\frac{k-1}{k}\right\}\exp\left\{\frac{1}{k}c\phi\right\},\\
&|D^2\omega| \le C\omega^{\frac{k-2}{k}}W_c^{\frac{2}{k}},\\
&\omega|\nabla\phi|^k \le CW_c
\end{aligned}$$

for some positive constant C. By Remark 2.1.17 or [27, Theorem 4.1] it follows that

$$\exp\left\{\frac{\phi(y)}{2}\right\} p_A(x,y,t) \le \frac{C}{t^{\frac{k}{2}}} \int_{\frac{t}{2}}^{t} \xi_c(x,s)\,ds$$

for all $x,\ y \in \mathbb{R}^N$, $0 < t \le 1$ and by (4.7)

$$p_A(x,y,t) \le C_3 \exp\left\{C_4 t^{\frac{1}{1-2\gamma}}\right\} \exp\left\{-\frac{\phi(y)}{2}\right\}$$

for suitable C_3, C_4 (we can neglect negative powers of t which can be included in the exponential changing the constant). By (4.1),

$$p(x,y,t) \leq C_3 \exp\left\{C_4 t^{\frac{1}{1-2\gamma}}\right\} \exp\left\{-\frac{\phi(x)}{2}\right\} = c(t) \exp\left\{-\frac{\phi(x)}{2}\right\}.$$

Using the symmetry of p_{-H} with respect to the variables $x,\ y$ we have

$$p(x,y,t) \leq c(t) \exp\left\{-\frac{\phi(y)}{2}\right\}.$$

Then we get

$$p(z,y,t) \leq c(t) \exp\left\{-\frac{\phi(z)}{4}\right\} \exp\left\{-\frac{\phi(y)}{4}\right\}$$

and, by the semigroup law,

$$\begin{aligned} p(x,y,t) &= \int_{\mathbb{R}^N} p(x,z,\frac{t}{2}) p(z,y,\frac{t}{2})\, dz \\ &\leq c(\frac{t}{2})^2 \exp\left\{-\frac{\phi(x)}{2}\right\} \exp\left\{-\frac{\phi(y)}{4}\right\} \int_{\mathbb{R}^N} \exp\left\{-\frac{\phi(z)}{4}\right\} dz \\ &= K_1 c(\frac{t}{2})^2 \exp\left\{-\frac{\phi(x)}{2}\right\} \exp\left\{-\frac{\phi(y)}{4}\right\}. \end{aligned}$$

As in the estimate above we deduce

$$\begin{aligned} p(x,y,t) &\leq K_1 c(\frac{t}{2}) c(\frac{t}{4})^2 \exp\left\{-\frac{\phi(y)}{2}\right\} \exp\left\{-\frac{\phi(x)}{2}\right\} \int_{\mathbb{R}^N} \exp\left\{-\frac{\phi(z)}{4}\right\} dz \\ &= c_1(t) \exp\left\{-\frac{\phi(x)}{2}\right\} \exp\left\{-\frac{\phi(y)}{2}\right\}. \end{aligned}$$

Therefore

$$p(x,y,t) \leq C_1 \exp\left\{C_2 t^{\frac{1}{1-2\gamma}}\right\} \exp\left\{-\frac{\phi(y)}{2}\right\} \exp\left\{-\frac{\phi(x)}{2}\right\}$$

and

$$p_A(x,y,t) \leq C_1 \exp\left\{C_2 t^{\frac{1}{1-2\gamma}}\right\} \exp\left\{-\phi(y)\right\}.$$

□

4.2 Intrinsic ultracontractivity for e^{-tH}

Let us consider the Schrödinger operator $H = -\Delta + V$ where $0 \leq V(x) \to \infty$ as $|x| \to \infty$. Let $E > 0$ be the first eigenvalue of H and $\psi > 0$ be the corresponding eigenfunction. Then $\Delta\psi = (V - E)\psi$. As observed in the previous section, $-H + E$ is unitarily equivalent to the Kolmogorov operator $A = \Delta + 2\frac{\nabla\psi}{\psi} \cdot \nabla$, namely $-H + E = T^{-1} A T$ where T is the multiplication operator $Tu = \psi^{-1} u$.

If $\phi = -2\log\psi$, then $A = \Delta - \nabla\phi\cdot\nabla$ and $Tu = e^{\frac{\phi}{2}}u$. If ϕ satisfies the hypotheses of the Proposition 4.1.4 then we obtain upper bounds for the kernel of the semigroup generated by $-H+E$. Let us also observe that, if p_E and p are the kernels corresponding respectively to $-H+E$ and $-H$, then $p = p_E e^{-tE} \le p_E(x,y,t)$.

We start with $V(x) = |x|^\alpha$, $\alpha > 2$ and improve [13, Corollary 4.5.5]. In what follows the knowledge of the asymptotic behavior of the first eigenfunction ψ of H will play a major role. We recall that there exist $c_1,\ c_2 > 0$ such that

$$\begin{aligned} c_1|x|^{-\frac{\alpha}{4}-\frac{N-1}{2}} \exp\left\{-\frac{2}{2+\alpha}|x|^{1+\frac{\alpha}{2}}\right\} &\le \psi(x) \\ &\le c_2|x|^{-\frac{\alpha}{4}-\frac{N-1}{2}} \exp\left\{-\frac{2}{2+\alpha}|x|^{1+\frac{\alpha}{2}}\right\} \end{aligned} \tag{4.11}$$

for large $|x|$, see [13, Corollary 4.5.8]. Our methods, however, need also a precise asymptotic behavior of $\nabla\psi$. This can be obtained from [36, Chapter 6, Theorem 2.1] (as we shall do for other potentials) or using the following qualitative arguments for ODE's which we prefer to present in the following lemma.

Lemma 4.2.1. *Let ψ be the first eigenfunction of $-\Delta + V$ with $V(x) = |x|^\alpha$, $\alpha > 2$. Then*

$$\lim_{|x|\to\infty} \frac{|\nabla\psi|^2}{\psi^2}\cdot\frac{1}{|x|^\alpha} = 1.$$

PROOF. Since the potential is radial, the first eigenfunction is radial too, so, writing the Laplacian in polar coordinates, we have

$$\psi'' + \frac{N-1}{r}\psi' = (r^\alpha - E)\psi.$$

Setting $v = -\frac{\psi'}{\psi}$, the previous differential equation becomes

$$v' = v^2 - \frac{N-1}{r}v - (r^\alpha - E).$$

The right hand side of the previous equals 0 if

$$v = \frac{N-1}{2r} \pm \frac{1}{2}\sqrt{\frac{(N-1)^2}{r^2} + 4(r^\alpha - E)}.$$

Now we prove that there exists $r_0 > 0$ such that for $r \ge r_0$

$$v \ge \frac{N-1}{2r} + \frac{1}{2}\sqrt{\frac{(N-1)^2}{r^2} + 4(r^\alpha - E)}.$$

Since

$$\frac{d}{dr}(r^{N-1}\psi') = r^{N-1}(r^\alpha - E)\psi,$$

the asymptotic behavior of ψ (see (4.11)) shows that $r^{N-1}(r^\alpha - E)\psi$ is integrable in neighborhood of $+\infty$. This implies that there exists $\lim_{r\to\infty} r^{N-1}\psi'$ and it is equal to 0, by the asymptotic behavior of ψ, again. Moreover, if $r \geq E^{\frac{1}{\alpha}}$, $\frac{d}{dr}(r^{N-1}\psi') > 0$ and

$$r^{N-1}\psi' \leq \lim_{r\to\infty} r^{N-1}\psi' = 0.$$

This means that, for r large enough, $\psi' \leq 0$ and $v = -\frac{\psi'}{\psi} > 0$. From this we deduce that for r large enough v is in the region where $v' > 0$ and

$$v \geq \frac{N-1}{2r} + \frac{1}{2}\sqrt{\frac{(N-1)^2}{r^2} + 4(r^\alpha - E)}. \tag{4.12}$$

We are now interested in the asymptotic behavior of v. Let $\delta,\ k > 0$. Suppose that there exists a sequence $(r_n)_{n\in\mathbb{N}}$ such that $r_n \to \infty$ and

$$v(r_n) \geq \frac{N-1}{2r} + \frac{1}{2}\sqrt{\frac{(N-1)^2}{r^2} + 4[(k+2\delta)^\alpha - E]}. \tag{4.13}$$

Consider the following Cauchy problem in the interval $[k, k+\delta]$:

$$\begin{cases} z' = z^2 - \frac{N-1}{k}z - [(k+\delta)^\alpha - E] \\ z(k) = \frac{N-1}{2k} + \frac{1}{2}\sqrt{\frac{(N-1)^2}{k^2} + 4[(k+2\delta)^\alpha - E]}. \end{cases}$$

In $[k, k+\delta]$,

$$v' \geq v^2 - \frac{N-1}{k}v - [(k+\delta)^\alpha - E]. \tag{4.14}$$

Let us observe that $z(k) > \frac{N-1}{2k} + \frac{1}{2}\sqrt{\frac{(N-1)^2}{k^2} + 4[(k+\delta)^\alpha - E]}$, i.e. $z(k)$ is greater than the largest zero of $z^2 - \frac{N-1}{k}z - [(k+\delta)^\alpha - E]$. Integrating the differential equation satisfied by z, we obtain

$$\int_{z(k)}^{z(r)} \frac{dw}{w^2 - \frac{N-1}{k}w - [(k+\delta)^\alpha - E]} = r - k$$

and, taking $r = k + \delta$,

$$\delta \leq \int_{z(k)}^{\infty} \frac{dw}{w^2 - \frac{N-1}{k}w - [(k+\delta)^\alpha - E]}.$$

After a simple change of variable in the integral above,

$$\delta \leq \int_0^\infty \frac{ds}{s^2 + 2sz(k) - \frac{N-1}{k}s + (k+2\delta)^\alpha - (k+\delta)^\alpha}.$$

The right hand side in the previous inequality goes to 0 for k tending to $+\infty$ by dominated convergence. This means that, if k is large enough, the solution z of the Cauchy problem in $[k, k+\delta]$ blows up before the point $k+\delta$. So, choosing $k = r_n$, for r_n large enough z_{r_n} blows up. By (4.13) and (4.14), $v(r) \geq z_{r_n}$ and so v blows up too. Since this is a contradiction, there exists $\overline{r}$ (depending on δ) such that, for $r \geq \overline{r}$,

$$v(r) \leq \frac{N-1}{r} + \frac{1}{2}\sqrt{\frac{(N-1)^2}{r^2} + 4[(r+2\delta)^\alpha - E]}. \tag{4.15}$$

Finally, from (4.12), (4.15) and the arbitrariness of $\delta > 0$

$$\lim_{r\to\infty} \frac{v(r)}{r^{\frac{\alpha}{2}}} = 1.$$

□

Theorem 4.2.2. *Let p be the kernel of the semigroup generated by $\Delta - V$ with $V(x) = |x|^\alpha$ for some $\alpha > 2$. Then*

$$p(x,y,t) \leq C \exp\left\{ct^{-\frac{\alpha+2}{\alpha-2}}\right\} \psi(x)\psi(y)$$

for $x, y \in \mathbb{R}^N$ and $0 < t \leq 1$.

Proof. Let $\phi = -2\log\psi$, as before. Then ϕ satisfies (4.5), (4.6) with $\gamma = \frac{\alpha}{2+\alpha}$ and (4.8).

In fact, rewriting (4.5) in terms of ψ, we can prove that for all $\varepsilon > 0$ there exists $C_\varepsilon > 0$ such that

$$\operatorname{div}\left(-2\frac{\nabla\psi}{\psi}\right) = -2\frac{\Delta\psi}{\psi} + 2\frac{|\nabla\psi|^2}{\psi^2} \leq 4\varepsilon\frac{|\nabla\psi|^2}{\psi^2} + C_\varepsilon$$

or, equivalently, since ψ is an eigenfunction with eigenvalue E,

$$(1-\varepsilon)\frac{|\nabla\psi|^2}{\psi^2} \leq (V - E) + C_\varepsilon.$$

This follows immediately from Lemma 4.2.1. Moreover (4.6) and (4.8) follow by Lemma 4.2.1 too. For example observe that (4.6) is equivalent to

$$\frac{|\nabla\psi|}{\psi} \geq C_1 \log^\gamma \psi^{-2} - C_2$$

for some $\gamma > \frac{1}{2}$ and positive $C_1,\ C_2$. The last is true for $\gamma = \frac{\alpha}{2+\alpha}$ and in virtue of (4.11) and Lemma 4.2.1. Arguing in similar way (4.8) also follows.

At this point Proposition 4.1.4 gives

$$p(x,y,t) \leq C \exp\left\{ct^{-\frac{\alpha+2}{\alpha-2}}\right\} \exp\left\{-\frac{\phi(y)}{2}\right\} \exp\left\{-\frac{\phi(x)}{2}\right\}$$

for all $x,\ y \in \mathbb{R}^N$ and this concludes the proof. □

Comparing the last theorem with [13, Corollary 4.5.5] we conclude that the limit value $b = \frac{\alpha+2}{\alpha-2}$ is allowed.

Proceeding in a similar way we prove the following bound when the potential is $\exp\{|x|^\alpha\}$.

Theorem 4.2.3. *Let p the kernel of the semigroup generated by $\Delta - V$ with $V(x) = \exp\{|x|^\alpha\}$ for some positive α. Then for $x, y \in \mathbb{R}^N$ and $0 < t \le 1$*

$$p(x,y,t) \le C \exp\left\{ct^{\frac{1}{1-2\gamma}}\right\} \psi(x)\psi(y)$$

with $\gamma = 1$ if $\alpha \ge 1$ and for any $\frac{1}{2} < \gamma < 1$ if $\alpha < 1$. Here ψ is the first eigenfunction of $\Delta - V$ and

$$\psi(r) = Cr^{-\frac{N-1}{2}} \exp\left\{-\frac{r^\alpha}{4}\right\} \exp\left\{-\int_0^r \exp\left\{\frac{s^\alpha}{2}\right\} ds\right\} \{1 + \varepsilon(r)\}$$

with $\varepsilon(r) \to 0$ for $r \to \infty$.

Proof. Let $\psi > 0$ the first eigenfunction of the operator $-\Delta + V$ corresponding to the eigenvalue E. Since the potential is radial, the first eigenfunction is radial too, therefore, writing the Laplacian in polar coordinates, we have

$$\psi''(r) + \frac{N-1}{r}\psi'(r) = (\exp\{r^\alpha\} - E)\psi(r).$$

The function $v(r) = r^{\frac{N-1}{2}}\psi(r)$ satisfies the differential equation

$$v''(r) = v(r)\left(\exp\{r^\alpha\} - E + \frac{N-1}{2}\frac{N-3}{2}\frac{1}{r^2}\right).$$

By [36, Theorem 2.1, Chapter 6], a solution of the previous differential equation is given by

$$v(r) = \exp\left\{-\frac{r^\alpha}{4}\right\} \exp\left\{-\int_0^r \exp\left\{\frac{s^\alpha}{2}\right\} ds\right\} \{1 + \varepsilon(r)\}$$

where $\varepsilon(r)$ is a function such that $|\varepsilon(r)|$, $\frac{1}{2}\exp\{-\frac{r^\alpha}{2}\}|\varepsilon'(r)|$ goes to 0 if r goes to ∞. Then

$$\psi(r) = r^{-\frac{N-1}{2}} v(r) = r^{-\frac{N-1}{2}} \exp\left\{-\frac{r^\alpha}{4}\right\} \exp\left\{-\int_0^r \exp\left\{\frac{s^\alpha}{2}\right\} ds\right\} \{1 + \varepsilon(r)\}.$$

After simple computations we obtain

$$\psi'(r) = \psi(r)\left(-\frac{N-1}{2r} - \frac{\alpha}{4}r^{\alpha-1} - \exp\left\{\frac{r^\alpha}{2}\right\} + \frac{\varepsilon'(r)}{1+\varepsilon(r)}\right).$$

It follows that $\phi = \log \psi^{-2}$ satisfies the hypothesis in Proposition 4.1.4. In particular, choosing $\gamma = 1$ if $\alpha \ge 1$ and any $\frac{1}{2} < \gamma < 1$ if $\alpha < 1$, (4.6) is verified and the claim follows. $\square$