Kernel Estimates for Schrödinger Operators*

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Dedicated to G. Da Prato on the occasion of his 70^{th} *birthday*

Abstract

We prove short time estimates for the heat kernel of Schrödinger operators with unbounded potential in $\mathbf{R}^N$.
Mathematics subject classification (2000): 35K65, 35B65, 47D07, 60J35.
Keywords: Heat kernels, Schrödinger operators, parabolic regularity.

1 Introduction

In this paper we prove short time estimates for the heat kernel p of the Schrödinger operator

$$H = -\Delta + V \tag{1.1}$$

where the potential V is nonnegative and belongs to $C^{\alpha}_{\rm loc}(\mathbf{R}^N)$ for some $0 < \alpha \le 1$. The solution of the parabolic problem

$$\begin{cases} u_t(x,t) = -Hu(x,t), & x \in \mathbf{R}^N,\ t > 0, \\ u(x,0) = f(x), & x \in \mathbf{R}^N, \end{cases} \tag{1.2}$$

where $f \in L^2(\mathbf{R}^N)$, is given by the semigroup of selfadjoint integral operators $(e^{-tH})_{t\ge 0}$

$$e^{-tH}f(x) = \int_{\mathbf{R}^N} p(x,y,t) f(y)\,dy, \quad t > 0,\ x \in \mathbf{R}^N. \tag{1.3}$$

Due to the local regularity of the potential V, the heat kernel p is a positive function symmetric with respect to x and y which belongs to $C^{2+\alpha,2+\alpha,1+\alpha/2}_{\rm loc}(\mathbf{R}^N \times \mathbf{R}^N \times (0,\infty))$ and solves the equation $\partial_t p = -H_x p$, $t > 0$.

The kernel p is pointwise dominated by the heat kernel of the Laplacian in $\mathbf{R}^N$, that is $p(x,y,t) \le (4\pi t)^{-N/2} \exp\{-|x-y|^2/(4t)\}$ holds. Much deeper upper bounds have been obtained by Davies and Simon if, for example, $V(x) = |x|^\alpha$ with $\alpha > 2$, see [3] or also [2, Section 4.5]. In this case $p(x,y,t) \le c(t)\psi(x)\psi(y)$, where ψ is the ground state of H and the function c has quite an explicit behaviour near 0.

In this paper we prove upper bounds like $p(x,y,t) \le c(t)\phi(x)\phi(y)$ for a large class of potentials tending to ∞ as $|x| \to \infty$, under the main assumption that $\omega = 1/\phi$ satisfies $\omega(x) \to +\infty$ as $|x| \to \infty$ and $H\omega \ge g \circ \omega$ where g is a convex function growing faster than linearly. The behaviour

*Work partially supported by GNAMPA-INdAM.
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of $c(t)$ near 0 is also shown to be precise. Similar bounds are also proved for the derivatives of p. Our analysis provides a family of such estimates e.g. for $V(x) = |x|^\alpha$ for every $\alpha > 0$ but does not allow to prove that of Davies and Simon since $1/\psi$ does not satisfy our assumption if ψ is the ground state of H. Estimates of our form for the heat kernel of more general (even nonsymmetric) operators have been obtained recently in [7] using ultracontractivity methods in weighted spaces. In particular, we show that our Example 3.3 can be deduced from [7, Theorem 1.2]. Due to the behaviour of $c(t)$ near 0, however, the upper bound of Example 3.4 seems not to fall in the range of application of [7].

We also refer the reader to the papers [5] and [15] for bounds on the heat kernels associated with potentials of polynomial type, different from ours. In particular, potentials not tending to infinity are treated in [5] and lower bounds can be found in [15].

The plan of the paper is the following.

In Section 2, we recall the construction of the generator of the Schrödinger semigroup by the form method and some known results on local regularity of p. We show how the integrability of certain unbounded functions with respect to $p(x, y, t)\,dy$ can be obtained via Lyapunov function techniques. This allows us to indicate some growth conditions on the potential V which imply precise estimates of the L^1-norm of Lyapunov functions with respect to the kernel p.

In Section 3, we use parabolic regularity techniques to deduce pointwise bounds on p from the L^1 bounds of the previous section. We give several examples and show the optimality of such estimates with respect to t. In particular, in the case of polynomial potentials the estimate is similar to that obtained in [2, Corollary 4.5.5]. Similar techniques have been employed in [8] in the elliptic case, to obtain upper and lower bounds for the density of invariant measures of certain diffusion processes.

In Section 4, based on a functional analytic approach similar to the one used in [2, Chapter 4], we show pointwise estimates for the derivatives of the kernel p. Basically, we prove that an estimate like $p(x, y, t) \le c(t)\phi(x)\phi(y)$, where $1/\phi$ is a Lyapunov function for H, extends to the complex half plane $\{\mathrm{Re}\ z > 0\}$, and then we estimate $\partial_t p$ using Cauchy's theorem. Estimates for the derivatives of p with respect to the space variables are then deduced from recent results on elliptic regularity for operators with unbounded coefficients.

Finally, let us comment on the oscillation condition (H1)(a), namely DV small compared with $V^{3/2}$, which allows us to use the results of [11], yielding

$$\|u\|_{W^{2,1}_k(Q_T)} + \|Vu\|_{L^k(Q_T)} \le C\|f\|_{L^k(Q_T)}$$

if u solves $\partial_t u - \Delta u + Vu = f$, $u(0) = 0$. This estimate, crucial in our approach, is closely related to the characterisation of the domain of $-H$ in $L^p(\mathbf{R}^n)$ as the intersection of the Sobolev space $W^{2,p}(\mathbf{R}^N)$ and the domain of the potential V. Such a characterisation holds under (H1)(a) but also if V satisfies a reverse Hölder inequality ((RH) in short), in particular if V is a positive polynomial, see [14]. Simple examples show that (H1)(a) and (RH) are independent. However, the above discussion suggests the conjecture that our estimates could be extended to the case of potentials satisfying (RH).

Notation. $B_R(x)$ denotes the open ball in $\mathbf{R}^N$ of radius R and centre x. If $x = 0$ we simply write B_R. For $0 \le a < b$, we use $Q(a, b) := \mathbf{R}^N \times (a, b)$ and $Q_T := Q(0, T)$. We write $C = C(a_1, \ldots, a_n)$ to point out that the constant C depends on the quantities $a_1, \ldots, a_n$.

If $u : \mathbf{R}^N \times J \to \mathbf{R}$, where $J \subset [0, \infty[$ is an interval, we use the following notation:

$$\partial_t u = \frac{\partial u}{\partial t}, \qquad D_i u = \frac{\partial u}{\partial x_i}, \qquad D_{ij} u = D_i D_j u,$$
$$Du = (D_1 u, \ldots, D_N u), \qquad D^2 u = (D_{ij} u),$$

and

$$|Du|^2 = \sum_{j=1}^{N} |D_i u|^2, \qquad |D^2 u|^2 = \sum_{i,j=1}^{N} |D_{ij} u|^2.$$

Next, we introduce some notation for function spaces. $C_b^j(\mathbf{R}^N)$ is the space of j times differentiable functions in $\mathbf{R}^N$, with bounded derivatives up to the order j. $C_c^\infty(\mathbf{R}^N)$ is the space of test functions. $C_b^\alpha(\mathbf{R}^N)$ denotes the space of all bounded and α-Hölder continuous functions on $\mathbf{R}^N$.

For $1 \le k \le \infty$, $j \in \mathbf{N}$, $W_k^j(\mathbf{R}^N)$ denotes the classical Sobolev space of all L^k–functions having weak derivatives in $L^k(\mathbf{R}^N)$ up to the order j. Its usual norm is denoted by $\|\cdot\|_{j,k}$ and by $\|\cdot\|_k$ if $j = 0$.

Let us now define some spaces of functions of two variables following basically the notation of [6]. $C^{2,1}(Q(a,b))$ is the space of all functions u such that Du, $D_{ij}u$ and $\partial_t u$ are continuous in $Q(a,b)$. For $0 < \alpha \le 1$ we denote by $C_b^{2+\alpha,1+\alpha/2}(Q(a,b))$ the space of all bounded function u such that Du, $D_{ij}u$ and $\partial_t u$ are bounded and α-Hölder continuous in $Q(a,b)$ with respect to the parabolic distance $d((x,t),(y,s)) := |x-y| + |t-s|^{\frac{1}{2}}$. Spaces of locally Hölder continuous functions are defined, as usual, requiring that the Hölder condition holds in every compact subset.

We shall also use parabolic Sobolev spaces. We denote by $W_k^{2,1}(Q(a,b))$ the space of functions $u \in L^k(Q(a,b))$ having weak space derivatives $D_x^\alpha u \in L^k(Q(a,b))$ for $|\alpha| \le 2$ and weak time derivative $\partial_t u \in L^k(Q(a,b))$ equipped with the norm

$$\|u\|_{W_k^{2,1}(Q(a,b))} := \|u\|_{L^k(Q(a,b))} + \|\partial_t u\|_{L^k(Q(a,b))} + \sum_{1 \le |\alpha| \le 2} \|D_x^\alpha u\|_{L^k(Q(a,b))}.$$

2 Local regularity and integrability of Schrödinger kernels

Let us start with some known properties of H, for which we refer e.g. to [13], [2].

As a first step we construct a semigroup in $L^2(\mathbf{R}^N)$ generated by a suitable realisation of $-H$. Following [2], consider the quadratic form

$$Q(f) = \int_{\mathbf{R}^N} |Df|^2 + V|f|^2 \, dx, \qquad f \in C_c^\infty(\mathbf{R}^N).$$

The form Q is closable, even under the weaker assumption $V \in L^1_{\mathrm{loc}}(\mathbf{R}^N)$, the domain of the closure is

$$\mathrm{Dom}(Q) = \Big\{ f \in W_2^1(\mathbf{R}^N) : \int_{\mathbf{R}^N} V|f|^2 < \infty \Big\},$$

and the following two conditions of Beurling-Deny are satisfied by Q:

(i) $f \in \mathrm{Dom}(Q)$ implies $|f| \in \mathrm{Dom}(Q)$ and $Q(|f|) \le Q(f)$

(ii) $0 \le f \in \mathrm{Dom}(Q)$ implies $f \wedge 1 \in \mathrm{Dom}(Q)$ and $Q(f \wedge 1) \le Q(f)$.

Then, the associated operator $-H_2$ in $L^2(\mathbf{R}^N)$ generates a symmetric sub-Markov semigroup $(e^{-tH_2})_{t \ge 0}$, where

$$\begin{aligned} D(H_2) &= \Big\{ f \in \mathrm{Dom}(Q) : \exists g \in L^2(\mathbf{R}^N) \text{ such that} \\ &\qquad \int_{\mathbf{R}^N} Df \cdot D\phi + Vf\phi = \int_{\mathbf{R}^N} g\phi \text{ for all } \phi \in C_c^\infty(\mathbf{R}^N) \Big\} \\ &= \Big\{ f \in \mathrm{Dom}(Q) : f \in W^2_{2,\mathrm{loc}}(\mathbf{R}^N), Hf \in L^2(\mathbf{R}^N) \Big\}, \end{aligned}$$

by local elliptic regularity. We also recall that $(e^{-tH_2})_{t\geq 0}$ is a *symmetric sub-Markov semigroup* if each operator e^{-tH_2} is symmetric, $e^{-tH_2} \geq 0$ for all $t \geq 0$, and $\|e^{-tH_2}f\|_\infty \leq \|f\|_\infty$ for all $f \in L^2(\mathbf{R}^N) \cap L^\infty(\mathbf{R}^N)$ and all $t \geq 0$. Furthermore, by [2, Theorem 1.3.3], we know that the semigroup $(e^{-tH_2})_{t\geq 0}$ extends to a contraction semigroup in $L^p(\mathbf{R}^N)$, for all $1 \leq p \leq \infty$.

Let us recall some properties of the integral kernel p in (1.3).

Proposition 2.1 *The kernel $p = p(x, y, t)$ is a positive continuous function in $\mathbf{R}^N \times \mathbf{R}^N \times (0, \infty)$ such that $p(x, y, t) = p(y, x, t)$. For every $y \in \mathbf{R}^N$, $p(\cdot, y, \cdot)$ belongs to $C^{2+\alpha,1+\alpha/2}_{\mathrm{loc}}(\mathbf{R}^N \times (0, \infty))$ and solves the equations $\partial_t p + H_x p = 0$. By symmetry one has also $\partial_t p + H_y p = 0$.*

PROOF. Since p is bounded in $\mathbf{R}^N \times \mathbf{R}^N \times [a, +\infty[$ for every $a > 0$, by the Gaussian estimates, the proof of [9, Theorem 4.4] ensures that $p(\cdot, y, \cdot) \in C^{2+\alpha,1+\alpha/2}_{\mathrm{loc}}(\mathbf{R}^N \times (0, \infty))$ for every $y \in \mathbf{R}^N$. If $f \in C_c^\infty(\mathbf{R}^N)$ and $u(x, t) = e^{-tH} f(x)$, then

$$0 = \partial_t u(x, t) + H_x u(x, t) = \int_{\mathbf{R}^N} (\partial_t p(x, y, t) + H_x p(x, y, t)) f(y)\, dy$$

and therefore, by the arbitrariness of f, $\partial_t p + H_x p = 0$. The last assertion follows by a similar argument. □

It follows from the continuity of p and the domination with the heat kernel in $\mathbf{R}^N$ that the semigroup preserves $C_b(\mathbf{R}^N)$. It is not strongly continuous in $C_b(\mathbf{R}^N)$, but we have the following properties which are consequence of the classical Schauder estimates, see [9].

Theorem 2.2 *For $f \in C_b(\mathbf{R}^N)$, let $u(x, t) = e^{-tH} f(x)$, for $t \geq 0$, $x \in \mathbf{R}^N$. Then*

(i) *the function u belongs to $C^{2+\alpha,1+\alpha/2}_{\mathrm{loc}}(\mathbf{R}^N \times (0, \infty))$ and satisfies the equation $\partial_t u(x, t) = \Delta u(x, t) - V(x)u(x, t)$. Moreover, if $f \in C_c^2(\mathbf{R}^N)$, then $\partial_t u(x, t) = -e^{-tH} H f(x)$.*

(ii) *$e^{-tH} f(x) \to f(x)$ as $t \to 0$, uniformly on compact sets of $\mathbf{R}^N$.*

(iii) *Let (g_n) be a bounded sequence in $C_b(\mathbf{R}^N)$ and suppose that $g_n(x) \to g(x)$ for every $x \in \mathbf{R}^N$ with $g \in C_b(\mathbf{R}^N)$. Then $e^{-tH} g_n(x) \to e^{-tH} g(x)$ in $C^{2,1}(\mathbf{R}^N \times (0, \infty))$.*

Remark 2.3 Since $C_c^\infty(\mathbf{R}^N)$ is a core of H as an operator on $L^2(\mathbf{R}^N)$ (see [12, Theorem X. 28]) and H_2 is closed and coincides with H on $C_c^\infty(\mathbf{R}^N)$, both operators coincide. Thus the minimal semigroup generated by $-H$ and constructed by localisation methods (see [9] and [1, Theorem 3.1]) coincides with the semigroup constructed by the form method.

Now we turn our attention to integrability properties of p and show how they can be deduced from the existence of suitable *Lyapunov functions*, that is of $C^{2+\alpha}_{\mathrm{loc}}$-functions $W : \mathbf{R}^N \to [0, \infty)$ such that $\lim_{|x|\to\infty} W(x) = +\infty$ and $-HW \leq \lambda W$ for some $\lambda > 0$. Note that a Lyapunov function for H always exists, since $V \geq 0$ (take for example $W(x) = 1 + |x|^2$, $x \in \mathbf{R}^N$), and therefore the maximum principle holds for bounded $C^{2,1}$ solutions of (1.2), see e.g. [9, Theorem 3.7].

In the proof of Proposition 2.5 below we need to approximate the semigroup $(e^{-tH})_{t\geq 0}$ by semigroups generated by operators with bounded potentials. This is done in the next lemma.

Lemma 2.4 *Take $0 \leq \eta \in C^\infty(\mathbf{R})$ decreasing with $\eta(s) = 1$ for $s \leq 1$, $\eta(s) = 0$ for $s \geq 2$, and define $V_n(x) = \eta\left(\left|\frac{x}{n}\right|\right) V(x)$, $H_n = -\Delta + V_n$. Consider the analytic semigroups $(e^{-tH_n})_{t\geq 0}$ generated by H_n in $C_b(\mathbf{R}^N)$. Then, for every $f \in C_b^{2+\alpha}(\mathbf{R}^N)$ the function $e^{-tH_n} f(x)$ converges to $e^{-tH} f(x)$ in $C^{2,1}(\mathbf{R}^N \times [0, T])$.*

PROOF. Let $u_n(t,x) = e^{-tH_n} f(x)$, $u(x,t) = e^{-tH} f(x)$ and observe that the sequence u_n converges pointwise as $n \to \infty$ if f is only a $C_b(\mathbf{R}^N)$ function. In fact, assuming $f \geq 0$, then $0 \leq u \leq u_{n+1} \leq u_n$, by the maximum principle. Let us fix a radius $\varrho > 0$. If $n > \varrho + 1$ the Schauder estimates for the operator H (see e.g. [4, Theorem 8.1.1]) yield

$$\|u_n\|_{C^{2+\alpha,1+\alpha/2}(B_\varrho \times [0,T])} \leq C\left(\|u_n\|_{L^\infty(\mathbf{R}^N \times [0,\infty))} + \|f\|_{C^{2+\alpha}(\mathbf{R}^N)}\right) \leq C\|f\|_{C^{2+\alpha}(\mathbf{R}^N)}.$$

By Ascoli's theorem, (u_n) converges to a function v in $C^{2,1}(\mathbf{R}^N \times [0,\infty))$. Since $\partial_t u_n + Hu_n = 0$ in $B_\varrho \times (0,T]$ for $n > \varrho$ we have $\partial_t v + Hv = 0$ in $\mathbf{R}^N \times (0,T]$. Moreover, $v(x,0) = f(x)$ and $|v(x,t)| \leq \|f\|_\infty$, since this is true for the u_n and we have only to prove that $u = v$. The function $w = u - v$ belongs to $C^{2,1}(\mathbf{R}^N \times [0,T])$, is bounded and satisfies $\partial_t w + Hw = 0$, $w(x,0) = 0$ and hence $w = 0$, by the maximum principle. □

The issue of the following result is the integrability of Lyapunov functions with respect to the measures $p(x,y,t)\,dy$ is given by the following result. This is a variant of [10, Lemma 3.9], where the case of a Kolmogorov operator is considered, rather than Schrödinger semigroups.

Proposition 2.5 *Let W be a Lyapunov function, $\lambda > 0$, $HW \geq \lambda W$. Then W is integrable with respect to the measures $p(x,y,t)dy$. The function*

$$\zeta(x,t) = \int_{\mathbf{R}^N} p(x,y,t)W(y)\,dy, \tag{2.1}$$

satisfies the inequality

$$\zeta(t,x) \leq e^{\lambda t} W(x).$$

Moreover, $|HW|$ is integrable with respect to $p(x,y,t)dy$, $\zeta \in C^{2,1}(\mathbf{R}^N \times (0,\infty)) \cap C(\mathbf{R}^N \times [0,\infty))$ and the inequality

$$\partial_t \zeta(x,t) \leq -\int_{\mathbf{R}^N} p(x,y,t)HW(y)\,dy$$

holds.

PROOF. For $\alpha \geq 0$, set $W_\alpha := W \wedge \alpha$ and $\zeta_\alpha(x,t) := \int_{\mathbf{R}^N} p(x,y,t)W_\alpha(y)\,dy$.

For all $\varepsilon \in (0,1)$ we choose $\psi_\varepsilon \in C^\infty(\mathbf{R})$ such that $\psi_\varepsilon(t) = t$ for $t \leq \alpha$, ψ_ε constant in $[\alpha+\varepsilon,\infty)$, $\psi_\varepsilon' \geq 0$, and $\psi_\varepsilon'' \leq 0$. Since $\psi_\varepsilon'' \leq 0$ one deduces that

$$t\psi_\varepsilon'(t) \leq \psi_\varepsilon(t), \quad t \geq 0. \tag{2.2}$$

Now we approximate H and $(T(t))_{t\geq 0}$ by $H_n := -\Delta + V_n$ and $(T_n(t))_{t\geq 0}$ as in Lemma 2.4, and we denote by $p_n(x,y,t)$ the kernel of $(T_n(t))_{t\geq 0}$. Since $\psi_\varepsilon \circ W \in C_b^{2+\alpha}(\mathbf{R}^N)$ we have

$$\partial_t T_n(t)(\psi_\varepsilon \circ W)(x) = -\int_{\mathbf{R}^N} p_n(x,y,t)H_n(\psi_\varepsilon \circ W)(y)\,dy.$$

On the other hand, by (2.2), we obtain

$$\begin{aligned} H_n(\psi_\varepsilon \circ W)(x) &= \psi_\varepsilon'(W(x))H_nW(x) - V_n(x)\left[\psi_\varepsilon'(W(x))W(x) - \psi_\varepsilon(W(x))\right] \\ &\quad -\psi_\varepsilon''(W(x))|DW(x)|^2 \\ &\geq \psi_\varepsilon'(W(x))H_nW(x). \end{aligned}$$

Thus,

$$\partial_t T_n(t)(\psi_\varepsilon \circ W)(x) \leq -\int_{\mathbf{R}^N} p_n(x,y,t)\psi_\varepsilon'(W(y))H_nW(y)\,dy$$

and also

$$\partial_t T_n(t)(\psi_\varepsilon \circ W)(x) \le -\int_{\mathbf{R}^N} p_n(x,y,t)\psi'_\varepsilon(W(y))HW(y)\,dy,$$

if n is sufficiently large since, for fixed ε, the function $\psi'_\varepsilon(W(y))$ has compact support. Letting $n \to \infty$ and using Lemma 2.4 we deduce

$$\partial_t e^{-tH}(\psi_\varepsilon \circ W)(x) \le -\int_{\mathbf{R}^N} p(x,y,t)\psi'_\varepsilon(W(y))HW(y)\,dy. \tag{2.3}$$

Next we observe that $\psi_\varepsilon \circ W \le \alpha+1$, $\psi'_\varepsilon(t) \to \chi_{(-\infty,\alpha]}(t)$, and $\psi_\varepsilon \circ W \to W_\alpha$ pointwise as $\varepsilon \to 0$. From Theorem 2.2(iii) we deduce that $e^{-tH}(\psi_\varepsilon \circ W) \to e^{-tH}W_\alpha$ in $C^{2,1}(\mathbf{R}^N \times (0,\infty))$. So, letting $\varepsilon \to 0$ in (2.3) and using dominated convergence in the right hand side (all the integrals can be taken on the compact set $\{W \le \alpha+1\}$, where HW is bounded) we get

$$\partial_t \zeta_\alpha(x,t) \le -\int_{\{W\le\alpha\}} p(x,y,t)HW(y)\,dy. \tag{2.4}$$

To conclude we proceed as in the proof of [10, Lemma 3.9]. From (2.4) we obtain

$$\partial_t \zeta_\alpha(x,t) \le \lambda\zeta_\alpha(x,t) \tag{2.5}$$

and hence, by Gronwall's lemma, $\zeta_\alpha(x,t) \le e^{\lambda t}W_\alpha(x)$. Letting $\alpha \to \infty$ we obtain $\zeta(x,t) \le e^{\lambda t}W(x)$, and therefore W is integrable with respect to the measure $p(x,y,t)dy$. The inequality $0 \le \zeta_\alpha \le \zeta$ and the interior Schauder estimates show that the family (ζ_α) is relatively compact in $C^{2,1}(\mathbf{R}^N \times (0,\infty))$. Since $\zeta_\alpha \to \zeta$ pointwise as $\alpha \to \infty$, it follows that $\zeta \in C^{2,1}(\mathbf{R}^N \times (0,\infty))$. Moreover, the inequality $\zeta_\alpha(x,t) \le \zeta(x,t) \le e^{\lambda t}W(x)$ implies that $\zeta(\cdot,t) \to W(\cdot)$ as $t \to 0$, uniformly on compact sets. Set $E = \{x \in \mathbf{R}^N : -HW(x) \ge 0\}$. Then

$$-\int_E p(x,y,t)HW(y)\,dy \le \lambda\int_E p(x,y,t)W(y)\,dy \le \lambda\zeta(x,t) < \infty. \tag{2.6}$$

Moreover, letting $\alpha \to \infty$ in (2.4), we obtain that

$$\partial_t\zeta(x,t) \le \liminf_{\alpha\to+\infty}\left(-\int_{\{W\le\alpha\}} p(x,y,t)HW(y)\,dy\right).$$

This fact and (2.6) imply that $|HW|$ is integrable with respect to $p(x,y,t)dy$ and that the above $\liminf$ is a limit, so that the proof is complete. □

As we will see in the next proposition, if we assume that HW tends to $+\infty$ faster than W, one obtains, by Proposition 2.5, that the function ζ in (2.1) is bounded with respect to the space variables, see [10, Theorem 3.10].

Proposition 2.6 *Assume that the Lyapunov function W satisfies the inequality $HW \ge g(W)$, where $g : [0,\infty) \to \mathbf{R}$ is a differentiable convex function such that $g(0) \le 0$, $\lim_{s\to+\infty} g(s) = +\infty$ and $1/g$ is integrable in a neighbourhood of $+\infty$. Then for every $a > 0$ the function ζ defined in (2.1) is bounded in $\mathbf{R}^N \times [a,\infty)$.*

Proof. Observe that $g(s) \le sg'(s)$, since g is convex with $g(0) \le 0$. Let us prove that

$$\int_{\mathbf{R}^N} p(x,y,t)g(W(y))\,dy \ge g(\zeta(x,t)). \tag{2.7}$$

Fix x and t and set $s_0 = \zeta(x,t)$. Then, for all $y \in \mathbf{R}^N$ we have

$$g(W(y)) \ge g(s_0) + g'(s_0)(W(y) - s_0)$$

and therefore, multiplying by $p(x,y,t)$ and integrating

$$\int_{\mathbf{R}^N} p(x,y,t)g(W(y))\,dy \geq g(s_0)\int_{\mathbf{R}^N} p(x,y,t)\,dy + g'(s_0)s_0\Big(1-\int_{\mathbf{R}^N} p(x,y,t)\,dy\Big) \geq g(s_0).$$

From Proposition 2.5 and (2.7) we deduce

$$\partial_t\zeta(x,t) \leq -\int_{\mathbf{R}^N} p(x,y,t)HW(y)\,dy \leq -\int_{\mathbf{R}^N} p(x,y,t)g(W(y))\,dy \leq -g(\zeta(x,t))$$

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

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

Let ℓ denote the greatest zero of g. Then $z(x,t) \leq \ell$ if $W(x) \leq \ell$. On the other hand, if $W(x) > \ell$, then z is decreasing and satisfies

$$t = \int_{z(x,t)}^{W(x)} \frac{ds}{g(s)} \leq \int_{z(x,t)}^{\infty} \frac{ds}{g(s)}. \tag{2.8}$$

This inequality easily yields that for every $a > 0$ there is a constant $C(a)$ such that $z(x,t) \leq C(a)$ for every $t \geq a$ and $x \in \mathbf{R}^N$. □

Next, we state a condition under which certain exponentials are Lyapunov functions. When dealing with Lyapunov functions, what is relevant is the behaviour as $|x| \to \infty$, hence we shall frequently give explicit formulae that could be singula at some point, but can be smoothed in an arbitrary way to fulfill the C^2 hypothesis.

Proposition 2.7 *Assume that*

$$\liminf_{|x|\to\infty} \frac{V(x)}{|x|^\beta} \geq c > 0, \tag{2.9}$$

for some $\beta > 0$. Then $W(x) = \exp\{\delta|x|^{1+\beta/2}\}$ (smoothed near $x = 0$) is a Lyapunov function for $0 < \delta < 2\sqrt{c}/(\beta+2)$. Moreover, if $\beta > 2$, there exist positive constants c_1, c_2 such that

$$\zeta(x,t) \leq c_1 \exp\left\{c_2 t^{-\frac{\beta+2}{\beta-2}}\right\} \tag{2.10}$$

for $x \in \mathbf{R}^N,\ t > 0$.

Proof. Let $W(x) = \exp\{\delta|x|^{1+\beta/2}\}$. We obtain, by a straightforward computation,

$$\begin{aligned} -HW(x) &= \delta(\beta+2)|x|^{\frac{\beta}{2}} e^{\delta|x|^{1+\frac{\beta}{2}}} \left(\frac{2N+\beta-2}{2|x|} + \frac{\delta(\beta+2)}{2}|x|^{\frac{\beta}{2}} - \frac{2V(x)}{\delta(\beta+2)|x|^{\frac{\beta}{2}}}\right) \\ &\leq C_1|x|^{\frac{\beta}{2}} e^{\delta|x|^{1+\frac{\beta}{2}}} \left(1 + \left(\frac{\delta(\beta+2)}{2} - \frac{2c}{\delta(\beta+2)}\right)|x|^{\frac{\beta}{2}}\right) \\ &\leq -C_2|x|^{\beta} e^{\delta|x|^{1+\frac{\beta}{2}}} \leq 0 \end{aligned}$$

for $|x|$ large. This shows that W is a Lyapunov function. Finally, if $\beta > 2$ it follows that $HW \geq g(W)$ with $g(s) = C_3 s(\log s)_+^{(2\beta)/(\beta+2)} - C_4$, for suitable $C_3, C_4 > 0$. Then Proposition 2.6 yields the boundedness of $\zeta(\cdot,t)$. To obtain (2.10) we recall that $\zeta \leq z$ where z satisfies (2.8). If ℓ denotes the zero of g and $z(x,t) \leq 2\ell$ we have simply to choose a suitable c_1. If $z(x,t) \geq 2\ell$, then

$$t \leq \int_z^\infty \frac{ds}{g(s)} \leq C_5 \int_z^\infty \frac{ds}{s(\log s)^{(2\beta)/(\beta+2)}} \leq C_6(\log z)^{(2-\beta)/(\beta+2)}$$

and (2.10) follows. □

The right hand side of (2.10) becomes very big as $t \to 0$. In order to have a milder behaviour we investigate when polynomials are Lyapunov functions.

Proposition 2.8 *Assume that condition (2.9) holds for some $\beta > 0$. Then $W(x) = \left(1 + |x|^2\right)^\alpha$ is a Lyapunov function for every $\alpha > 0$ and there exists a positive constant c such that*

$$\zeta(x,t) \le c t^{-(2\alpha)/\beta} \tag{2.11}$$

for $x \in \mathbf{R}^N,\ 0 < t \le 1$.

Proof. We have

$$\begin{aligned} -HW(x) &= \left(1+|x|^2\right)^\alpha \left(\frac{2\alpha N}{1+|x|^2} + \frac{4\alpha(\alpha-1)|x|^2}{(1+|x|^2)^2} - V(x) \right) \\ &\le -C_1 \left(1+|x|^2\right)^{\alpha+\beta/2} = -C_1 W^\gamma \end{aligned}$$

for $|x|$ large and $\gamma = 1 + \beta/(2\alpha) > 1$. This shows that $HW \ge g(W)$ with $g(s) = C_2 s^\gamma - C_3$ for suitable $C_2, C_3 > 0$. Proceeding as in the proof of (2.10) one shows (2.11), the only difference being that the function $t^{-(2\alpha)/\beta}$ goes to 0 as $t \to +\infty$, and then the estimate is not true, in general, for all $t > 0$. □

An inspection of the above proof shows that polynomials are Lyapunov functions for H when V has only a logarithmic behaviour at infinity. The proof is similar to that of the two propositions above.

Proposition 2.9 *Assume that*

$$\liminf_{|x|\to\infty} \frac{V(x)}{(\log|x|)^\beta} > 0 \tag{2.12}$$

for some $\beta > 1$. Then $W(x) = \left(1+|x|^2\right)^\alpha$ is a Lyapunov function for every $\alpha > 0$ and there exist positive constants c_1, c_2 such that

$$\zeta(x,t) \le c_1 \exp\left\{ c_2 t^{-\frac{1}{\beta-1}} \right\} \tag{2.13}$$

for $x \in \mathbf{R}^N,\ t > 0$.

3 Pointwise bounds on kernels

To obtain pointwise bounds on p we need the following assumption depending on suitable weight functions.

(H1) (a) $0 \le V \in C^1(\mathbf{R}^N)$ and for every $\gamma > 0$ there exists $C_\gamma > 0$ such that $|DV| \le \gamma V^{\frac{3}{2}} + C_\gamma$.

(b1) $0 < \omega \in C^2(\mathbf{R}^N)$ is a Lyapunov function such that for every $\gamma > 0$ there exists $C_\gamma > 0$ such that

$$\frac{|D\omega|^2}{\omega^2} + \frac{|\Delta\omega|}{\omega} \le \gamma V + C_\gamma.$$

(b2) $0 < \omega \in C^2(\mathbf{R}^N)$ verifies the inequality

$$\frac{|D\omega|^2}{\omega^2} + \frac{|\Delta\omega|}{\omega} \le \gamma V + C_\gamma$$

for some $\gamma, C_\gamma > 0$ and moreover there are $k > (N+2)/2$ and a Lyapunov function $\tilde\omega$ such that $(1 + V^k)\omega \le \tilde\omega$.

We denote by ζ_ω and $\zeta_{\tilde{\omega}}$ the function defined by (2.1) and relative to ω, $\tilde{\omega}$, respectively, and fix $0 < a_0 < a < b < b_0 < T$ assuming that $b_0 - b \geq a - a_0$. In all the proofs of this section the variable x is used as a parameter and hence all differential operators in the space variable act with respect to y. For simplicity we write Δ for Δ_y and so on. The following statement contains two similar estimates: one is obtained assuming (H1)(a) and (b1) and will be used in Example 3.3, the other is obtained assuming (H1)(a) and (b2) and will be used in Example 3.4.

Theorem 3.1

(i) Assume (H1)(a), (b1). *Then*

$$\omega(y)p(x,y,t) \leq \frac{C}{(a-a_0)^{\frac{N+2}{2}}} \int_{a_0}^{b_0} \zeta_\omega(x,t)\, dt \tag{3.1}$$

for $a \leq t \leq b$ and $y \in \mathbf{R}^N$. Moreover

$$\|\omega p\|_{W_k^{2,1}(Q(a,b))} + \|V\omega p\|_{L^k(Q(a,b))} \leq \frac{C}{(a-a_0)^{\frac{N}{2}(1-\frac{1}{k})+2-\frac{1}{k}}} \int_{a_0}^{b_0} \zeta_\omega(x,t)\, dt \tag{3.2}$$

if $k > (N+2)/2$.

(ii) Assume (H1)(a), (b2). *Then*

$$\omega(y)p(x,y,t) \leq \frac{C}{(a-a_0)^{\frac{N+2}{2}}} \int_{a_0}^{b_0} \zeta_{\tilde{\omega}}(x,t)\, dt \tag{3.3}$$

for $a \leq t \leq b$ and $y \in \mathbf{R}^N$. Moreover

$$\|\omega p\|_{W_k^{2,1}(Q(a,b))} + \|V\omega p\|_{L^k(Q(a,b))} \leq \frac{C}{(a-a_0)^{\frac{N}{2}(1-\frac{1}{k})+2-\frac{1}{k}}} \int_{a_0}^{b_0} \zeta_{\tilde{\omega}}(x,t)\, dt \tag{3.4}$$

where k is the parameter in (H1)(b2).

Proof of (i). First observe that, since p satisfies Gaussian estimates, it belongs to $L^k(Q(a,b))$ for every $1 < k < \infty$. Let η be a smooth function such that $\eta(t) = 1$ for $a \leq t \leq b$ and $\eta(t) = 0$ for $t \leq a_0$ and $t \geq b_0$, $0 \leq |\eta'| \leq \frac{2}{a-a_0}$ and set $q = \eta^k p$. Then q belongs to $L^k(Q_T) \cap W_k^{2,1}(B_R \times [0,T])$ for every $R > 0$ and solves the parabolic problem

$$\begin{cases} \partial_t q - \Delta q + Vq = k\eta^{k-1}p\eta_t & \text{in } Q_T \\ q(y,0) = 0 & y \in \mathbf{R}^N. \end{cases}$$

Since both q and the right hand side belong to $L^k(Q_T)$, then $q \in W_k^{2,1}(Q_T)$ and $Vq \in L^k(Q_T)$, by Theorem 5.2. In particular $V^{\frac{1}{2}}Dq \in L^k(Q_T)$, by Lemma 5.1.

Set $\omega_\varepsilon = \omega/(1+\varepsilon\omega)$. Since

$$\frac{D\omega_\varepsilon}{\omega_\varepsilon} = \frac{D\omega}{\omega(1+\varepsilon\omega)}, \quad \frac{\Delta\omega_\varepsilon}{\omega_\varepsilon} = \frac{\Delta\omega}{\omega(1+\varepsilon\omega)} - \frac{2\varepsilon}{(1+\varepsilon\omega)^2}\frac{|D\omega|^2}{\omega},$$

then ω_ε satisfies (H1)(b1) with the same constants C_γ as ω.

The function $\omega_\varepsilon q$ satisfies

$$\begin{cases} \partial_t(\omega_\varepsilon q) - \Delta(\omega_\varepsilon q) = -V\omega_\varepsilon q + k\eta^{k-1}p\omega_\varepsilon\eta_t - q\Delta\omega_\varepsilon - 2D\omega_\varepsilon \cdot Dq & \text{in } Q_T \\ \omega_\varepsilon(y)q(y,0) = 0 & y \in \mathbf{R}^N. \end{cases}$$

Observe that $V\omega_\varepsilon q$ belongs to $L^k(Q_T)$, since ω_ε is bounded and $Vq \in L^k(Q_T)$. Similarly, the second and the third term in the right hand side of the equation above are in $L^k(Q_T)$, using (H1). Concerning the last term we have

$$|D\omega_\varepsilon \cdot Dq| \le C\omega_\varepsilon\big(1+V^{\frac{1}{2}}\big)|Dq|$$

and hence it belongs to $L^k(Q_T)$, too. This implies that $\omega_\varepsilon q$ belongs to $W^{2,1}_k(Q_T)$. Since

$$D\omega_\varepsilon \cdot Dq = \frac{D\omega_\varepsilon}{\omega_\varepsilon}\cdot D(\omega_\varepsilon q) - \frac{|D\omega_\varepsilon|^2}{\omega_\varepsilon} q,$$

we rewrite the above equation in the following form that allows us to apply Theorem 5.2.

$$\begin{cases} \partial_t(\omega_\varepsilon q) - \Delta(\omega_\varepsilon q) + V\omega_\varepsilon q = k\eta^{k-1}p\omega_\varepsilon\eta_t - 2\frac{D\omega_\varepsilon}{\omega_\varepsilon}D(\omega_\varepsilon q) - q\Delta\omega_\varepsilon + 2\frac{|D\omega_\varepsilon|^2}{\omega_\varepsilon}q & \text{in } Q_T \\ \omega_\varepsilon(y)q(y,0) = 0 & y \in \mathbf{R}^N. \end{cases} \tag{3.5}$$

We fix $k > (N+2)/2$ and estimate the L^k-norm of the right hand side above. We have

$$\|\eta^{k-1}p\omega_\varepsilon\eta_t\|_{L^k(Q_T)} \le \frac{C}{a-a_0}\|\omega_\varepsilon q\|^{\frac{k-1}{k}}_{L^\infty(Q_T)}\left(\int_{Q(a_0,b_0)}\omega p\right)^{\frac{1}{k}}$$

and

$$\left\|q\left(\Delta\omega_\varepsilon - 2\frac{|D\omega_\varepsilon|^2}{\omega_\varepsilon}\right)\right\|_{L^k(Q_T)} \le \gamma\|V\omega_\varepsilon q\|_{L^k(Q_T)} + C_\gamma\|\omega_\varepsilon q\|^{\frac{k-1}{k}}_{L^\infty(Q_T)}\left(\int_{Q_T}\omega q\right)^{\frac{1}{k}}.$$

Moreover, using Lemma 5.1 with $\sigma = 1$ and the interpolative inequality

$$\|D(\omega_\varepsilon q)\|_{L^k(Q_T)} \le \delta\|\omega_\varepsilon q\|_{W^{2,1}_k(Q_T)} + C_\delta\|\omega_\varepsilon q\|_{L^k(Q_T)} \qquad \forall\ \delta > 0$$

we get

$$\begin{aligned}\left\|\frac{D\omega_\varepsilon}{\omega_\varepsilon}D(\omega_\varepsilon q)\right\|_{L^k(Q_T)} &\le \gamma\|V^{\frac{1}{2}}D(\omega_\varepsilon q)\|_{L^k(Q_T)} + C_\gamma\|D(\omega_\varepsilon q)\|_{L^k(Q_T)} \\ &\le C\gamma\left(\|\omega_\varepsilon q\|_{W^{2,1}_k(Q_T)} + \|V\omega_\varepsilon q\|_{L^k(Q_T)}\right) \\ &\quad + C_\gamma\left(\delta\|\omega_\varepsilon q\|_{W^{2,1}_k(Q_T)} + C_\delta\|\omega_\varepsilon q\|_{L^k(Q_T)}\right). \end{aligned} \tag{3.6}$$

Therefore, setting

$$\Lambda = \frac{C}{a-a_0}\left(\int_{Q(a_0,b_0)}\omega p\right)^{\frac{1}{k}} = \frac{C}{a-a_0}\left(\int_{a_0}^{b_0}\zeta_\omega(x,t)\,dt\right)^{\frac{1}{k}}$$

we obtain from Theorem 5.2

$$\begin{aligned}\|\omega_\varepsilon q\|_{W^{2,1}_k(Q_T)} + \|V\omega_\varepsilon q\|_{L^k(Q_T)} &\le C\Bigg(\|\omega_\varepsilon q\|^{\frac{k-1}{k}}_{L^\infty(Q_T)}\Lambda(1+C_\gamma+C_\gamma C_\delta) \\ &\quad + (\gamma + C_\gamma\delta)\|\omega_\varepsilon q\|_{W^{2,1}_k(Q_T)} + \gamma\|V\omega_\varepsilon q\|_{L^k(Q_T)}\Bigg),\end{aligned}$$

with C independent of ε. Choosing first a small γ and then a small δ we obtain

$$\|\omega_\varepsilon q\|_{W^{2,1}_k(Q_T)} + \|V\omega_\varepsilon q\|_{L^k(Q_T)} \le C\|\omega_\varepsilon q\|^{\frac{k-1}{k}}_{L^\infty(Q_T)}\Lambda. \tag{3.7}$$

Now we use the interpolative estimate (see Proposition 5.4)

$$\|\omega_\varepsilon q\|_{L^\infty(Q_T)} \le C\|\omega_\varepsilon q\|_{L^1(Q_T)}^{1-\theta}\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)}^{\theta}$$

with

$$\theta = \frac{N+2}{(N+2)(1-1/k)+2}$$

to obtain

$$\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)} \le C\|\omega_\varepsilon q\|_{L^1(Q_T)}^{\left(1-\frac{N+2}{2k}\right)\left(1-\frac{1}{k}\right)}\Lambda^{\frac{(N+2)(1-\frac{1}{k})+2}{2}} \le C\|\omega q\|_{L^1(Q_T)}^{\left(1-\frac{N+2}{2k}\right)\left(1-\frac{1}{k}\right)}\Lambda^{\frac{(N+2)(1-\frac{1}{k})+2}{2}}.$$

Using again the interpolative estimate above we finally get

$$\|\omega_\varepsilon q\|_{L^\infty(Q_T)} \le C\|\omega_\varepsilon q\|_{L^1(Q_T)}^{1-\theta}\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)}^{\theta} \le C\|\omega q\|_{L^1(Q_T)}^{1-\frac{N+2}{2k}}\Lambda^{\frac{N+2}{2}}$$

and, estimating the integrals of ωq through the function ζ_ω, we obtain

$$\omega_\varepsilon(y)p(x,y,t) \le \frac{C}{(a-a_0)^{\frac{N+2}{2}}}\int_{a_0}^{b_0}\zeta_\omega(x,t)\,dt$$

for $a \le t \le b$ and $y \in \mathbf{R}^N$. Since the above constant C does not depend on ε, letting $\varepsilon \to 0$ we conclude the proof of the pointwise estimate (3.1).

To prove (3.2) we use (3.7) to get

$$\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)} + \|V\omega_\varepsilon q\|_{L^k(Q_T)} \le \frac{C}{(a-a_0)^{\frac{N}{2}\left(1-\frac{1}{k}\right)+2-\frac{1}{k}}}\int_{a_0}^{b_0}\zeta_\omega(x,t)\,dt.$$

Since $\omega_\varepsilon q \to \omega q$, $V\omega_\varepsilon q \to V\omega q$ in $L^k(Q_T)$, by the above estimate and a weak compactness argument we conclude the proof of (i).

Proof of (ii). We follow essentially the same path as for (i), with the difference that the constant γ is not arbitrary, but fixed in (b2). Therefore, we use the arbitrariness of σ in Lemma 5.1, obtaining the inequality

$$\begin{aligned}\left\|\frac{D\omega_\varepsilon}{\omega_\varepsilon}D(\omega_\varepsilon q)\right\|_{L^k(Q_T)} &\le C\gamma\left(\sigma\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)} + \frac{c}{\sigma}\|V\omega_\varepsilon q\|_{L^k(Q_T)}\right)\\ &\quad + C_\gamma\left(\delta\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)} + C_\delta\|\omega_\varepsilon q\|_{L^k(Q_T)}\right)\end{aligned} \tag{3.8}$$

in place of (3.6). Setting

$$\tilde\Lambda = \frac{C}{a-a_0}\left(\int_{Q(a_0,b_0)}\tilde\omega p\right)^{\frac{1}{k}} = \frac{C}{a-a_0}\left(\int_{a_0}^{b_0}\zeta_{\tilde\omega}(x,t)\,dt\right)^{\frac{1}{k}}$$

and using the estimate $\omega \le \tilde\omega$, we obtain

$$\begin{aligned}\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)} &\le C\Big[\|\omega_\varepsilon q\|_{L^\infty(Q_T)}^{\frac{k-1}{k}}\tilde\Lambda + (1+C_\gamma+C_\gamma C_\delta)(\gamma\sigma + C_\gamma\delta)\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)}\\ &\quad + \Big(\gamma + \frac{c}{\sigma}\Big)\|V\omega_\varepsilon q\|_{L^k(Q_T)}\Big].\end{aligned}$$

Choosing δ and σ small enough and using the inequalities

$$\|V\omega_\varepsilon q\|_{L^k(Q_T)} \le \|\omega_\varepsilon q\|_{L^\infty(Q_T)}^{\frac{k-1}{k}}\tilde\Lambda$$

and $V^k\omega \le \tilde\omega$, we deduce

$$\|\omega_\varepsilon q\|_{W_k^{2,1}(Q_T)} \le C\|\omega_\varepsilon q\|_{L^\infty(Q_T)}^{\frac{k-1}{k}}\tilde\Lambda$$

instead of (3.7). From now on, the proof of (i) can be repeated. □

Choosing $k > N+2$ we obtain a pointwise estimate for Dp, see also the next section for further estimates of the derivatives of p.

Proposition 3.2 *Assume* (H1)(a),(b1) *and suppose moreover that* $|D\omega| \le C\omega$ *for a suitable* $C > 0$. *Then*

$$\omega(y)|Dp(x,y,t)| \le \frac{C}{(a-a_0)^{\frac{N+3}{2}}} \int_{a_0}^{b_0} \zeta_\omega(x,t)\, dt$$

for $a \le t \le b$ *and* $y \in \mathbf{R}^N$.

Proof. We apply Theorem 3.1(i) with $k > N+2$ and we use the interpolative estimate

$$\|D(\omega q)\|_{L^\infty(Q_T)} \le C\|\omega q\|_{L^1(Q_T)}^{1-\eta} \|\omega q\|_{W_k^{2,1}(Q_T)}^{\eta}$$

with

$$\eta = \frac{N+3}{(N+2)(1-1/k)+2}.$$

The result then follows by an explicit computation and estimating the L^1-norm of ωq through ζ_ω. □

Let us present now some examples. In the first we use part (i) of Theorem 3.1, in the second part (ii).

Example 3.3 Assume that condition (2.9) holds. We fix $\alpha > 0$ and consider the Lyapunov function $\omega(y) = (1+|y|^2)^\alpha$. We apply Theorem 3.1(i) with $a_0 = t/2, a = t, b_0 = 2t$ and deduce, using Proposition 2.8,

$$p(x,y,t) \le \frac{C}{t^{\frac{N}{2}+\frac{2\alpha}{\beta}}}(1+|y|^2)^{-\alpha}$$

for $0 < t \le 1$. Since p is symmetric with respect to x, y, we get

$$p(x,y,t) \le \frac{C}{t^{\frac{N}{2}+\frac{2\alpha}{\beta}}}(1+|x|^2)^{-\frac{\alpha}{2}}(1+|y|^2)^{-\frac{\alpha}{2}}, \quad 0 < t \le 1. \tag{3.9}$$

Let us show now that this estimate is precise with respect to t, following the method of [2, Theorem 4.5.10]. Assuming that $V(x) = |x|^\beta$ and that

$$p(x,y,t) \le c(t)(1+|x|^2)^{-\frac{\alpha}{2}}(1+|y|^2)^{-\frac{\alpha}{2}}.$$

Choose $|x_0| \ge 1$ and consider the ball $B_1(x_0)$ of centre x_0 and radius 1. We denote by H_0 the operator H with Dirichlet boundary conditions in $B_1(x_0)$. Since $V \le c|x_0|^\beta$ in $B_1(x_0)$, with c independent of x_0, the maximum principle yields

$$e^{-tH} \ge e^{-tH_0} \ge e^{-tc|x_0|^\beta} e^{t\Delta_{B_1(x_0)}},$$

as operators acting on $L^2(B_1(x_0))$ and where the Laplacian is considered with Dirichlet boundary conditions. Considering the corresponding kernels and using the estimate $p_0(x_0,x_0,t) \ge ct^{-N/2}$, see [2, Lemma 3.3.3], where p_0 is the kernel of the Dirichlet Laplacian in $B_1(x_0)$, we obtain

$$t^{-\frac{N}{2}} e^{-tc|x_0|^\beta} \le p(x_0,x_0,t) \le c(t)(1+|x_0|^2)^{-\alpha}.$$

Choosing $|x_0|^\beta = t^{-1}$ it follows that

$$c(t) \ge \frac{C}{t^{\frac{N}{2}+\frac{2\alpha}{\beta}}}$$

for small t.

We notice that estimate (3.9) can be deduced also from [7, Theorem 1.2]. With the notation there, $\mu = N$ and it is possible to choose $\xi = \eta = (1+|x|^2)^{-\alpha/2}$, $\alpha > 0$. An elementary computation gives then $\nu = 4\alpha/\beta$ and (3.9) follows.

Example 3.4 Assume now that condition (2.9) holds for some $\beta > 2$. We apply Theorem 3.1(ii) with $a_0 = t/2, a = t, b_0 = 2t$, $\omega(y) = \exp\left\{\delta|y|^{1+\beta/2}\right\}$, $\tilde{\omega}(y) = \exp\left\{\delta'|y|^{1+\beta/2}\right\}$, with $\delta < \delta' < 2\sqrt{c}/(\beta+2)$. Notice that (H1)(b2) holds with $\gamma > 2\delta^2(1+\beta/2)^2$. Using Proposition 2.7 (and neglecting negative powers of t which can be included in the exponential below, changing the constant c), we obtain $p(x,y,t) \le c(t)\phi(y)$, where

$$c(t) = \exp\left\{ct^{-\frac{\beta+2}{\beta-2}}\right\}, \qquad \phi(y) = \exp\left\{-\delta|y|^{1+\beta/2}\right\}$$

Using the symmetry of p in x, y and proceeding as above one would only obtain $p(x,y,t) \le c(t)\sqrt{\phi(x)\phi(y)}$. This was not a problem in the example above since all polynomials were Lyapunov functions, whereas, in the present situation, we have an upper bound on δ'. To get a better estimate we proceed as follows.

Using the symmetry of p with respect to the variables x, y we have $p(x,y,t) \le c(t)\phi(x)$. Then we get $p(z,y,t) \le c(t)\phi(z)^\alpha\phi(y)^{1-\alpha}$ for every $0 < \alpha < 1$ and, by the semigroup law,

$$\begin{aligned} p(x,y,t) = \int_{\mathbf{R}^N} p(x,z,\frac{t}{2})p(z,y,\frac{t}{2})\,dz &\le c(t/2)^2\phi(x)\phi(y)^{1-\alpha}\int_{\mathbf{R}^N}\phi(z)^\alpha\,dz \\ &= K_1 c(t/2)^2\phi(x)\phi(y)^{1-\alpha}. \end{aligned}$$

Finally

$$\begin{aligned} p(x,y,t) = \int_{\mathbf{R}^N} p(x,z,\frac{t}{2})p(z,y,\frac{t}{2})\,dz &\le K_1 c(t/2)c(t/4)^2\phi(x)\phi(y)\int_{\mathbf{R}^N}\phi(z)^{1-\alpha}\,dz \\ &\le c_1(t)\phi(x)\phi(y), \end{aligned}$$

with $c_1(t) = \exp\left\{c_1 t^{-\frac{\beta+2}{\beta-2}}\right\}$ for a suitable $c_1 > 0$.

This estimate is similar to [2, Corollary 4.5.5] where, however, the result is more precise with respect to the spatial variables, the choice of ϕ as the ground state of H being possible (in particular the limit case $\delta = 2\sqrt{c}/(\beta+2)$ is allowed).

Also in this case we prove that the estimate above is precise, concerning the function $c(t)$, for $V(x) = |x|^\beta$. Proceeding as in Example 3.3 we find the inequality

$$c(t) \ge t^{-\frac{N}{2}}\exp\left\{-ct|x|^\beta + 2\delta|x|^{1+\frac{\beta}{2}}\right\}$$

for large $|x|$. Setting $|x| = Mt^{-2/(\beta-2)}$ it follows that

$$c(t) \ge t^{-\frac{N}{2}}\exp\left\{-cM^\beta + 2\delta M^{1+\frac{\beta}{2}}\right\}t^{-\frac{\beta+2}{\beta-2}}.$$

Since $\beta > 2$ the bracket is negative for large M and the estimate $c(t) \ge \exp\left\{ct^{-\frac{\beta+2}{\beta-2}}\right\}$ follows for a suitable $c > 0$.

Example 3.5 Assume now that condition (2.12) holds. Proceeding as above and using Proposition 2.9 we obtain

$$p(x,y,t) \le \exp\left\{ct^{-\frac{1}{\beta-1}}\right\}(1+|x|^2)^{-\frac{\alpha}{2}}(1+|y|^2)^{-\frac{\alpha}{2}}.$$

The same method as in the example above shows that the behaviour with respect to the time variable is precise also in this case.

4 Estimates for derivatives of kernels

Estimates for the first order derivatives of p with respect to the variable y have been already obtained in Proposition 3.2 where the weight was assumed at most of exponential type. Estimates for $D_{yy}p$ or for $\partial_t p$ can be obtained with similar methods, differentiating the equation satisfied by p and assuming more regularity on V. We prefer here to follow a functional analytic approach based on [2, Chapter 4], that gives quite precise results in the examples discussed at the end of the previous section.

We assume the following condition, which holds in all the examples of Section 3.

(H2) The kernel p satisfies the estimate

$$p(x,y,t) \le c(t)\phi(x)\phi(y)$$

for $0 < t \le T$, $x, y \in \mathbf{R}^N$, a suitable non increasing function c and a positive function ϕ such that $\omega = 1/\phi$ is a Lyapunov function for H.

We consider the Hilbert space $L^2(\phi^2)$ of all measurable functions in $\mathbf{R}^N$ which are square integrable with respect to the measure $\phi^2(y)\,dy$. The map

$$U : L^2(\phi^2) \to L^2(\mathbf{R}^N), \qquad Uf = \phi f$$

is an isometry with inverse

$$U^* = U^{-1} : L^2(\mathbf{R}^N) \to L^2(\phi^2), \qquad U^{-1}g = \phi^{-1}g.$$

The operator $H_1 = U^{-1}HU$ is self-adjoint in $L^2(\phi^2)$ and $e^{-tH_1} = U^{-1}e^{-tH}U$. It is elementary to check that the integral kernel of the operator e^{-tH_1} with respect to the measure $\phi^2(y)\,dy$ is given by $p(x,y,t)\phi^{-1}(x)\phi^{-1}(y)$ so that (H2) can be restated in an equivalent way by saying that e^{-tH_1} can be extended to a bounded operator from $L^1(\phi^2)$ to $L^\infty(\mathbf{R}^N)$ whose norm does not exceed $c(t)$.

Lemma 4.1 *Assume* (H2). *Then there exists a constant $K > 0$ such that for every $0 < t \le T$ and $f \in L^1(\mathbf{R}^N)$*

$$\|U^{-1}e^{-tH}Uf\|_{L^1(\mathbf{R}^N)} \le K\|f\|_{L^1(\mathbf{R}^N)}.$$

Proof. Indeed, by Proposition 2.5 and since p is symmetric in x, y, we have

$$\int_{\mathbf{R}^N} p(x,y,t)\phi^{-1}(x)\,dx \le e^{\lambda t}\phi^{-1}(y)$$

and therefore

$$\begin{aligned}\int_{\mathbf{R}^N}\left|\int_{\mathbf{R}^N}\phi^{-1}(x)p(x,y,t)\phi(y)f(y)\,dy\right|dx &\le \int_{\mathbf{R}^N}\phi(y)|f(y)|\,dy\int_{\mathbf{R}^N}p(t,x,y)\phi^{-1}(x)\,dx \\ &\le e^{\lambda t}\int_{\mathbf{R}^N}|f(y)|\,dy.\end{aligned}$$

□

Proposition 4.2 *Assume* (H2). *Then there exists a constant $K > 0$ such that, for all $z \in \mathbf{C}$ with $0 < \operatorname{Re} z \le T$,*

$$|p(x,y,z)| \le Kc(\operatorname{Re} z/2)\phi(x)\phi(y), \quad x,\, y \in \mathbf{R}^N.$$

Proof. Let $z = t + is$ with $0 < t \le T$. Then

$$U^{-1}e^{-zH}U = U^{-1}e^{-\frac{t}{2}H}UU^{-1}e^{-isH}UU^{-1}e^{-\frac{t}{2}H}U.$$

From (H2) we have

$$\|U^{-1}e^{-\frac{t}{2}H}U\|_{L^1(\phi^2)\to L^\infty(\mathbf{R}^N)} \le c(t/2)$$

and

$$\|U^{-1}e^{-\frac{t}{2}H}U\|_{L^\infty(\mathbf{R}^N)\to L^\infty(\mathbf{R}^N)} \le K$$

for $0 < t \le T$, by Lemma 4.1 since the operator is self-adjoint. Thus the Riesz-Thorin theorem yields

$$\|U^{-1}e^{-\frac{t}{2}H}U\|^2_{L^2(\phi^2)\to L^\infty(\mathbf{R}^N)} \le Kc(t/2).$$

Now, since the norm of $U^{-1}e^{-isH}U$, as an operator from $L^2(\phi^2)$ to itself, is 1, and $U^{-1}e^{-\frac{t}{2}H}U$ is self-adjoint, we infer

$$\begin{aligned}\|U^{-1}e^{-zH}U\|_{L^1(\phi^2)\to L^\infty(\mathbf{R}^N)} &\le \|U^{-1}e^{-\frac{t}{2}H}U\|^2_{L^2(\phi^2)\to L^\infty(\mathbf{R}^N)}\\ &\le Kc(t/2)\end{aligned}$$

and the statement follows. □

Theorem 4.3 *Under assumption* (H2) *the estimate*

$$|\partial_t^n p(x,y,t)| \le \frac{K2^n n!}{t^n}c(t/4)\phi(x)\phi(y)$$

holds for $0 < t \le T$, $x, y \in \mathbf{R}^N$, $n \in \mathbf{N}$ *and a suitable* $K > 0$.

Proof. The proof follows by the Cauchy estimates of the derivatives of holomorphic functions, applying Proposition 4.2 to the ball of centre t and radius $t/2$ in the complex plane. □

Finally we prove pointwise estimates for Δp.

Theorem 4.4 *Assume* (H2) *and also that* V *satisfies* (H1)(a) *and* $\omega = 1/\phi$ *satisfies* (H1)(b1). *Then*

$$|\Delta_x p(x,y,t)| + |\Delta_y p(x,y,t)| + (V(x)+V(y))\,p(x,y,t) \le \frac{K_1}{t}c(t/4)\phi(x)\phi(y) \tag{4.1}$$

for $0 < t \le T$, $x, y \in \mathbf{R}^N$ *and a suitable* $K_1 > 0$.

Proof. Set $c_1(t) = (2K/t)c(t/4)$, where K is the constant given by Theorem 4.3. Since p is symmetric in x, y, then $\Delta_x p(x,y,t) = \Delta_y p(y,x,t)$ and therefore it suffices to prove only the estimates for $\Delta_y p(x,y,t)$ and $V(y)p(x,y,t)$. Let us fix $x \in \mathbf{R}^N$, $t > 0$. Then $p(x,\cdot,t) \in C_0(\mathbf{R}^N)$ satisfies $\Delta_y p - Vp = \partial_t p$. Since $\partial_t p \in C_0(\mathbf{R}^N)$, by Theorem 4.3, Theorem 5.3 yields $\Delta_y p, Vp \in C_0(\mathbf{R}^N)$. Let $\omega = 1/\phi$, $\omega_\varepsilon = \omega/(1+\varepsilon\omega)$. Then we have, see (3.5),

$$-\Delta(\omega_\varepsilon p) + V\omega_\varepsilon p = -2\frac{D\omega_\varepsilon}{\omega_\varepsilon}D(\omega_\varepsilon p) - p\Delta\omega_\varepsilon + 2\frac{|D\omega_\varepsilon|^2}{\omega_\varepsilon}p - \partial_t(\omega_\varepsilon p). \tag{4.2}$$

Clearly $\omega_\varepsilon p \in C_0(\mathbf{R}^N) \cap W^{2,p}_{\rm loc}(\mathbf{R}^N)$ for every $p < \infty$ and $V\omega_\varepsilon p \in C_0(\mathbf{R}^N)$, since ω_ε is bounded. Let us verify that $\Delta(\omega_\varepsilon p) \in C_0(\mathbf{R}^N)$. Since ω_ε is bounded, $\omega_\varepsilon \Delta p \in C_0(\mathbf{R}^N)$, and $p\Delta\omega_\varepsilon \in C_0(\mathbf{R}^N)$ because it is pointwise dominated (using (H1)) by $V\omega_\varepsilon p$. Finally,

$$\begin{aligned}\|D\omega_\varepsilon \cdot Dp\|_{L^\infty(\mathbf{R}^N)} &\le C\left(\|V^{1/2}\omega_\varepsilon Dp\|_{L^\infty(\mathbf{R}^N)} + \|\omega_\varepsilon Dp\|_{L^\infty(\mathbf{R}^N)}\right)\\ &\le \frac{C}{\varepsilon}\left(\|Vp\|_{L^\infty(\mathbf{R}^N)} + \|\Delta p\|_{L^\infty(\mathbf{R}^N)} + \|Dp\|_{L^\infty(\mathbf{R}^N)}\right),\end{aligned}$$

by [11, Proposition 2.3] and hence $D\omega_\varepsilon \cdot Dp \in C_0(\mathbf{R}^N)$. Thus $\Delta(\omega_\varepsilon p) = \omega_\varepsilon \Delta p + p\Delta\omega_\varepsilon + 2D\omega_\varepsilon \cdot Dp \in C_0(\mathbf{R}^N)$. We now apply Theorem 5.3 and from (4.2), using (H1), Theorem 4.3 and the inequality $\omega_\varepsilon \leq \omega$, we obtain

$$\begin{aligned} \|\Delta(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + \|V\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)} \leq\ & C\Big(C_\gamma c(t)\phi(x) + \gamma\|V\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)} + c_1(t)\phi(x) \\ & +\gamma\|V^{\frac{1}{2}}D(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + C_\gamma\|D(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)}\Big). \end{aligned} \tag{4.3}$$

Since

$$\|V^{\frac{1}{2}}D(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} \leq C\left(\|\Delta(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + \|V\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)}\right), \tag{4.4}$$

by [11, Proposition 2.3], and

$$\|D(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} \leq C\|\Delta(\omega_\varepsilon p)\|^{\frac{1}{2}}_{L^\infty(\mathbf{R}^N)}\|\omega_\varepsilon p\|^{\frac{1}{2}}_{L^\infty(\mathbf{R}^N)},$$

choosing γ small enough we obtain

$$\|\Delta(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + \|V\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)} \leq Cc_1(t)\phi(x).$$

Letting $\varepsilon \to 0$ we immediately obtain $V(y)\omega(y)p(x,y,t) \leq Cc_1(t)\phi(x)$. Moreover, writing again

$$\Delta(\omega_\varepsilon p) = \omega_\varepsilon\Delta p + 2\frac{D\omega_\varepsilon}{\omega_\varepsilon}\cdot D(\omega_\varepsilon p) + p\left(\Delta\omega_\varepsilon - 2\frac{|D\omega_\varepsilon|^2}{\omega_\varepsilon}\right)$$

we obtain

$$\begin{aligned} \|\omega_\varepsilon\Delta p\|_{L^\infty(\mathbf{R}^N)} \leq\ & \|\Delta(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + C\|V\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)} + \\ & C\left(\|V^{\frac{1}{2}}D(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + \|\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)}\right) \\ \leq\ & C\left(\|\Delta(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + \|V\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)} + \|\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)}\right) \leq Cc_1(t)\phi(x) \end{aligned}$$

and the thesis follows letting $\varepsilon \to 0$. □

Corollary 4.5 *Under the assumptions of the previous theorem we have also*

$$|D_y p(x,y,t)| + |D_x p(x,y,t)| \leq \frac{K}{\sqrt{t}}c(t/4)\phi(x)\phi(y) \tag{4.5}$$

$0 < t \leq T$, $x, y \in \mathbf{R}^N$.

Proof. The thesis follows from (H2) and Theorem 4.4 using the inequality

$$\|D_y(\omega p)\|_{L^\infty(\mathbf{R}^N)} \leq \|\Delta(\omega p)\|^{\frac{1}{2}}_{L^\infty(\mathbf{R}^N)}\|\omega p\|^{\frac{1}{2}}_{L^\infty(\mathbf{R}^N)}.$$

The proof for $D_x p$ is similar. □

Remark 4.6 Theorem 4.4 and Corollary 4.5 apply directly to the case described in Example 3.3, thanks to hypothesis (H1)(b1). In the case described in Example 3.4, we obtain slightly weaker estimates, assuming, in addition, that $V(x)e^{-\varepsilon|x|^{1+\beta/2}}$ is bounded for every $\varepsilon > 0$. In fact, with the notation of Example 3.4, (H2) holds with $\phi(x) = e^{-\delta|x|^{1+\beta/2}}$, but we get

$$|\Delta_x p(x,y,t)| + |\Delta_y p(x,y,t)| + (V(x) + V(y))\,p(x,y,t) \leq \frac{K_1}{t}c(t/4)\bar{\phi}(x)\bar{\phi}(y)$$

with $\bar\phi(x) = e^{-\bar\delta|x|^{1+\beta/2}}$ for every $0 < \bar\delta < \delta$ instead of (4.1) and K_1 depending on $\bar\delta$. Setting $\bar\omega = 1/\bar\phi$ and arguing as in the proof of Theorem 4.4, we get (4.3) with $\bar\omega_\varepsilon = \bar\omega/(1+\varepsilon\bar\omega)$ in place of ω_ε. Next, notice that the inequality in (H1)(b2) holds for $\bar\omega$ and $\bar\omega_\varepsilon$ with $\gamma > 2\bar\delta^2(1+\beta/2)^2$. Moreover,

$$\begin{aligned}\|V\bar\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)} &\le \sup_{y\in\mathbf{R}^N} |V(y)\bar\omega_\varepsilon(y)c(t)\phi(x)\phi(y)| \le \sup_{y\in\mathbf{R}^N} |V(y)e^{(\bar\delta-\delta)|y|^{1+\frac{\beta}{2}}}|\; c(t)\phi(x) \\ &\le Cc(t)\bar\phi(x) \end{aligned} \tag{4.6}$$

and [11, Proposition 2.3] gives

$$\|V^{\frac12}D(\bar\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} \le \sigma\|\Delta(\bar\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + \frac{c}{\sigma}\|V\bar\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)}$$

for small $\sigma > 0$. Coming back to (4.3), with $\bar\omega_\varepsilon$ in place of ω_ε, using (4.6) we get

$$\begin{aligned}\|\Delta(\bar\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} &\le C\Big(C_\gamma c(t)\bar\phi(x) + \gamma\|V\bar\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)} + c_1(t)\phi(x) \\ &\quad +\gamma\left(\sigma\|\Delta(\bar\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + \frac{c}{\sigma}\|V\bar\omega_\varepsilon p\|_{L^\infty(\mathbf{R}^N)}\right) + C_\gamma\|D(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)}\Big) \\ &\le C\gamma\sigma\|\Delta(\bar\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + CC_\gamma\|D(\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} + Cc_1(t)\bar\phi(x),\end{aligned}$$

where $c_1(t) = (2K/t)c(t/4)$ as in the proof of Theorem 4.4. Therefore, choosing σ small enough and using (4.6) once again, we deduce

$$\|\Delta(\bar\omega_\varepsilon p)\|_{L^\infty(\mathbf{R}^N)} \le Cc_1(t)\bar\phi(x)$$

and conclude as for Theorem 4.4. Concerning Corollary 4.5, we get

$$|D_y p(x,y,t)| + |D_x p(x,y,t)| \le \frac{K}{\sqrt{t}}c(t/4)\bar\phi(x)\bar\phi(y)$$

instead of (4.5).

5 Appendix

In this section we collect some results used in the paper. We start by proving a regularity result for solution of parabolic problems involving operators with unbounded coefficients.

We consider the parabolic operator

$$B = \partial_t - \Delta + V$$

in $L^k(Q_T)$, $1 < k < \infty$, where the potential V satisfies (H1)(a).

Lemma 5.1 *Suppose that* (H1)(a) *holds. Then there exist two constants $c, \sigma_0 > 0$ such that for every $u \in W^{2,1}_k(Q_T)$ with $Vu \in L^k(Q_T)$ the following estimate holds for $0 < \sigma \le \sigma_0$*

$$\|V^{\frac12}Du\|_{L^k(Q_T)} \le \sigma\|u\|_{W^{2,1}_k(Q_T)} + \frac{c}{\sigma}\|Vu\|_{L^k(Q_T)}.$$

Proof. By density, it is sufficient to consider functions u with support contained in $B_R \times [0,T]$ for some $R > 0$. By [11, Proposition 2.3] there exist $\sigma_0, c > 0$ such that

$$\int_{\mathbf{R}^N} V^{\frac{k}{2}}(x)|Du(x,t)|^k\,dx \le \sigma^k\int_{\mathbf{R}^N}|\Delta u(x,t)|^k\,dx + \frac{c^k}{\sigma^k}\int_{\mathbf{R}^N} V^k(x)|u(x,t)|^k\,dx$$

for $\sigma \le \sigma_0$. The proof is easily concluded integrating with respect to t. □

Theorem 5.2 *Assume that V satisfies* (H1)(a). *Let $1 < k < \infty$ and let u be a function in $L^k(Q_T) \cap W_k^{2,1}(B_R \times [0,T])$ for every $R > 0$ solving*

$$\begin{cases} Bu = g & \text{in } \; Q_T \\ u(x,0) = 0 & x \in \mathbf{R}^N, \end{cases} \tag{5.1}$$

with $g \in L^k(Q_T)$. Then

$$\|u\|_{W_k^{2,1}(Q_T)} + \|Vu\|_{L^k(Q_T)} \le C\|g\|_{L^k(Q_T)}, \tag{5.2}$$

where C depends only upon N, k and the constants in (H1)(a).

Proof. Given $g \in L^k(Q_T)$ by [11, Proposition 6.5] there exists a (unique) $z \in W_k^{2,1}(Q_T)$ with $Vz \in L^k(Q_T)$ which solves (5.1) and satisfies the inequality

$$\|z\|_{W_k^{2,1}(Q_T)} + \|Vz\|_{L^k(Q_T)} \le C\|g\|_{L^k(Q_T)},$$

with C as in the statement. Therefore we have only to show that $u = z$. The function $w = u - z$ belongs to $L^k(Q_T) \cap W_k^{2,1}(B_R \times [0,T])$ for every $R > 0$ and satisfies

$$\int_{Q_T} w(-\partial_t \phi - \Delta\phi + V\phi) = 0$$

for every $\phi \in C^{2,1}(Q_T)$ vanishing at time T and having support in $B_R \times [0,T]$ for some $R > 0$. Since $w \in L^k(Q_T)$, by density the above equality holds for every $\phi \in W_{k'}^{2,1}(Q_T)$ such that ϕ vanishes at time T and $V\phi \in L^{k'}(Q_T)$. Given $\psi \in L^{k'}(Q_T)$, by [11, Proposition 6.5] again, we find $\phi \in W_{k'}^{2,1}(Q_T)$ with $\phi(\cdot, T) = 0$ and $V\phi \in L^{k'}(Q_T)$ such that $-\partial_t\phi - \Delta\phi + V\phi = \psi$. Therefore

$$\int_{Q_T} w\psi = 0$$

for every $\psi \in L^{k'}(Q_T)$ and $w = 0$. □

We used an analogue of the above results in the elliptic case for the sup-norm.

Theorem 5.3 *Let V satisfy* (H1)(a) *and let $u \in C_0(\mathbf{R}^N) \cap W_{\text{loc}}^{2,p}(\mathbf{R}^N)$ for all $p < \infty$ such that*

$$u - \Delta u + Vu = f$$

with $f \in C_0(\mathbf{R}^N)$. Then $Vu, \Delta u \in C_0(\mathbf{R}^N)$ and moreover

$$\|\Delta u\|_{L^\infty(\mathbf{R}^N)} + \|Vu\|_{L^\infty(\mathbf{R}^N)} \le C\left(\|f\|_{L^\infty(\mathbf{R}^N)} + \|u\|_{L^\infty(\mathbf{R}^N)}\right)$$

where C depends upon N and the constants in (H1)(a).

Proof. By [11, Proposition 4.2] there exists a unique $z \in C_0(\mathbf{R}^N) \cap W_{\text{loc}}^{2,p}(\mathbf{R}^N)$ for all $p < \infty$ such that $z - \Delta z + Vz = f$ which also satisfies the estimate in the statement. Therefore we have to show that $u = z$. The function $w = u - z$ belongs to $C_0(\mathbf{R}^N) \cap W_{\text{loc}}^{2,p}(\mathbf{R}^N)$ for all $p < \infty$ and satisfies $w - \Delta w + Vw = 0$. The maximum principle implies that $w = 0$ and concludes the proof. □

Now we prove the interpolative estimates we used in Section 3

Proposition 5.4 *(i) Assume that $k > (N+2)/2$. Then there exists $C > 0$ such that for every $u \in W^{2,1}_k(Q_T)$ the estimate*

$$\|u\|_{L^\infty(Q_T)} \le C\|u\|^{1-\theta}_{L^1(Q_T)}\|u\|^{\theta}_{W^{2,1}_k(Q_T)}$$

holds with

$$\theta = \frac{N+2}{(N+2)(1-1/k)+2}.$$

(ii) Assume that $k > N+2$. Then there exists $C > 0$ such that for every $u \in W^{2,1}_k(Q_T)$ the estimate

$$\|Du\|_{L^\infty(Q_T)} \le C\|u\|^{1-\eta}_{L^1(Q_T)}\|u\|^{\eta}_{W^{2,1}_k(Q_T)}$$

holds with

$$\eta = \frac{N+3}{(N+2)(1-1/k)+2}.$$

Proof. Let us prove (i). Since there exists a linear extension operator from $W^{2,1}_k(Q_T)$ to $W^{2,1}_k(Q)$, $Q = \mathbf{R}^{N+1}$ which is also continuous from $L^r(Q_T)$ to $L^r(Q)$ for $1 \le r \le \infty$, we may assume that $Q_T = Q$. Let R be a unit cube in Q. Since the embedding of $W^{2,1}_k(R)$ into $C(\overline{R})$ is compact, see [6, Lemma 3.3], a standard argument yields a constant $C > 0$ such that

$$\|u\|_{L^\infty(R)} \le C\left(\|u\|_{L^1(R)} + \|\partial_t u\|_{L^k(R)} + \|D^2 u\|_{L^k(R)}\right)$$

for every $u \in W^{2,1}_k(R)$. Then, obviously,

$$\|u\|_{L^\infty(Q)} \le C\left(\|u\|_{L^1(Q)} + \|\partial_t u\|_{L^k(Q)} + \|D^2 u\|_{L^k(Q)}\right) \tag{5.3}$$

for every $u \in W^{2,1}_k(Q)$. Applying (5.3) to the function $v(x,t) = u(\lambda x, \lambda^2 t)$, $\lambda > 0$, we get

$$\|u\|_{L^\infty(Q)} \le C\left(\lambda^{-(N+2)}\|u\|_{L^1(Q)} + \lambda^{2-\frac{N+2}{k}}\left(\|\partial_t u\|_{L^k(Q)} + \|D^2 u\|_{L^k(Q)}\right)\right)$$

and the statement follows minimising over $\lambda > 0$. The proof of (ii) is similar. □

References

[1] W. Arendt, G. Metafune, D. Pallara: Schrödinger operators with unbounded drift, *J. Oper. Theory* **55** (2006), 101-127.

[2] E.B. Davies: *Heat Kernels and Spectral Theory,* Cambridge University Press, 1989.

[3] E.B. Davies, B. Simon: Ultracontractivity and the heat kernel of Schrödinger operators and Dirichlet Laplacians, *J. Funct. Anal.* **59** (1984), 335-395.

[4] N.V. Krylov: *Lectures on Elliptic and Parabolic Problems in Hölder Spaces,* Graduate Studies in Mathematics 12, Amer. Math. Soc., 1996.

[5] K. Kurata: An estimate on the heat kernel of magnetic Schrödinger operators and uniformly elliptic operators with non-negative potentials, *J. London Math. Soc.* **62** (2000), 885-903.

[6] O.A. Ladyzhenskaya, V.A. Solonnikov, N.N. Ural'tseva: *Linear and Quasilinear Equations of Parabolic Type,* Amer. Math. Soc., 1968.

[7] V. Liskevich, Z. Sobol: Estimates of the kernel of semigroups associated with second-order elliptic operators with singular coefficients, *Potential Analysis* **18** (2003), 359-390.

[8] G. Metafune, D. Pallara, A. Rhandi: Global properties of invariant measures, *J. Funct. Anal.* **223** (2005), 396-424.

[9] G. Metafune, D. Pallara, M. Wacker: Feller semigroups on $\mathbf{R}^N$, *Semigroup Forum* **65** (2002), 159-205.

[10] G. Metafune, D. Pallara, M. Wacker: Compactness properties of Feller semigroups, *Studia Math.* **153** (2002), 179-206.

[11] G. Metafune, J. Prüss, A. Rhandi, R. Schnaubelt: L^p-regularity for elliptic operators with unbounded coefficients, *Advances in Diff. Equat.* **10** (2005), 1131-1164.

[12] M. Reed, B. Simon: *Methods of Modern Mathematical Physics, Vol. II,* Academic Press, 1975.

[13] B. Simon: Schrödinger semigroups, *Bull. Amer. Math. Soc.* **7** (1982), 447-526.

[14] Z. Shen: L^p-estimates for Schrödinger operators with certain potentials, *Ann. Inst. Fourier* **45** (1995), 513-546.

[15] A. Sikora: On-diagonal estimates on Schrödinger semigroup kernels and reduced heat kernels, *Commun. Math. Phys.* **188** (1997), 233-249.