

Introduction

In the last years, owing to their connections with probability and stochastic analysis, there has been an increasing interest towards linear elliptic and parabolic operators with unbounded coefficients. In literature, one can find a careful theory concerning solutions of Cauchy problems associated with the above mentioned operators in several function spaces. Many aspects such as existence, uniqueness, regularity, integral representation are object of study for numerous authors.

We will deal with elliptic operators of form

$$Au(x) = \sum_{i,j=1}^N a_{ij}(x)D_{ij}u(x) + \sum_{i=1}^N F_i(x)D_iu(x) - V(x)u(x)$$

with (a_{ij}) symmetric matrix satisfying the ellipticity condition, a_{ij} , F_i , V real-valued functions, V positive potential. Under hölderianity assumptions on the coefficients, an existence result for bounded classical solutions of the Cauchy problem

$$\begin{cases} u_t(x, t) = Au(x, t) & x \in \mathbb{R}^N, t > 0, \\ u(x, 0) = f(x) & x \in \mathbb{R}^N \end{cases}$$

with initial datum $f \in C_b(\mathbb{R}^N)$ holds (see [29], [4]). The solution is constructed through an approximation procedure as the limit of solutions of Cauchy Dirichlet problems in suitable bounded domains and is given by a certain semigroup $T(t)$ applied to the initial datum f .

Moreover it can be represented by the formula

$$u(x, t) = \int_{\mathbb{R}^N} p(x, y, t)f(y) dy \quad t > 0, x \in \mathbb{R}^N$$

where p is a positive function called integral kernel. In the first four chapters of this work, our attention is mainly devoted to the study of the integral kernel p just introduced. In particular we prove upper bounds on these kernels. We examined separately operators containing only the second and the first order parts and Schrödinger operators characterized by a vanishing drift term ($F = 0$) and second order part given by the Laplacian. The case of the whole operator is not contemplated. The semigroup associated with the Schrödinger operator can be built under weaker assumptions on the potential by means of the quadratic

form method. It is sufficient the requirement $V \in L^1_{loc}(\mathbb{R}^N)$ to obtain a strongly continuous analytic semigroup on $L^2(\mathbb{R}^N)$ that can be extrapolated to $L^p(\mathbb{R}^N)$ for $1 \leq p \leq \infty$ and that admits an integral representation.

If A is given by $\Delta - V$, the kernel p is pointwise dominated by the heat kernel of the Laplacian in \mathbb{R}^N , that is

$$p(x, y, t) \leq \frac{1}{(4\pi t)^{\frac{N}{2}}} \exp\left\{-\frac{|x-y|^2}{4t}\right\}, \quad \forall x, y \in \mathbb{R}^N.$$

For the presence of the positive potential, one expects more decay in the space variables.

Deeper upper bounds for $V(x) = |x|^\alpha$ with $\alpha > 2$ can be found for example in [13, Section 4.5]. Davies and Simon prove that $p(x, y, t) \leq c(t)\psi(x)\psi(y)$, where ψ is the ground state of $-A$, that is the eigenfunction corresponding to the smallest eigenvalue, and c has an explicit behaviour near 0. Similar estimates can be found in [28] where upper bounds like $p(x, y, t) \leq c(t)\phi(x)\phi(y)$ are obtained for a large class of potential tending to infinity as $|x| \rightarrow \infty$ under the main assumption that $\omega = 1/\phi$ satisfies $\omega(x) \rightarrow \infty$ as $|x| \rightarrow \infty$ and $-A\omega \geq g\omega$ where g is a convex function growing faster than linearly. The behaviour of $c(t)$ near 0 is also shown to be precise. The authors are able to deduce estimates for $V(x) = |x|^\alpha$ for every $\alpha > 0$ but the Davies and Simon bounds cannot be achieved since the ground state does not satisfy their assumptions.

Sikora proves another kind of estimates for $V(x) = |x|^\alpha$, $\alpha > 0$, see [45] where also lower bounds are proved. He obtains precise on-diagonal bounds of the form $p(x, x, t) \leq h(x, t)$ and then he deduces off-diagonal bounds from the semigroups law.

Potentials unbounded only in certain directions (like $x_1^2 x_2^2 x_3^2$ in \mathbb{R}^3) are considered by Kurata in [22] where upper bounds are proved. Such estimates are not sharp but their main concern is the applicability to degenerate non homogeneous potentials.

In the case of $V(x) = |x|^\alpha$ we obtain estimates similar to those of Sikora ([45]). However our method is not confined to special polynomial potentials but applies also to logarithmic, exponential growths or more generally to radial increasing potentials and potentials consisting of a radial part and lower order terms. Moreover our approach allows us to obtain more precise bounds.

On the other hand we consider also bounds similar to the Davies and Simon ones and, using the similarity between Schrödinger and Kolmogorov operators, we improve the estimates obtained by Davies and Simon for $V(x) = |x|^\alpha$ with $\alpha > 2$ and we show that the same technique works for other potentials too. As nice application, we see how the Sikora type estimates combined with a Tauberian theorem due to Karamata allow us to deduce some interesting information about the asymptotic distribution of the eigenvalues of $-A$. When V has a polynomial behaviour these results have been proved by Titchmarsh (see [51]) using cube-decomposition methods. Our approach allows us to treat also potentials with different growth.

Kolmogorov operators, that is elliptic operators with unbounded drift term and vanishing potential, have also been studied. Some results concerning pointwise upper bounds for their kernels can be found for example in [27] where the authors use Lyapunov functions techniques to prove estimates of the form $p(x, y, t) \leq c(t)\omega(y)$. We get inspiration from this paper to prove upper bounds like $p(x, y, t) \leq c(t)\omega(y, t)$.

In recent papers (see [6], [7] and [8]), Bogachev, Krylov, Röckner and Shaposhnikov prove existence and regularity properties for parabolic problems having measures as initial data, they also deduce uniform boundedness of solutions but we cannot compare their estimates with our results since the fundamental solution p is singular for $t = 0$.

Besides the kernel estimates, other aspects of Schrödinger operators were widely investigated. For example, an interesting problem is the characterization of the domain in which the operator generates a strongly continuous or an analytic semigroup. A natural question is under which conditions on the potential V the domain of $\Delta - V$ in $L^p(\mathbb{R}^N)$ coincides with the intersection of the domain of the Laplacian and the domain of the potential that is $W^{2,p}(\mathbb{R}^N) \cap D(V)$ where $D(V) = \{u \in L^p(\mathbb{R}^N) : Vu \in L^p(\mathbb{R}^N)\}$. By the classical theory for elliptic operators with bounded coefficients, the last description of the domain is true for bounded potentials but in general a greater effort is needed to get information on the domain in the unbounded case and additional assumptions have to be required.

Cannarsa and Vespri (see [10]) prove that, assuming an oscillation condition on the potential, namely $|\nabla V| = o(V^{\frac{3}{2}})$, the operator generates an analytic semigroup in $L^p(\mathbb{R}^N)$ for $1 \leq p \leq \infty$. Moreover with their approach they characterize for $1 < p < \infty$. We remark that they consider a more general operator containing also a drift term.

Metafun, Pruss, Rhandi and Schnaubelt (see [31]) improve the previous generation result. In particular they establish that, under suitable assumptions on the drift term and the oscillation assumption above on the potential, the whole elliptic operator A endowed with the natural domain $D(\Delta) \cap D(V)$ generates an analytic and contractive strongly continuous semigroup on $L^p(\mathbb{R}^N)$, $1 \leq p < \infty$, and on $C_0(\mathbb{R}^N)$. The precise description of the domain corresponds to good a priori estimates for the elliptic problem $\lambda u - Au = f$. Moreover the maximal regularity of type L^q for the inhomogeneous parabolic problem associated with the given operator is deduced.

On the other hand the equality $D(\Delta - V) = D(\Delta) \cap D(V)$ holds even if V belongs to suitable Reverse Hölder classes (see for example [41] and [3]). The oscillation condition and the reverse Hölder one are incomparable, it is easy to find examples of polynomials which satisfy a reverse Hölder inequality for which the oscillation condition fails and viceversa. The potential $V(x, y) = x^2 y^2$ does not satisfy $|DV| \leq \gamma V^{\frac{3}{2}}$ for any γ but it belongs to the reverse Hölder class B_p for every $1 < p \leq \infty$. The potential $V(x) = e^x$ in \mathbb{R} does not satisfy the

doubling property and then it does not belong to any reverse Hölder class but the oscillation condition obviously holds.

In [41] Shen proves the L^p boundedness of $D^2(-\Delta+V)^{-1}$ on \mathbb{R}^N for $1 < p < \infty$, assuming $V \in B_p$ and under the restrictions $N \geq 3$, $p \geq \frac{N}{2}$, he introduces an auxiliary function $m(x, V)$, which is well defined for $p \geq \frac{N}{2}$ and allows him to estimate the fundamental solution.

In a recent work, P. Auscher and B. Ben Ali, see [3], extend Shen's result removing the original restrictions on the space dimension and on p . In their proof they use a criterion to prove the L^p boundedness of certain operators in absence of kernels, see [42, Theorem 3.1], [2, Theorem 3.14], and some weighted mean value inequalities for nonnegative subharmonic functions with respect to Muckenhoupt weights.

Following Shen's approach, W. Gao and Y. Jiang extend the previous results to the parabolic case. In [18], they consider the parabolic operator $\partial_t - \Delta + V$ where $V \in B_p$ is a nonnegative potential depending only on the space variables and, under the assumptions $N \geq 3$ and $p > (N+2)/2$, they prove the boundedness of $V(\partial_t - \Delta + V)^{-1}$ in L^p .

We consider the parabolic Schrödinger operator, in particular we focus our attention on the validity of a priori estimates for solutions of $\lambda u - \partial_t u + \Delta u - Vu = f$ in $L^p(\mathbb{R}^{N+1})$ and consequently on the characterization of the domain. We improve the results of Gao and Jiang indeed a larger class of potentials is allowed. We obtain the L^p boundedness of $V(\partial_t - \Delta + V)^{-1}$ (and consequently of $\partial_t(\partial_t - \Delta + V)^{-1}$ and $D^2(\partial_t - \Delta + V)^{-1}$) if the potential V belongs to some parabolic Reverse Hölder class B_p for $1 < p < \infty$, without any restriction on the space dimension and on p ; moreover we remark that our potentials may also depend on the time variable. Our approach is similar to that of [3]. We use a more general version of the boundedness criterion in absence of kernels in homogeneous spaces (see Theorem D.1.1) and the Harnack inequality for subsolutions of the heat equation. A crucial role is played by some properties of the B_p weights originally proved in the classical case that is when \mathbb{R}^N is equipped with the Lebesgue measure and the Euclidean distance. Since we need parabolic cylinders instead of balls of \mathbb{R}^N , we use the more general theory of B_p weights in homogeneous spaces, as treated in [48, Chapter I].

The first chapter contains some introductory and known results. Specifically, following [29, Section 4], we assume local uniform ellipticity and local Hölderianity on the coefficients to prove that there exists a positive semigroup $(T(t))_{t \geq 0}$ such that, for any $f \in C_b(\mathbb{R}^N)$, $u(x, t) = T(t)f(x)$ is a classical solution of the Cauchy problem associated with $A = \sum_{i,j=1}^N a_{ij}D_{ij} + \sum_{i=1}^N F_i D_i - V$. $T(t)$ is the semigroup generated by A in a weak sense. The semigroup $(T(t))_{t \geq 0}$ has a smooth integral kernel whose behaviour will be examined later.

After that, in a special case we show how a different approach is possible. We sketch the construction of the semigroup generated by Schrödinger operators with locally integrable potentials by means of the quadratic form theory (see [13]). The semigroup generated by $\Delta - V$ is ultracontractive and, by the Dun-

ford Pettis Theorem, it admits an integral kernel.

In Chapter 2 we prove upper and lower bounds for heat kernels of Schrödinger semigroups and upper bounds for Kolmogorov semigroups. In both cases we consider the semigroup built under Hölderianity assumptions on the coefficients. First we analyse Kolmogorov operators. We assume the existence of a Lyapunov function for the operator A , i.e. a positive and smooth function V going to infinity for $|x| \rightarrow \infty$ such that $AV \leq \lambda V$ for some positive λ . This requirement is not restrictive since for the operators we are interested in through this chapter a function satisfying this property exists (see [27, Section 2]). This assumption insures that the domain of the weak generator coincides with the maximal domain.

We introduce Lyapunov functions for the parabolic operator $L = \partial_t + A$. The definition is a little bit different from the one given in the elliptic case. We say that a continuous function $W : [0, T] \times \mathbb{R}^N \rightarrow [0, +\infty)$ is a Lyapunov function for the operator L if it belongs to $C^{2,1}(Q_T)$, $\lim_{|x| \rightarrow \infty} W(x, t) = +\infty$ uniformly with respect to t in compact sets of $(0, T]$ and there exists $h : [0, T] \rightarrow [0, \infty)$ integrable in a neighborhood of 0 such that $LW(x, t) \leq h(t)W(x, t)$ for all $(x, t) \in Q_T$. Note that we do not require that $W(x, 0)$ tends to ∞ as $|x| \rightarrow \infty$. We prove that a similar function is integrable with respect to the kernel p , more precisely $\int_{\mathbb{R}^N} p(x, y, t)W(y, t) dy \leq e^{\int_0^t h(s) ds} W(x, 0)$. Assuming growth assumptions on the radial component of the drift, we provide a class of Lyapunov functions for L . To achieve the main result, we preliminarily establish some integrability and regularity results for the kernel. Then, by using the estimate of the L^1 -norm of Lyapunov functions stated before, we prove pointwise estimates of kernels of the form $p(x, y, t) \leq c(t)\omega(y, t)$. The main ingredient is an estimate of the L^∞ -norm of solutions of certain parabolic problems. We explicitly write the bounds so obtained in correspondence of some particular choices of the drift.

A similar method based upon the Lyapunov functions technique works also for Schrödinger operators. In the second part of the chapter we deduce upper bounds for Schrödinger semigroups even if a different approach gives sometimes more refined estimates as it will be shown in Chapter 3. Here we assume that the potential satisfies the oscillation hypothesis $|DV| \leq \gamma V^{\frac{3}{2}} + C_\gamma$ for small values of γ .

The integrability of Lyapunov functions, a parabolic regularity result and an interpolative estimate of the sup norm of functions in parabolic Sobolev spaces play a crucial role in the proof of the wished estimates which are of the Sikora form $p(x, y, t) \leq c(t)\omega(x, t)\omega(y, t)$ (see [45]). As application we see that this method enables us to deduce small times upper bounds for potentials growing in a polynomial, exponential or logarithmic way. The sharpness is discussed. For $V(x) = |x|^\alpha$, $0 < \alpha < 2$, $V(x) = \exp\{c|x|^\alpha\}$ and $V(x) = M \log(1 + |x|^2)$ our estimates are sharp, the method does not give a precise estimate of certain constants in ω which however will be obtained in the next chapter. The estimate for $V(x) = |x|^\alpha$, $\alpha > 2$, is exact concerning the decay in the space variable for a

fixed time, sharp estimates for such potential are proved in Chapter 3 by considering suitable space-time regions. Finally large time estimates are deduced by the previous ones by means of the symmetry of the kernel and by the semigroup law.

The third chapter is devoted to the study of upper and lower bounds of Schrödinger kernels. In some cases, the results here obtained cover the ones in the previous chapter.

Given a positive potential V , for each positive s we consider the new potential V_s equal to s in the level set corresponding to s and V otherwise. To obtain the bound on p , as in [45], we estimate the difference between the kernels p and p_s and then we use the triangle inequality. In [45], Sikora uses the functional calculus to estimate such a difference for the potential $V(x) = |x|^\alpha$. Our approach, though more elementary, yields more precise bounds and a wider class of potentials can be studied. Once the difference is estimated, we observe that, for radial potentials and in correspondence of a particular choice of s depending on the potential, the measure of the level set is known and the bound can be explicitly written as follows

$$p(x, x, t) \leq \frac{1}{(4\pi t)^{\frac{N}{2}}} \exp\{-tV(cx)\} + \frac{C(N)}{t^{\frac{N}{2}}} \frac{c^N \omega_N}{(1-c)^N} \exp\left\{-\frac{(1-c)^2|x|^2}{4t}\right\}$$

for all $0 < c < 1$.

Low-order perturbations of the potentials above can be estimated in similar way. We remark that we first obtain on diagonal estimates and then by the semigroup law we deduce off diagonal estimates.

The natural question is whether such estimates are sharp. Considering suitable space-time regions, one can control the gaussian term with the first addendum, moreover in these regions similar lower estimates are true and the sharpness follows.

As consequence we deduce a result concerning the asymptotic distribution of the eigenvalues of $-\Delta + V$. Denoted by $N(\lambda)$ the number of eigenvalues less than λ and λ_n the eigenvalues of $-\Delta + V$, the Karamata Theorem relates the asymptotic behaviour of $N(\lambda)$ for $\lambda \rightarrow \infty$ with the behaviour of $\sum_n e^{-\lambda_n t}$ for small values of t , by Mercer's Theorem we know that $\int_{\mathbb{R}^N} p(x, x, t) = \sum_{n=1}^{\infty} e^{-\lambda_n t}$, therefore we can use the upper and lower estimates for p to achieve information on $N(\lambda)$.

In Chapter 4, we prove once again upper bounds for Schrödinger semigroups. But this time we obtain Davies-type estimates. We recall that by a result due to Davies, if $V(x) = |x|^\alpha$, $\alpha > 2$, then for all $\frac{\alpha+2}{\alpha-2} < b < \infty$, $p(x, y, t) \leq c_1 \exp\{c_2 t^{-b}\} \psi(x) \psi(y)$ for all $x, y \in \mathbb{R}^N$, $0 < t \leq 1$, where ψ is the ground state of $-\Delta + |x|^\alpha$. Moreover the lower bound on b is sharp in the sense that if $p(x, y, t) \leq c(t) \psi(x) \psi(y)$ then $c(t) \geq c_1 \exp\{c_2 t^{-\frac{\alpha+2}{\alpha-2}}\}$. We improve this estimate indeed we show that $p(x, y, t) \leq c_1 \exp\{c_2 t^{-\frac{\alpha+2}{\alpha-2}}\} \psi(x) \psi(y)$ by using the similarity between Schrödinger and Kolmogorov operators. If the function

$|\nabla\phi|^2 - 2\Delta\phi$ is bounded from below in \mathbb{R}^N , then the operator $\Delta - \nabla\phi \cdot \nabla$ in $L^2(\mathbb{R}^N)$ is unitarily equivalent to the Schrödinger operator $\Delta - V$ 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 $\Delta - \nabla\phi \cdot \nabla = -T(\Delta - V)T^{-1}$ where T is the multiplication operator $Tu = e^{\frac{\phi}{2}}u$. Consequently the problems of finding estimates for the kernels of the two operators are equivalent. We prove estimates for the Kolmogorov kernel as in [27] and then we deduce estimates for the Schrödinger kernel.

The last chapter is aimed at the description of the domain of parabolic Schrödinger operators. As main result, we prove that, if the potential V is in a parabolic Reverse Hölder class B_p , then $\|Vu\|_{L^p(\mathbb{R}^{N+1})} \leq C\|\partial_t u - \Delta u + Vu\|_{L^p(\mathbb{R}^{N+1})}$ for all u in the maximal domain of the operator. By difference and by parabolic regularity, the estimates for the L^p norm of D^2u and $\partial_t u$ follow. Consequently we deduce that the domain of $\partial_t - \Delta + V$ is $W_p^{2,1}(\mathbb{R}^{N+1}) \cap D(V)$ where $D(V) = \{u \in L^p(\mathbb{R}^{N+1}) : Vu \in L^p(\mathbb{R}^{N+1})\}$.

Through this chapter, we define the parabolic reverse Hölder classes by replacing cubes or balls of \mathbb{R}^N in the classical definition with parabolic cylinders and we state some useful properties enjoyed by them. For instance B_p weights are in some Muckenhoupt classes A_p and satisfy a self improvement property due to Gehring. Some examples of B_p weights are provided.

We take care of giving a meaning to the operator. We get inspiration by an elliptic Kato's result (see [19]) to endow $\partial_t - \Delta + V$ in L^p with the maximal domain $\{u \in L^p(\mathbb{R}^{N+1}) : Vu \in L_{loc}^1(\mathbb{R}^{N+1}), (\partial_t - \Delta + V)u \in L^p(\mathbb{R}^{N+1})\}$. We prove that for every $\lambda > 0$, $\lambda + \partial_t - \Delta + V$ is invertible and, for every $1 \leq p < \infty$, C_c^∞ is a core for the operator. The main tool is a parabolic version of Kato's inequality originally proved in the elliptic case and which we generalized to the parabolic one.

Then we consider the operator on L^1 and we prove the apriori estimates. This is an easy task, indeed the claimed estimates for $p = 1$ immediately follow by approximation and integration by parts. These estimates will play a key role in the proof of the apriori estimates in the general case which is more involved and requires a greater effort. We use a powerful criterion to prove the boundedness of certain operators in absence of kernels. We turn our attention toward the operator $T = V(\partial_t + \Delta - V)^{-1} \cdot | \cdot |$. Its boundedness in L^1 , which follows by the previous apriori estimates, and a sort of reverse Hölder inequality which follows by the properties of the B_p weights and by the Harnack inequality for subsolution of the heat equation, thanks to the criterion mentioned above, give the boundedness in L^p . The main result immediately follows.

Appendix A, B and C contain respectively the Karamata Theorem and a weaker version of it used in Chapter 3 to study the asymptotic distribution of the eigenvalues of the Schrödinger operators, a preliminary inequality needed to prove an integration by parts formula (see [32]) and used in Chapter 5 to study the parabolic Schrödinger operator in an infinite cylinder $Q(S, T)$ and

some Embedding Theorems for parabolic Sobolev spaces useful in the second chapter.

The whole Appendix D is devoted to the boundedness criterion used in Chapter 3. It's worth it aiming the attention to such result which is extremely helpful and of own interest. A weaker version of such theorem appears in [42, Theorem 3.1], it is confined to the elliptic case and it is more restrictive concerning the exponents involved. Namely, Shen, inspired by a paper of Caffarelli and Peral (see [9]), proved that if T is a sublinear bounded operator on $L^2(\mathbb{R}^N)$ such that, given $p > 2$, there exist some positive constants $\alpha_2 > \alpha_1 > 1$, $N > 0$ for which

$$\left\{ \frac{1}{|B|} \int_B |Tf|^p dx \right\}^{\frac{1}{p}} \leq N \left\{ \left(\frac{1}{|\alpha_1 B|} \int_{\alpha_1 B} |Tf|^2 dx \right)^{\frac{1}{2}} + \sup_{B' \supset B} \left(\frac{1}{|B'|} \int_{B'} |f|^2 dx \right)^{\frac{1}{2}} \right\}$$

for any ball $B \subset \mathbb{R}^N$ and any bounded measurable function f with compact support contained in $\mathbb{R}^N \setminus \alpha_2 B$ then T is bounded in $L^q(\mathbb{R}^N)$ for any $2 < q < p$. Following [42, Theorem 3.1], we prove the result stated above in a more general setting, i.e. we replace balls of \mathbb{R}^N with parabolic cylinders and a whatever L^{p_0} space plays the role of the L^2 space in the assumptions. For the proof we need a revisited theory in the parabolic case concerning the Maximal Hardy-Littlewood functions, the Lebesgue points and a Calderón-Zygmund decomposition.

We remark that, since \mathbb{R}^{N+1} endowed with the parabolic distance is a homogeneous space, the result can be deduced by a more general version of this theorem formulated by Auscher and Martell (see [2, Section5]).

As application we provide an alternative proof of the classical apriori estimates for the operator $\partial_t - \Delta$ and of the classical Calderón-Zygmund Theorem. These operators are both bounded in L^2 and satisfy the assumption of Shen's Theorem, this can be proved by means of Cacioppoli-type estimates and by Sobolev Embedding Theorems in the parabolic case and by the mean value Theorem for harmonic functions in the elliptic one.

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