SHARP GAUSSIAN BOUNDS AND L^p -GROWTH OF SEMIGROUPS ASSOCIATED WITH ELLIPTIC AND SCHRÖDINGER OPERATORS

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ABSTRACT. We prove sharp large time Gaussian estimates for heat kernels of elliptic and Schrödinger operators, including Schrödinger operators with magnetic fields. Our estimates are then used to prove that for general (magnetic) Schrödinger operators $A = -\sum_{k=1}^d (\frac{\partial}{\partial x_k} - ib_k)^2 + V$, we have the L^∞ -estimate (for large t):

$$\|e^{-tA}\|_{L(L^\infty(\mathbb{R}^d))} \leq Ce^{-s(A)t}(t \ln t)^{d/4}$$

where $s(A) := \inf \sigma(A)$ is the spectral bound of A . The same estimate holds for elliptic and Schrödinger operators on general domains.

1. INTRODUCTION

Let Ω be an open subset of $\mathbb{R}^d$ ($d \geq 1$). Throughout this paper, A will denote one of the self-adjoint operators defined in (1), (2) or (3) below:

$$(1) \quad A = - \sum_{k,j=1}^d \frac{\partial}{\partial x_j} \left(a_{kj} \frac{\partial}{\partial x_k} \right) \quad \text{a uniformly elliptic operator.}$$

Here $a_{kj} = a_{jk} \in L^\infty(\Omega, \mathbb{R})$, $1 \leq k, j \leq d$, and satisfy the standard ellipticity condition $\eta I \leq (a_{kj})_{kj} \leq \mu I$, where η and μ are positive constants. If A is considered on $L^2(\Omega)$, we assume for simplicity that A is subject to Dirichlet boundary conditions.

$$(2) \quad A = -\Delta + V \quad \text{a Schrödinger operator.}$$

The operator A acts on $L^2(\mathbb{R}^d)$ (or $L^2(\Omega)$) and the potential $V = V^+ - V^-$ is such that the positive part $V^+ \in L^1_{loc}$ and the negative part V^- is in the Kato class (see, e.g., Simon [24]).

$$(3) \quad A = - \sum_{k=1}^d \left(\frac{\partial}{\partial x_k} - ib_k \right)^2 + V \quad \text{a Schrödinger operator with magnetic field.}$$

Here A acts on $L^2(\mathbb{R}^d)$, $b_k \in L^2_{loc}$ are real-valued functions for $1 \leq k \leq d$, and the potential V is as in (2).

In each of the three situations here, A is defined by the sesquilinear form method (as the operator associated with a densely defined closed symmetric form). It is a self-adjoint operator. Its associated semigroup e^{-tA} is given by a kernel $p(t, x, y)$,

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called the heat kernel of A . This kernel satisfies a Gaussian upper bound. More precisely, if A is as in (1), then

$$(4) \quad |p(t, x, y)| \leq C t^{-d/2} \exp \left\{ -c \frac{|x - y|^2}{t} \right\} \quad \forall t > 0.$$

This is due to Aronson [2]. See also the monographs of Davies [9] and Ouhabaz [20] for more information. If A is a Schrödinger operator as in (2) or (3), then

$$(5) \quad |p(t, x, y)| \leq C t^{-d/2} e^{wt} \exp \left\{ -c \frac{|x - y|^2}{t} \right\} \quad \forall t > 0,$$

where C, c, w are positive constants and $w = 0$ if $V^- = 0$; see Simon [24]. Sharper estimates are proved in Zhang [26] for Schrödinger operators with negative potentials.

More precise estimates are known in the case of uniformly elliptic operators. For such operators on the Euclidean space $\mathbb{R}^d$, Davies and Pang [7] proved that

$$(6) \quad |p(t, x, y)| \leq C t^{-d/2} \exp \left\{ -\frac{\rho(x, y)^2}{4t} \right\} \left[1 + \frac{\rho(x, y)^2}{t} \right]^{d/2} \quad \forall t > 0,$$

where ρ is defined by (11) below (with $\mathbb{R}^d$ instead of Ω).¹ Sikora [21] improved this result, showing that the power $d/2$ in the latter estimate can be replaced by $\frac{d-1}{2}$. Estimates like (6) have been proved for some nonsymmetric operators on domains in Ouhabaz [20]. For the magnetic Schrödinger operator $A = -\sum_{k=1}^d (\frac{\partial}{\partial x_k} - ib_k)^2$ (with $b_k \in L^2_{loc}$), one even has, by the well-known diamagnetic inequality, that

$$(7) \quad |p(t, x, y)| \leq (4\pi t)^{-d/2} \exp \left\{ -\frac{|x - y|^2}{4t} \right\} \quad \forall t > 0.$$

The obvious disadvantage of the estimates (4), (5), (6) or (7) is that they do not give precise information on the asymptotic behavior of the heat kernel for large t . Beyond the classical case of a bounded domain Ω , there are many Schrödinger operators (including magnetic ones with $V = 0$) for which the spectral bound $s(A) := \inf \sigma(A) > 0$ (here $\sigma(A)$ denotes the spectrum of A). In that case, one aims to get exponential decay (with respect to t) in the behavior of the heat kernel. In the context of Riemannian manifolds with Ricci curvature bounded from below, Davies [10] has proved the following estimate for the heat kernel of the Laplace-Beltrami operator $-\Delta$:

$$(8) \quad |p(t, x, y)| \leq \frac{C}{\sqrt{v(x, r)v(y, r)}} e^{-s(-\Delta)t} \exp \left\{ -\frac{\rho(x, y)^2}{4t} \right\}$$

where C is a positive constant, $r = \min\{1, \sqrt{t}, \frac{t}{\rho(x, y)}\}$, $v(x, r)$ is the volume of the ball of center x and radius r , and $\rho(x, y)$ is the Riemannian metric. Davies' proof for (8) relies heavily on the parabolic Harnack inequality.

In the present paper we consider general Schrödinger operators and uniformly elliptic operators on arbitrary domains. In these cases, it is not clear how one can apply the technique in [10]. We shall use a different method and prove precise

¹The results in [7] hold on some Riemannian manifolds.

Gaussian upper bounds. For example, if $A = -\sum_{k=1}^d (\frac{\partial}{\partial x_k} - ib_k)^2 + V$ is as in (3), our estimate reads as follows:

$$(9) \quad |p(t, x, y)| \leq C e^{-s(A)t} t^{-d/2} \exp \left\{ -\frac{|x-y|^2}{4t} \right\} \left[1 + \delta t + \frac{|x-y|^2}{t} \right]^{d/2} \quad \forall t > 0.$$

We also obtain a Gaussian lower bound of a similar type for a class of Schrödinger operators $-\Delta + V$.

In order to prove (9) we start from (4) and (5). We use the perturbation method of Davies which is based on $L^1 - L^\infty$ estimates of the semigroup $T_\lambda(t) := e^{-\lambda\phi} e^{-tA} e^{\lambda\phi}$ (for an appropriate function ϕ and $\lambda \in \mathbb{R}$). The idea now is to make use of $L^2 - L^2$ estimates of the perturbed semigroup $T_\lambda(t)$, from which we obtain a good estimate for the $L^1 - L^\infty$ norm that implies (9). In a sense, we show that (4) and (5) are automatically improved to (9). The proof is quite elementary and can be used in other circumstances. If A is as in (1), we could consider other boundary conditions, e.g., the Neumann or mixed boundary conditions. For the latter conditions, we assume that Ω has the extension property. Also, we could consider Schrödinger operators (2) and (3) on domains (again with Dirichlet or Neumann boundary conditions). The Gaussian estimate (5) for magnetic Schrödinger operators on domains follows from the diamagnetic inequality proved by Liskevich and Manavi [16] and by Hundertmark and Simon [15].

Note also that our results hold in the case where the potential V in example (2) is replaced by a measure with appropriate conditions on its negative and positive parts.

We mention that the power $d/2$ in the term $\left[1 + \delta t + \frac{|x-y|^2}{t} \right]^{d/2}$ cannot be improved in the general case we consider here. The obvious reason is that $s(A)$ may be an eigenvalue of A , in which case, one sees immediately by letting $t \rightarrow \infty$ that (9) cannot hold with some power strictly less than $d/2$ in the last term. Note that in the case of a magnetic Schrödinger operator (with $V = 0$) in two dimensions, a better estimate than (9) was proved by Loss and Thaller [18]. See also Erdős [12] for further information.

Another aim of the present paper is to investigate the growth of $\|e^{-tA}\|_{\mathcal{L}(L^\infty)}$, i.e., the norm of e^{-tA} as an operator on L^∞ . We apply our Gaussian upper bound (9) to prove that for $t \geq 1$,

$$(10) \quad \|e^{-tA}\|_{\mathcal{L}(L^\infty)} \leq C e^{-s(A)t} (1 + t \ln t)^{d/4}.$$

Here A is as in (1), (2) or (3).

The growth of the L^∞ -norm for Schrödinger semigroups $(e^{-t(-\Delta+V)})_{t \geq 0}$ has been investigated. Simon [22] proved that for V in a certain class of potentials, the Schrödinger semigroup satisfies

$$\|e^{-t(-\Delta+V)}\|_{\mathcal{L}(L^\infty)} \leq C e^{-s(-\Delta+V)t} (1+t)^{d/2}.$$

The question of whether the growth $t^{d/2}$ in this estimate can be improved arose in Simon [22].² This question has been answered only for a very restricted class of potentials; see Simon [23] and Davies and Simon [6]. Our L^∞ -estimate (10) gives an answer to this question. The estimate (10) holds for general Schrödinger operators (including magnetic ones). We do not make use of any special properties of the potential V nor of the magnetic field. The power $d/4$ in (10) cannot be improved

²See also [24], p. 471.

in general. Indeed, it is proved in [23], among other things, that for $d = 4$, there exist potentials V for which $s(-\Delta + V) = 0$ and $\|e^{-t(-\Delta+V)}\|_{\mathcal{L}(L^\infty)}$ grows at least as $\frac{t}{\ln t}$. For some particular potentials, the exact behavior of $\|e^{-t(-\Delta+V)}\|_{\mathcal{L}(L^\infty)}$ was given in [6].

2. HEAT KERNEL BOUNDS

Let A be one of the operators described in (1), (2) or (3). Denote by $s(A) := \inf \sigma(A)$ its spectral bound, that is,

$$s(A) = \inf \left\{ \int_{\Omega} Au(x) \overline{u(x)} dx, u \in D(A), \|u\|_2 = 1 \right\}.$$

Before we state the main result of this section, let us define the following metric associated with the uniformly elliptic operator (1):

$$(11) \quad \rho(x, y) = \sup \{ \phi(x) - \phi(y), \phi \in C_c^\infty(\mathbb{R}^d) \text{ such that } \sum_{k,j=1}^d a_{kj} \frac{\partial \phi}{\partial x_k} \frac{\partial \phi}{\partial x_j} \leq 1 \text{ a.e. on } \Omega \}.$$

In our notation, $C_c^\infty(O)$ (where O is any open subset of $\mathbb{R}^d$) denotes the space of real-valued, infinitely differentiable functions with compact support in O .

Theorem 1. 1) Assume that A is as in (1). There exists a positive constant C such that

$$0 \leq p(t, x, y) \leq C e^{-s(A)t} t^{-d/2} \exp \left\{ -\frac{\rho(x, y)^2}{4t} \right\} \left[1 + s(A)t + \frac{\rho(x, y)^2}{t} \right]^{d/2} \quad \forall t > 0.$$

2) Assume that A is as in (2) or (3). There exist two constants $C > 0$ and $w \geq 0$ such that

$$|p(t, x, y)| \leq C e^{-s(A)t} t^{-d/2} \exp \left\{ -\frac{|x - y|^2}{4t} \right\} \left[1 + s(A)t + wt + \frac{|x - y|^2}{t} \right]^{d/2} \quad \forall t > 0.$$

The constant w depends only on V^- , and $w = 0$ if $V^- = 0$.

Assertion 1) can also be found in Ouhabaz [20]. As mentioned above, we show that the estimates here follow easily from the less sharp bounds (4) and (5).

Proof. Let $\lambda \in \mathbb{R}$ and $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ be a C^∞ -function with compact support such that

$$\sum_{k,j=1}^d b_{kj} \frac{\partial \phi}{\partial x_k} \frac{\partial \phi}{\partial x_j} \leq 1 \quad \text{a.e. on } \Omega.$$

Here,

$$b_{kj} = a_{kj} \text{ if } A \text{ is as in (1) and } b_{kj} = \delta_{kj} \text{ if } A \text{ is as in (2) or (3)}.$$

Denote by $\mathfrak{a}$ the symmetric form associated with the self-adjoint operator A . In each of the above examples, $\mathfrak{a}$ is the closure of the form initially defined on $C_c^\infty(\Omega)$. One checks easily that³

$$\Re \mathfrak{a}(e^{\lambda \phi} u, e^{-\lambda \phi} u) = \mathfrak{a}(u, u) - \lambda^2 \sum_{k,j=1}^d \int_{\Omega} b_{kj} \frac{\partial \phi}{\partial x_k} \frac{\partial \phi}{\partial x_j} |u|^2 dx.$$

³One checks this first for $u \in C_c^\infty(\Omega)$, and then uses standard approximation arguments.

Therefore,

$$(12) \quad \Re \mathfrak{a}(e^{\lambda\phi}u, e^{-\lambda\phi}u) \geq (s(A) - \lambda^2) \int_{\Omega} |u|^2 dx.$$

On the other hand, $\mathfrak{a}(e^{\lambda\phi}\cdot, e^{-\lambda\phi}\cdot)$ is the form associated with the semigroup $(T_{\lambda}(t))_{t \geq 0} := (e^{-\lambda\phi}e^{-tA}e^{\lambda\phi})_{t \geq 0}$, whose kernel is

$$k(t, x, y) = p(t, x, y)e^{\lambda(\phi(y) - \phi(x))}.$$

Now using (4) and (5), we obtain⁴

$$\begin{aligned} |k(t, x, y)| &\leq Ct^{-d/2}e^{wt} \exp\left\{-c\frac{|x-y|^2}{t}\right\} \exp\{\lambda(\phi(x) - \phi(y))\} \\ &\leq Ct^{-d/2}e^{wt} \exp\left\{-c\frac{|x-y|^2}{t}\right\} \exp\{|\lambda|c_1|x-y|\} \\ &\leq Ct^{-d/2}e^{wt} \exp\left\{-c\frac{|x-y|^2}{2t}\right\} \exp\{c_2\lambda^2 t\}, \end{aligned}$$

where c_1, c_2 are positive constants independent of ϕ and λ . This implies, in particular, that for each $t > 0$, $T_{\lambda}(t)$ is bounded from $L^2(\Omega)$ into $L^\infty(\Omega)$ with the $L^2 - L^\infty$ norm estimate:

$$(13) \quad \|T_{\lambda}(t)\|_{2,\infty} \leq Ct^{-d/4} \exp\{(c_2\lambda^2 + w)t\}.$$

From (12) and (13) we conclude by Lemma 2 below that

$$(14) \quad \|T_{\lambda}(t)\|_{2,\infty} \leq Cet^{-d/4}e^{(-s(A)+\lambda^2)t}[1 + s(A)t + wt + c_2\lambda^2 t]^{d/4} \quad \forall t > 0.$$

The same estimate holds for the adjoint $T_{-\lambda}(t)$ of $T_{\lambda}(t)$. Therefore,

$$(15) \quad |k(t, x, y)| \leq C't^{-d/2}e^{(-s(A)+\lambda^2)t}[1 + s(A)t + wt + c_2\lambda^2 t]^{d/2} \quad \forall t > 0,$$

where C', c_2 are positive constants independent of λ and ϕ . The last estimate yields

$$|p(t, x, y)| \leq C't^{-d/2}e^{(-s(A)+\lambda^2)t}e^{\lambda(\phi(x) - \phi(y))}[1 + s(A)t + wt + c_2\lambda^2 t]^{d/2}.$$

Choosing $\lambda = \frac{(\phi(y) - \phi(x))}{2t}$ and optimizing over ϕ , we obtain the theorem. $\square$

The following simple lemma was used in the proof. It is taken from Ouhabaz [20] (see pp. 159–160). It is implicit in Coulhon [5].

Lemma 2. *Assume that a strongly continuous semigroup $(T(t))_{t \geq 0}$, acting on $L^2(X, \mu)$, satisfies*

$$\|T(t)\|_{\mathcal{L}(L^2)} \leq Me^{-\beta t} \quad \forall t > 0$$

and $T(t)$ is bounded from $L^2(X, \mu)$ into $L^\infty(X, \mu)$ with the $L^2 - L^\infty$ norm estimate

$$\|T(t)\|_{2,\infty} \leq Ct^{-d/4}e^{\alpha t} \quad \forall t > 0,$$

for some positive constants C, d , and some $\alpha \geq -\beta$. Then

$$\|T(t)\|_{2,\infty} \leq CMe^{-\beta t}e^{\alpha t}[1 + (\alpha + \beta)t]^{d/4} \quad \forall t > 0.$$

It is a classical fact that for Schrödinger operators $-\Delta + V$ on $L^2(\mathbb{R}^d)$ Gaussian lower bounds follow from upper ones.

⁴Here $w = 0$ in case (1) and also in cases (2) and (3) if $V^- = 0$.

Corollary 3. *Let $A = -\Delta + V$ acting on $L^2(\mathbb{R}^d)$ and assume that V^+, V^- are both in the Kato class. Then*

$$p(t, x, y) \geq C e^{s(-\Delta-V)t} t^{-d/2} \exp \left\{ -\frac{|x-y|^2}{4t} \right\} \\ \times \left[1 + s(A)t + wt + \frac{\rho(x, y)^2}{t} \right]^{-d/2} \quad \forall t > 0.$$

Proof. The idea to derive lower bounds from upper bounds relies on the Feynman-Kac formula. This idea is taken from Simon [24]. Denote by X_t the d -dimensional Brownian motion. We have for every nonnegative $f \in C_c^\infty(\mathbb{R}^d)$,

$$\begin{aligned} e^{t\Delta} f(x) &= \int f(X_t) dP_x \\ &\leq \left(\int e^{-\int_0^t V(X_s) ds} f(X_t) dP_x \right)^{1/2} \left(\int e^{\int_0^t V(X_s) ds} f(X_t) dP_x \right)^{1/2} \\ &= \left(e^{-t(-\Delta+V)} f(x) \right)^{1/2} \left(e^{-t(-\Delta-V)} f(x) \right)^{1/2} \\ &\leq \frac{1}{\varepsilon} e^{-t(-\Delta+V)} f(x) + \varepsilon e^{-t(-\Delta-V)} f(x). \end{aligned}$$

The last inequality holds for all $\varepsilon > 0$. We deduce from this and assertion 2) of Theorem 1⁵ that

$$p(t, x, y) \geq \left(\varepsilon (4\pi)^{-d/2} - \varepsilon^2 C e^{-s(-\Delta-V)t} \left[1 + s(-\Delta-V)t + wt + \frac{|x-y|^2}{t} \right]^{d/2} \right) \\ \times t^{-d/2} \exp \left\{ -\frac{|x-y|^2}{4t} \right\}.$$

We optimize over ε and obtain the Gaussian lower bound. $\square$

3. L^p -GROWTH OF SCHRÖDINGER SEMIGROUPS

The Gaussian upper bound of the heat kernel implies uniform boundedness of $\|e^{-tA}\|_{\mathcal{L}(L^\infty)}$ for $t \in [0, 1]$. In the sequel, we shall consider only the large time $t \geq 1$.

Theorem 4. *Let A be as in (1), (2) or (3). Then there exist two constants C and w such that for every $t \geq 1$,*

$$\|e^{-tA}\|_{\mathcal{L}(L^\infty)} \leq C e^{-s(A)t} (1 + (s(A) + w)t \ln t)^{d/4}.$$

The constant $w = 0$ if $V^- = 0$ or if A is as in (1).

Proof. If A is as in (1), then the heat kernel bound (4) holds. We may assume that $s(A) > 0$, otherwise the theorem follows immediately from (4).

Similarly, if A is as in (2) or (3), then (5) holds and we may assume that $s(A) + w > 0$.

As a consequence of Theorem 1, there exists two positive constants C and δ such that

$$(16) \quad |p(t, x, y)| \leq C t^{-d/2} e^{-s(A)t} \exp \left\{ -\delta \frac{|x-y|^2}{t} \right\} [1 + s(A)t + wt]^{d/2}.$$

⁵Which we apply to the heat kernel of $-\Delta - V$.

On the other hand,

$$\begin{aligned} \int_{\Omega} |p(t, x, y)|^2 dy &= \|e^{-(t-1)A}(p(1, x, \cdot))\|_2^2 \\ &\leq e^{-s(A)2(t-1)} \|p(1, x, \cdot)\|_2^2 \\ &\leq M e^{-s(A)2t}. \end{aligned}$$

Thus,

$$(17) \quad \int_{\Omega} |p(t, x, y)|^2 dy \leq M e^{-s(A)2t} \quad \text{for all } t \geq 1.$$

Now let $\epsilon \in (0, 1)$ and let $p_{\epsilon} \in (0, 1)$ such that $\frac{1-\epsilon}{2} + \frac{\epsilon}{p_{\epsilon}} = 1$. We have by Hölder's inequality,

$$\int_{\Omega} |p(t, x, y)| dy \leq \left(\int_{\Omega} |p(t, x, y)|^2 dy \right)^{\frac{1-\epsilon}{2}} \left(\int_{\Omega} |p(t, x, y)|^{p_{\epsilon}} dy \right)^{\frac{1+\epsilon}{2}}.$$

Using (16) we obtain for $t \geq 1$, that

$$\begin{aligned} &\int_{\Omega} |p(t, x, y)|^{p_{\epsilon}} dy \\ &\leq C^{p_{\epsilon}} t^{-p_{\epsilon}d/2} [1 + s(A)t + wt]^{p_{\epsilon}d/2} e^{-s(A)tp_{\epsilon}} \int_{\Omega} \exp \left\{ -\delta p_{\epsilon} \frac{|x-y|^2}{t} \right\} dy \\ &\leq C' t^{-p_{\epsilon}d/2} [1 + s(A)t + wt]^{p_{\epsilon}d/2} e^{-s(A)tp_{\epsilon}} t^{d/2} p_{\epsilon}^{-d/2}. \end{aligned}$$

Using this, (17), and the expression $p_{\epsilon} = \frac{2\epsilon}{1+\epsilon}$, we see that there exists a constant K independent of ϵ and $t \geq 1$ such that

$$\int_{\Omega} |p(t, x, y)| dy \leq K e^{-s(A)t} t^{d/4} t^{\epsilon d/4} \epsilon^{-d/4}.$$

We optimize over ϵ . The RHS has its minimum for $\epsilon = \frac{1}{\ln t}$ and this proves the theorem. $\square$

As mentioned in the introduction, a result of Simon [23] shows that for $d = 4$, there exist potentials V for which $\|e^{-t(-\Delta+V)}\|_{\mathcal{L}(L^{\infty})}$ grows at least as $\frac{t}{\ln t}$. This shows that the power $d/4$ in the last theorem cannot be improved for general Schrödinger operators.

Remarks. 1) If Ω has finite measure $|\Omega|$, one has a better estimate. More precisely,

$$\|e^{-tA}\|_{\mathcal{L}(L^{\infty}(\Omega))} \leq C \sqrt{|\Omega|} e^{-s(A)t}.$$

This follows immediately from (17).

2) Since $\|e^{-tA}\|_{\mathcal{L}(L^2)} \leq e^{-s(A)t}$, one has by interpolation and duality the following estimate for every $p \in [1, \infty]$:

$$\|e^{-tA}\|_{\mathcal{L}(L^p)} \leq C e^{-s(A)t} [1 + (s(A) + w)t \ln t]^{\frac{d}{2}|\frac{1}{2} - \frac{1}{p}|} \quad \text{for all } t \geq 1.$$

3) It is known that the Gaussian upper bound of the heat kernel implies that the spectrum of the generator on L^p , $1 \leq p < \infty$ is p -independent (see [14], [1], [11],

[20]). One obtains from this that for every $\varepsilon > 0$, there exists a constant C_ε such that

$$\|e^{-tA}\|_{\mathcal{L}(L^p)} \leq C_\varepsilon e^{-s(A)t} e^{\varepsilon t}.$$

Our results show that the exponential term $e^{\varepsilon t}$ can be improved into $(t \ln t)^{d/4}$ for large t .

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