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ESTIMATES OF GLOBAL BOUNDS FOR SOME SCHRÖDINGER HEAT KERNELS ON MANIFOLDS

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ABSTRACT. We establish global bounds for the heat kernel of Schrödinger operators $-\Delta + V$ where V is a certain long range potential. As a consequence we find some conditions for the heat kernel to have global Gaussian lower and upper bound. Some of the conditions are sharp if the potential does not change sign. We also provide a generalized Liouville theorem for Schrödinger operators and a refined version of the trace formula of Sa Barreto and Zworski [SZ].

1. Introduction

A fundamental result proved in [A] states that the fundamental solution of a second order uniformly parabolic equation in divergence form has Gaussian lower and upper bounds. However, in general, these bounds are not global in time since the parameters in these bounds depend, in an implicit manner, on the lower order terms of the equation. The following example illustrates the need for a better understanding of the bounds. By standard estimates, the fundamental solution of $\Delta + V - \partial_t$ with $V \in L^\infty$ satisfies

$$\frac{c_n e^{-\|V\|_\infty t}}{t^{n/2}} e^{-\frac{|x-y|^2}{4t}} \leq G(x, t; y, 0) \leq \frac{c_n e^{\|V\|_\infty t}}{t^{n/2}} e^{-\frac{|x-y|^2}{4t}}.$$

The presence of the functions $e^{\|V\|_\infty t}$and $e^{-\|V\|_\infty t}$ masks a wealth of information and makes the bounds less useful when $t \to \infty$.

An important question arises:

Does there exist a global estimate on the heat kernel of $-\Delta + V$, which reveals an explicit dependence on the potential V?

Many authors have studied the above the problem. We refer the reader to [Si1], [M], [DS], [NS], [LY], [N], [SZ], [Se], [Zg2], [Zo2] and the papers quoted there.

Let us sketch two interesting recent results in [SZ] and [Se]. In the main Lemma 3.2 in [SZ], Sa Barreto and Zworski proved that the heat kernel of $-\Delta + V$ has global Gaussian upper bound provided that V has super exponential decay and $-\Delta + V$ has no negative eigenvalue and 0 is not a pole of the resolvent. On the other hand, Semenov [Se] proved that $-\Delta + V$ with $V \geq 0$ has a global Gaussian lower bound if and only if $\Delta^{-1} V \in L^\infty(\mathbf{R}^n)$. As indicated below in Remark 1.1, this class of functions, also called Green bound functions, belong to short range potentials since these functions essentially decay faster than $1/|x|^2$ near infinity.

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These works show that knowledge of the global behavior of the fundamental solution is instrumental in various fields such as scattering theory, spectrum analysis. As pointed out in [Zg3], information on global bounds is also related to the study of global solutions to semilinear parabolic equations.

In the first part of the paper we obtain a global lower bound for the heat kernel of V which not only recaptures all the previous lower bounds obtained in the papers quoted above but also covers far wider choices of potential V. For instance Theorem A below is valid for long range potentials that are just L^∞ bounded near infinity. When V satisfies $|V(x)| \to \infty$ as $|x| \to \infty$, global estimates for the heat kernel are well-known. For example, see Section 4.5 in [D]. While the paper [Se] deals with short range potentials essentially having faster than quadratic decay. Our result seems to fill the gap when the potential is long range, i.e., when V is bounded or decays to zero near infinity at slower than quadratic rate.

In the second part of the paper, we obtain several necessary and sufficient conditions on a class of potentials V so that the heat kernel of $L = -\Delta + V$ has global Gaussian upper bound. In contrast, previous papers [SZ] and [Se] established only certain sufficient conditions.

In [Zo2], the equivalence of the subcriticality of L to a number of important properties of L was established, assuming that the potential V is Green tight (see Definition 1.1 below). In this paper we shall introduce two more equivalent conditions: global Gaussian bound and uniform stability. As an application we offer a generalized Liouville theorem and an improvement of a trace formula recently obtained in [SZ] (see Section 4 below).

In addition to establishing the above new estimates in the Euclidean setting, we will also generalize them to the case of complete noncompact manifolds where new difficulties arise (see the remark after Corollary A).

Let us fix a number of notations and assumptions. Unless stated otherwise, $\mathbf{M}$ is always an n-dimensional complete noncompact Riemannian manifold with nonnegative Ricci curvature. G stands for the heat kernel of the operator $-\Delta + V$ on $\mathbf{M}$; G_0 is the heat kernel of $-\Delta$, the Laplace Beltrami operator in $\mathbf{M}$. Γ_0 and Γ will be the Green's functions of $-\Delta$ and $-\Delta + V$ respectively. We always assume that the manifold is nonparabolic, i.e., $\Gamma_0 \geq 0$. If $c > 0$ and $t > s$, then we write

$$(1.1) \qquad G_c = G_c(x, t; y, s) \equiv \frac{1}{|B(x, (t-s)^{1/2})|} \exp\left(-c\frac{|x-y|^2}{t-s}\right).$$

Let $V = V(x)$ be any Borel measurable function and $t > 0$; then we write

$$(1.2) \qquad K_V(t) = \sup_x \int_0^t \int_{\mathbf{M}} G_c(x, t; y, s)|V(y)|\, dy\, ds.$$

The value of $K_V(t)$ depends on c which is chosen to be sufficiently small. Note that

$K_V(t)$ is locally finite if $V \in L^p_{\text{loc}}$ with $p > n/2$ is merely bounded near infinity. To better state Theorems B and C and following [Zo1] we have:

Definition 1.1. (a) A Borel measurable function V is called Green-bound in $\mathbf{M}$ if $\sup_x \int_{\mathbf{M}} \Gamma_0(x, y)|V(y)|\,dy < \infty$.

(b) A Borel measurable function V is called Green-tight in $\mathbf{M}$ if

$$\lim_{R\to\infty} \sup_x \int_{|y|\geq R} \Gamma_0(x, y)|V(y)|\,dy = 0.$$

Remark 1.1. Any functions $V(x)$ satisfying $|V(x)| \leq C/(1+|x|^q)$ with $q > 2$ are Green-tight functions in $\mathbf{M}$. For a proof and other properties, please see [Zo1]. It is also clear that V is a Green bound function if and only if $\Delta^{-1}V \in L^\infty$. A Green tight function is a Green bound function.

Remark 1.2. Throughout the paper we assume that the potential V restricted to any compact set is in the Kato class K_n, which allows singularities worse than those in L^p_{loc}, $p > n/2$. A Borel measurable function V is in K_n if $\lim_{r\to 0}[\sup_x \int_{|x-y|\leq r} \frac{|V(y)|}{|x-y|^{n-2}}\,dy] = 0$. More properties about this natural class of functions can be found in [AS] and [Si2].

The main results of the paper are the next three theorems. Theorem A covers both long range and short range potentials. Here we say a potential has short range if it is Green bound. We stress that Theorem A holds for all complete noncompact manifolds with nonnegative Ricci curvature and no extra assumptions are needed. Let $V^+ = V^+(x) = \max\{V(x), 0\}$.

THEOREM A (GLOBAL LOWER BOUND). *There exist positive constants c_1, c_2 depending only on $\mathbf{M}$ such that*

$$G(x,t;y,0) \geq \begin{cases} \frac{c_1}{|B(x,t^{1/2})|} e^{-c_2 K_{V^+}(t)}, & d(x,y)^2 \leq t, \\ \frac{c_1}{|B(x,t^{1/2})|} e^{-c_2 \frac{d(x,y)^2}{t}[1+K_{V^+}(\frac{t^2}{d(x,y)^2})]}, & d(x,y)^2 \geq t. \end{cases}$$

We emphasize that for each t, $K_V(t)$ is easy to compute for all V (in the local Kato class) which are L^∞ bounded near infinity. In particular this includes long range potentials behaving like $\frac{a}{d(x)^k}$ (near infinity) with any $k \in [0, 2]$. This makes the result new even in the Euclidean case. The next corollaries indicate the powerful nature of the above estimates.

COROLLARY A. *If $V \geq 0$, then the heat kernel of $-\Delta + V$ has global Gaussian lower and upper bound if and only if V is Green bound.*

We remark that the result in Corollary A in the Euclidean case has been proven recently in [Se], which uses a semigroup method. We are not able to generalize that method to the present setting which is inhomogeneous in nature. For example the L^1 to L^∞ norm of the semigroup generated by $-\Delta$, which is $c/t^{n/2}$ in $\mathbf{R}^n$, may be difficult to compute or define in the general case. Therefore a different approach is needed. We mention that Corollary A on the manifold case was first proved directly in [Zg1] and was used to study some nonlinear problems.

In the special case $V = V^+ = 1$, we have $K_V(s) \le Cs$ for $s = t$ or $s = \frac{t^2}{d(x,y)^2}$. Theorem A then implies $G(x, t; y, 0) \ge CG_c(x, t; y, 0)e^{-ct}$. Since $G = G_0 e^{-t}$, this indicates that the on-diagonal part of the lower bound in Theorem A is sharp up to a constant.

The next corollary deals with long range potentials having quadratic or slower decay. Potentials with quadratic decay lie just beyond Green bound functions. From [BG], we know this is a very subtle situation. The same result was obtained in [Zg3] by a different method.

COROLLARY B. *Let* $\mathbf{M} = \mathbf{R}^n$ *and* $n \ge 3$.

(*a*) *If* $0 \le V(x) \le \frac{a}{1+d^2(x,0)}$ *with* $a > 0$, *then there exist constants* $c > 0$, $\alpha > 0$ *depending only on* $\mathbf{M}$ *and* a *such that*

$$G(x, t; y, 0) \ge \frac{c}{t^\alpha}, \qquad d(x, y)^2 \le t.$$

(*b*) *If* $0 \le V(x) \le \frac{a}{1+d^k(x,0)}$ *for any* $0 \le k < 2$, *then there exist constants* $c_1, c_2 > 0$ *such that*

$$G(x, t; y, 0) \ge c_1 e^{-c_2 t^{1-(k/2)}}/t^{n/2}, \qquad d(x, y)^2 \le t.$$

THEOREM B. *Let* $\mathbf{M} = \mathbf{R}^n$ *with* $n \ge 3$. *Suppose* V *is Green tight. Then the following are equivalent.*

(*a*) G, *the heat kernel of* $-\Delta + V$, *has global Gaussian bounds, i.e., there are positive constants* a *and* c *such that*

$$\frac{1}{c(t-s)^{n/2}} e^{-\frac{|x-y|^2}{a(t-s)}} \le G(x, t; y, s) \le \frac{c}{(t-s)^{n/2}} e^{-a\frac{|x-y|^2}{t-s}},$$

for all $t > s$ *and all* $x, y \in \mathbf{R}^n$, $n \ge 3$.

(*b*) *For* Γ, *the Green's function of* $-\Delta + V$, *there is a positive constant* b *such that, for all* $x, y \in \mathbf{R}^n$,

$$b^{-1}\Gamma_0(x, y) \le \Gamma(x, y) \le b\Gamma_0(x, y).$$

(*c*) *The operator* $-\Delta + V$ *is subcritical, i.e., there exists* $\epsilon > 0$ *such that* $-\Delta + (1+\epsilon)V \ge 0$.

(*d*) *Gaugeability, i.e.,* $u_0(x) \equiv E^x[e^{-\int_0^\infty V(X_t)\,dt}]$ *is bounded in* $\mathbf{R}^n$.

(*e*) *Uniform stability, i.e.,* $\|p_t\|_{\infty,\infty} < C < \infty$.

Remark 1.3. In the above, $\{X_t : t > 0\}$ is the set of Brownian motions in $\mathbf{M}$ and E^x is the expectation on the Brownian paths starting from x. p_t is the semigroup generated by $-\Delta + V$, which is also denoted by $e^{-t(-\Delta+V)}$ for convenience.

There are many other conditions equivalent to the subcriticality of an operator. We refer to [Zo2] for details.

Remark 1.4. The function u_0 in (d) is a solution of $-\Delta u + Vu = 0$. A proof can be found in [Zo2].

The classical Liouville theorem states that all bounded harmonic functions are constants. This was later generalized to manifolds by S. T. Yau. The next theorem provides a similar result for Schrödinger operators on manifolds. In the Euclidean case it has been proven by Z. Zhao [Zo3] using probability. The current result will be proved by analytical means. To achieve this we make crucial use of the Gaussian upper bound similar to that in Theorem B and the deep results in [Li].

THEOREM C (Generalized Liouville Theorem). *Let* $\mathbf{M}$ *be a complete noncompact manifold with Euclidean growth, which means* $|B(x,r)| \geq Cr^n$ *for* $C > 0$. *Suppose* $V = V(x)$ *satisfies* $|V(x)| \leq \frac{C}{1+d(x,x_0)^a}$ *for* $a > 2$, $n \geq 3$, *and the heat kernel* $-\Delta + V$ *has global Gaussian upper bound. Then bounded solutions to the Schrödinger equation*

$$-\Delta u + Vu = 0 \tag{1.3}$$

are unique up to a constant. More precisely, if u_1 *and* u_2 *are two bounded nontrivial solutions to* (1.3), *then* $u_1 = cu_2$ *for a constant* c.

Remark 1.5. If $\mathbf{M} = \mathbf{R}^n$, then by Theorem B, the above condition that the heat kernel p_t has global Gaussian upper bound can be replaced by $-\Delta + V$ subcritical. Note that the result in [Zo3] is slightly stronger than Theorem C in the Euclidean case since only the conditions that V is Green tight and $-\Delta + V$ is subcritical are required in [Zo3]. However we are not able to generalize the method in [Zo3] to the manifold case. By Theorem A in [Zg2], which holds for heat kernels p_t of $-\Delta + V$ on all noncompact complete manifolds with Ricci ≥ 0, there exists a $\delta > 0$ such that p_t has global Gaussian upper bound provided that $V^+(x) \leq \frac{\delta}{1+d(x,x_0)^\alpha}$ for $\alpha > 2$.

Recently Grigo'yan and Hansen [GH] have obtained a different Liouville type property for (1.3). They obtained conditions on V so that the only bounded solution to (1.3) is 0. If one assumes a priori that (1.3) has a positive bounded solution then a result similar to Theorem C in $\mathbf{R}^n$ was established by B. Simon ([Si], Theorem 3.4).

We will prove Theorems A, B, C in Sections 2, 3 and 4 respectively. More applications and examples are given in Section 4.

2. Proof of Theorem A

Clearly we only need to prove the theorem when $V \geq 0$ i.e. $V = V^+$.

Step 1. We prove that there exists $\epsilon > 0$ depending only on $\mathbf{M}$ such that the following holds. For any $T > 0$, suppose $K_V(T) \le \epsilon$, then G, the heat kernel of $-\Delta + V$, satisfies

$$G(x, t; y, s) \ge C/|B(x, (t-s)^{1/2})| \tag{2.1}$$

for all $0 < s < t \le T$ and $d(x, y)^2 \le t - s$. Here C is a positive constant independent of T.

By Duhamel's principle, we have

$$\begin{aligned} G(x, t; y, s) &= G_0(x, t; y, s) \\ &\quad - \int_s^t \int_{\mathbf{M}} G(x, t; z, \tau)\, V(z)\, G_0(z, \tau; y, s)\, dz\, d\tau, \end{aligned} \tag{2.2}$$

where $x, y \in \mathbf{M}$ and $s < t$.

Iterating (2.2) we obtain

$$\begin{aligned} G(x, t; y, s) &= G_0(x, t; y, s) + \Sigma_{k=1}^{\infty} G_0 * (HG_0)^{*k}(x, t; y, s) \\ &\equiv G_0(x, t; y, s) + \Sigma_{k=0}^{\infty} J_k(x, t; y, s) \end{aligned} \tag{2.2$'$}$$

where $HG_0(x, t; y, s) \equiv -V(x) G_0(x, t; y, s)$.

First of all, by [LY], there is a constant A such that

$$G_0(x, t; y, s) \le \frac{A}{|B(x, (t-s)^{1/2})|} \exp\left(-\alpha \frac{d(x, y)^2}{t-s}\right) \le \frac{A}{|B(x, (t-s)^{1/2})|}. \tag{2.3}$$

Next,

$$\begin{aligned} |J_1(x, t; y, s)| &= \left| \int_s^t \int_D G_0(x, t; z, \tau) V(z) G_0(z, \tau; y, s)\, dz\, d\tau \right| \\ &\le A^2 \int_s^t \int_{\mathbf{M}} \frac{1}{|B(x, (t-\tau)^{1/2})|} \exp\left(-\alpha \frac{d(x, z)^2}{t-\tau}\right) \\ &\quad \times \frac{|V(z)|}{|B(y, (\tau - s)^{1/2})|} \exp\left(-\alpha \frac{d(z, y)^2}{\tau - s}\right) dz d\tau \\ &= A^2 \int_s^{\frac{t+s}{2}} \int_D \cdots dz\, d\tau + \epsilon A^2 \int_{\frac{t+s}{2}}^t \int_D \cdots dz\, d\tau. \end{aligned}$$

When $\tau \in [s, \frac{t+s}{2}]$, $t - \tau \ge (t-s)/2$; when $\tau \in [\frac{t+s}{2}, t]$, $\tau - s \ge (t-s)/2$. Hence

$$\begin{aligned} &|J_1(x, t; y, s)| \\ &\le \frac{CA^2}{|B(x, (t-s)^{1/2})|} \int_s^{\frac{t+s}{2}} \int_D |V(z)| \frac{1}{|B(y, (\tau-s)^{1/2})|} \exp\left(-\alpha \frac{d(z, y)^2}{\tau - s}\right) dz\, d\tau \\ &\quad + \frac{CA^2}{|B(x, (t-s)^{1/2})|} \int_{\frac{t+s}{2}}^t \int_D \frac{1}{|B(x, (t-\tau)^{1/2})|} \exp\left(-\alpha \frac{d(x, z)^2}{t-\tau}\right) |V(z)|\, dz\, d\tau. \end{aligned}$$

Here we have used the fact that $|B(x, (t-s)^{1/2})|$ is comparable to $|B(y, (t-s)^{1/2})|$, which is due to the inequality $d(x, y)^2 \le t - s$ and the doubling property.

Hence we have

$$|J_1(x, t; y, s)| \le \frac{CA^2}{|B(x, (t-s)^{1/2})|} K_V(t). \tag{2.4}$$

Following an induction argument as in [Zg2], for $k \ge 1$ we have

$$|J_k(x, t; y, s)| \le \frac{[C_0 K_V(t)]^k}{|B(x, (t-s)^{1/2})|}, \tag{2.5}$$

Substituting the above estimate in (2.2′), we obtain

$$G(x, t; y, s) \ge G_0(x, t; y, s) - \Sigma_{k=1}^{\infty} \frac{[C_0 K_V(t)]^k}{|B(x, (t-s)^{1/2})|}.$$

If $d(x, y)^2 \le t - s$, then $G_0(x, t; y, s) \ge C/|B(x, (t-s)^{1/2})|$. Since $K_V(t) \le K_V(T) \le \epsilon$, clearly we can choose ϵ so small that

$$G(x, t; y, s) \ge C/|B(x, (t-s)^{1/2})|, \tag{2.6}$$

when $d(x, y)^2 \le t - s$ and $0 < s < t \le T$. Obviously ϵ can be chosen to depend on $\mathbf{M}$ only.

Step 2. We prove that, for all $t > 0$,

$$G(x, t; y, 0) \ge \frac{c_1}{|B(x, t^{1/2})|} e^{-c_2 K_{V+}(t)}, \quad d(x, y)^2 \le t.$$

Here c_1 and c_2 depend only on $\mathbf{M}$.

Fixing any $t > 0$, we assume $K_V(t) > \epsilon$ where ϵ is the constant from step 1. Otherwise step 1 already establishes the result. Let $\eta = \epsilon / K_V(t)$. Then $\eta < 1$ and $K_{\eta V}(t) = \epsilon$. Let $\tilde{G}$ be the heat kernel of $-\Delta + \eta V$. By step 1, for such a fixed t, we have

$$\tilde{G}(x, t; y, 0) \ge \frac{C}{|B(x, t^{1/2})|}, \quad d(x, y)^2 \le t.$$

The bridge between $\tilde{G}$ and G is built by the Feynman-Kac formula, which is well-known to hold for the current case since $-\Delta$ is essentially self adjoint and it generates a contraction semigroup when $\mathbf{M}$ has nonnegative Ricci curvature (see [D]). We point out that one can also use the Trotter [T] product formula, which uses only analytic method, to obtain the same result.

Let $\{X_t : t > 0\}$ be the Brownian motions in $\mathbf{M}$ and E^x be the expectation on the Brownian paths starting from x. Using Hölder's inequality on the Feynman-Kac formula, for any nonnegative $f \in C_0^\infty(\mathbf{M})$ one has

$$\begin{aligned}
&\int_{\mathbf{M}} \tilde{G}(x,t;y,0) f(y)\,dy \\
&\quad = \left[E^x \exp\left(-\eta \int_0^t V(X_\tau)\,d\tau \right) f(X_t) \right] \\
&\quad = \left[E^x \exp\left(-\eta \int_0^t V(X_\tau)\,d\tau \right) f^\eta(X_t) f^{1-\eta}(X_t) \right] \\
&\quad \le \left[E^x \exp\left(- \int_0^t V(X_\tau)\,d\tau \right) f(X_t) \right]^\eta \left[E^x f(X_t) \right]^{1-\eta} \\
&\quad = \left[\int_{\mathbf{M}} G(x,t;y,0) f(y)\,dy \right]^\eta \left[\int_{\mathbf{M}} G_0(x,t;y,0) f(y)\,dy \right]^{1-\eta}.
\end{aligned}$$

By choosing a sequence approximating the Dirac δ function, we deduce that

$$\tilde{G}(x,t;y,0) \le [G(x,t;y,0)]^\eta [G_0(x,t;y,0)]^{1-\eta}.$$

Noting that G_0 is the heat kernel of the free Laplacian, we have

$$\tilde{G}(x,t;y,0) \le C[G(x,t;y,0)]^\eta [1/|B(x,t^{1/2})|]^{1-\eta},$$

which yields, via the lower bound for $\tilde{G}$,

$$\begin{aligned}
G(x,t;y,0) &\ge C\left[|B(x,t^{1/2})|^{1-\eta} \tilde{G}(x,t;y,0) \right]^{1/\eta} \\
&\ge C\left[|B(x,t^{1/2})|^{1-\eta} \frac{C}{|B(x,t^{1/2})|} \right]^{1/\eta} = \frac{C^{1/\eta}}{|B(x,t^{1/2})|} = \frac{e^{-cK_V(t)\epsilon^{-1}}}{|B(x,t^{1/2})|}
\end{aligned}$$

where $d(x,y)^2 \le t-s$ and $t > s$. This completes step 2.

Step 3. We establish the off-diagonal lower bound.

To this end, we follow a standard path in [FS]. One can also see Theorem 3.3.4 in [D]. For completeness we present a proof modeling that in [D]. We remind the reader that in [D] the lower order terms are zero.

Let $t > 0$ and $x, y \in \mathbf{M}$ be arbitrary. Suppose $l = l(s)$ is a minimal geodesic connecting x and y which is parametrized by length. If we put

$$x_r = l(rd(x,y)/M)$$

for $0 \le r \le M$ then

$$d(x_r, x_{r+1}) \le \frac{1}{2}(t/M)^{1/2}$$

if and only if

$$4d(x,y)^2/t \le M.$$

We take M to be the smallest integer which satisfies this inequality. Then

$$G(x,t;y,0) \ge \int G(x,\frac{t}{M};y_1,0)G\left(y_1,\frac{t}{M};y_2;0\right)\cdots G\left(y_{M-1},\frac{t}{M};y;0\right)dy_1\cdots dy_{M-1}$$

where we integrate y_r over the set

$$\left\{y_r : d(y_r,x_r) < \frac{1}{4}(t/M)^{1/2}\right\}.$$

Applying (2.6), for y_r in the region above, by the doubling property we have

$$\begin{aligned} G\left(y_{r-1},\frac{t}{M};y_r,0\right) &\ge Ce^{-cK_V(t/M)}/|B(y_r,(t/M)^{1/2})| \\ &\ge Ce^{-cK_V(t/M)}/|B(x_r,(t/M)^{1/2})|. \end{aligned}$$

This yields the bound

$$\begin{aligned} G(x,t;y,0) &\ge \Pi_{r=0}^{M-1}\left[\frac{Ce^{-cK_V(t/M)}}{|B(x_r,(t/M)^{1/2})|}\right]\Pi_{r=1}^{M-1}\left[C|B(x_r,(t/M)^{1/2})|\right] \\ &\ge C^M e^{-cMK_V(t/M)}/|B(x,(t/M)^{1/2})|. \end{aligned}$$

Since M is close to $4d(x,y)^2/t$, by the doubling condition the above implies that for some $c_1, c_2 > 0$,

$$G(x,t;y,0) \ge c_1^{-1}G_{c_2^{-1}}(x,t;y,0)e^{-c_2\frac{d(x,y)^2}{t}K_V\left(\frac{t^2}{d(x,y)^2}\right)}.$$

for all $x, y \in \mathbf{M}$, all $t > 0$.

Proof of Corollary A. Suppose $V \ge 0$ is Green bound. Then, for all $t > 0$,

$$K_V(t) \le \sup_x \int_{\mathbf{M}} V(y)\Gamma_0(x,y)\,dy \le C < \infty.$$

The global Gaussian lower bound follows immediately from Theorem A. The Gaussian upper bound always holds since $V \ge 0$.

Now suppose G, the heat kernel of $-\Delta + V$, has global Gaussian lower and upper bound. By Duhamel's principle,

$$G(x,t;y,s) = G_0(x,t;y,s) - \int_s^t \int_{\mathbf{M}} G(x,t;z,\tau)\,V(z)\,G_0(z,\tau;y,s)\,dz\,d\tau,$$

where as before, G_0 is the heat kernel of the Laplacian. By assumption, there are positive numbers c_1 and c_2 such that $G(x,t;z,\tau) \geq c_1 G_{c_2}(x,t;z,\tau)$. Hence

$$c_1 \int_s^t \int_{\mathbf{M}} G_{c_2}(x,t;z,\tau)\, V(z)\, G_0(z,\tau;y,s)\, dz\, d\tau \leq G_0(x,t;y,s) - G(x,t;z,\tau).$$

Integrating the above inequality with respect to x , we deduce that for some $C > 0$,

$$\int_s^t \int_{\mathbf{M}} V(z)\, G_0(z,\tau;y,s)\, dz\, d\tau \leq C,$$

which implies

$$\sup_{y\in\mathbf{M}} \int_{\mathbf{M}} \Gamma_0(y,z) V(z)\, dz \leq C.$$

This means V is Green bound. $\square$

Proof of Corollary B. Suppose $0 \leq V(x) \leq \frac{C}{1+|x-x_0|^k}$, for $k \in [0,2]$. For $t > 1$ we have

$$\begin{aligned}
K_V(t) &\leq C + C \sup_x \int_1^t \int_{\mathbf{R}^n} \frac{1}{s^{n/2}} e^{-c\frac{|x-y|^2}{s}} \frac{1}{1+|x_0-y|^k}\, dy\, ds \\
&\leq C + C \sup_x \int_1^t \int_{|x_0-y|^2\leq s} \frac{1}{s^{n/2}} e^{-c\frac{|x-y|^2}{s}} \frac{1}{1+|x_0-y|^k}\, dy\, ds \\
&\quad + C \sup_x \int_1^t \int_{|x_0-y|^2\geq s} \frac{1}{s^{n/2}} e^{-c\frac{|x-y|^2}{s}} \frac{1}{1+|x_0-y|^k}\, dy\, ds \\
&\leq C + C \sup_x \int_1^t \int_{|x_0-y|^2\leq s} \frac{1}{s^{n/2}} \frac{1}{1+|x_0-y|^k}\, dy\, ds \\
&\quad + C \sup_x \int_1^t \int_{|x_0-y|^2\geq s} \frac{1}{s^{n/2}} e^{-c\frac{|x-y|^2}{s}} \frac{1}{s^{k/2}}\, dy\, ds \\
&\leq C + \sup_x \int_1^t \frac{1}{s^{n/2}} \int_{|x_0-y|^2\leq s} \frac{1}{1+|x_0-y|^k}\, dy\, ds + C \int_1^t \frac{1}{s^{k/2}}\, ds \\
&\leq C + C \int_1^t \frac{1}{s^{k/2}}\, ds.
\end{aligned}$$

If $k = 2$, then $K_V(t) \leq c + \beta \ln t$. Here β is a nonnegative number. When $|x-y|^2 \leq 1$ and $t > 1$, using Theorem A we have

$$G(x,t;y,0) \geq \frac{C}{t^{n/2}} e^{-c_2(C+\beta\ln t)} = \frac{C}{t^{(n+2c_2\beta)/2}}.$$

If $0 \le k < 2$, then $K_V(t) \le ct^{1-(k/2)}$. Using Theorem A again, when $|x-y|^2 \le 1$ and $t > 1$ we have

$$G(x,t;y,0) \ge \frac{Ce^{-ct^{1-(k/2)}}}{t^{n/2}}. \qquad \square$$

3. Proof of Theorem B

We shall follow the chart: $(a) \Rightarrow (b) \Rightarrow (c) \iff (d) \iff (e)$ and $(c) \Rightarrow (a)$. The proof is divided into several steps.

Step 1. $(a) \Rightarrow (b)$ is trivial since $\Gamma(x,y) = \int_0^\infty G(x,t;y,0)\,dt$.

Next we show that $(b) \Rightarrow (c)$. To this end we first prove that the operator $-\Delta + (1+\epsilon)V$ has a positive Green's function when ϵ is sufficiently small. Let Γ_ϵ denote the Green's function of $-\Delta + (1+\epsilon)V$. Then, formally,

$$\Gamma_\epsilon(x,y) = \Gamma(x,y) - \epsilon \int_{\mathbf{R}^n} \Gamma_\epsilon(x,z)\, V(z)\, \Gamma(z,y)\,dz. \tag{3.1}$$

We use the word formally since the existence of Γ_ϵ is not yet justified.

Iterating (3.1) we obtain

$$\begin{aligned} \Gamma_\epsilon(x,y) &= \Gamma(x,y) + \Sigma_{k=1}^\infty \Gamma * (-\epsilon V\Gamma)^{*k}(x,y) \\ &\equiv \Gamma(x,y) + \Sigma_{k=0}^\infty I_k(x,y) \end{aligned} \tag{3.2}$$

By (b), there is a positive constant c_3 such that

$$c_3^{-1}\Gamma_0(x,y) \le \Gamma(x,y) \le c_3^{-1}\Gamma_0(x,y), \tag{3.3}$$

for all $x, y \in \mathbf{R}^n$. Hence

$$\begin{aligned} |I_1| &\le \epsilon \int_{\mathbf{R}^n} \Gamma_0(x,z)|V(z)|\Gamma_0(z,y)\,dz \\ &\le \epsilon \int_{|x-z|\ge|x-y|/2} \Gamma_0(x,z)|V(z)|\Gamma_0(z,y)\,dz \\ &\quad + \epsilon \int_{d(z,y)\ge|x-y|/2} \Gamma_0(x,z)|V(z)|\Gamma_0(z,y)\,dz \end{aligned}$$

Hence

$$|I_1| \le C\epsilon K(V)\Gamma_0(x,y)$$

where $K(V) = \sup_x \int_{\mathbf{R}^n} \Gamma_0(x,y)|V(y)|\,dy$.

By an induction, for $k = 1, 2, \ldots$ we have

$$|I_k| \le [\epsilon C K(V)]^k \Gamma_0(x,y). \tag{3.4}$$

Using the lower bound in (3.3) together with (3.2) and (3.4), we deduce that

$$\Gamma_\epsilon(x,y) \geq \frac{1}{c_3}\Gamma_0(x,y) - \Sigma_{k=1}^{\infty}[\epsilon CK(V)]^k\Gamma_0(x,y) \geq c_4\Gamma_0(x,y) > 0$$

when ϵ is sufficiently small. From here it is standard to show that Γ_ϵ is a positive Green's function for $-\Delta + (1+\epsilon)V$. Now we can follow the Allegretto-Piepenbrink theory (see [Si2]) to show that the operator $-\Delta + (1+\epsilon)V \geq 0$, and hence the operator $-\Delta + V$ is subcritical by definition. Indeed let $f \in C_0^\infty(\mathbf{R}^n)$; we choose a point x_0 outside of the support of f. Then $u = \Gamma_\epsilon(x, x_0)$ is a positive solution of $-\Delta u + (1+\epsilon)Vu = 0$ in $\mathbf{R}^n - \{x_0\}$ (see Theorem 6.4 in [CZ]). By Theorem C.8.2 in [Si2], we have $\int_{\mathbf{R}^n}(|\nabla f|^2 + (1+\epsilon)Vf^2)\,dx \geq 0$. Since f is arbitrary, we know that $-\Delta + (1+\epsilon)V$ is a nonnegative operator in $\mathbf{R}^n$.

Step 2. From [Zo2] we know that (c) is equivalent to (d). Now we prove that (d) is equivalent to (e).

First we show that (e) $\Rightarrow$ (d). By the positivity of p_t, it is clear that

$$\|p_t\|_{\infty,\infty} = \|p_t 1\|_\infty = \sup_x E^x\left[e^{-\int_0^t V(X_\tau)}\,d\tau\right].$$

Assuming p_t has uniform stability, then $\|p_t\|_{\infty,\infty} \leq C$. Hence $E^x[e^{-\int_0^t V(X_\tau)d\tau}] \leq C$. By Fatou's lemma, we have

$$u_0(x) = E^x\left[e^{-\int_0^\infty V(X_\tau)\,d\tau}\right] \leq C.$$

This proves (d), i.e., gaugeability.

Next we prove that $(d) \Rightarrow (e)$.

Again let $u_0 = E^x[e^{-\int_0^\infty V(X_\tau)d\tau}]$. We claim that there exist $A, B > 0$ such that $B \leq u_0(x) \leq A < \infty$ for all $x \in \mathbf{R}^n$. Since V is Green tight, we have

$$\sup_{x\in\mathbf{R}^n} E^x \int_0^\infty |V(X_t)|\,dt \leq \sup_x \int_{\mathbf{R}^n} \Gamma_0(x,y)|V(y)|\,dy < C < \infty.$$

By Jensen's inequality,

$$u_0 = E^x[e^{-\int_0^\infty V(X_t)\,dt}] \geq e^{-E^x\int_0^\infty V(X_t)\,dt} \geq B > 0.$$

The upper bound holds by assumption. This proves the claim. By Theorem 2 of [Zo2], u_0 is a solution to $-\Delta u + Vu = 0$. Hence $p_t u_0 = u_0$. Therefore

$$p_t 1(x) \leq \frac{1}{B} p_t u_0(x) = \frac{1}{B} u_0(x) \leq \frac{A}{B}.$$

Therefore $\|p_t\|_{\infty,\infty} = \|p_t 1\|_\infty \leq A/B$.

Step 3. Finally we only need to show that (c) $\Rightarrow$ (a) since we already proved that (a) $\Rightarrow$ (c).

We will follow the arguments in Lemma 3.2 in [SZ], which uses a combination of ideas in [D] and [Si2]. For this reason we will be brief. Since $-\Delta + V$ is subcritical, there is an $\epsilon > 0$ such that $-\Delta + (1+2\epsilon)V \geq 0$. Hence

$$-\Delta + (1+\epsilon)V \geq -\epsilon\Delta. \tag{3.5}$$

Since (c) is equivalent to (e), we know that $\|p_t\|_{\infty,\infty} \leq C < \infty$, which, by duality and interpolation, implies $\|p_t\|_{1,1}$, $\|p_t\|_{2,2} \leq C < \infty$. Hence we can apply Theorem 2.4.2 in [D] to conclude that

$$\|e^{-t(-\Delta+(1+\epsilon)V)}\|_{2,\infty} \leq C(V)t^{-n/4}.$$

As in [SZ], one obtains

$$e^{-t(-\Delta+(1+\epsilon)V)}(x,y) \leq C(V)/t^{n/2}. \tag{3.6}$$

Let $1 < q, q' < \infty$ satisfy $\frac{1}{q} + \frac{1}{q'} = 1$. Applying Hölder's inequality to the Feynman-Kac formula, we obtain

$$e^{-t(-\Delta+V)}(x,y) \leq \left[e^{-t(-\Delta+qV)}(x,y)\right]^{1/q}\left[e^{-t(-\Delta)}(x,y)\right]^{1/q'}. \tag{3.7}$$

Taking $q = 1+\epsilon$, using (3.6) and (3.7), the Gaussian upper bound follows. The Gaussian lower bound is a consequence of Corollary A as follows.

First we use Corollary A with V is replaced by V^+. We stress that we did not use the condition that $-\Delta + V$ is subcritical in the proof of the global lower bound. As V^+ is Green bound, we know that the heat kernel of $-\Delta + V^+$ has global Gaussian lower bound. By the maximum principle, we know that the heat kernel of $-\Delta + V$ is not smaller than that of $-\Delta + V^+$. Hence the former must also have global Gaussian lower bound. This completes the proof Theorem B.

4. Proof of Theorem C and other applications and examples

Proof of Theorem C. First we claim that any bounded solution to

$$-\Delta u + Vu = 0 \tag{4.1}$$

satisfies the following integral equation for a suitable constant C:

$$u(x) = C - \int_{\mathbf{M}} \Gamma(x,y)V(y)u(y)\,dy.$$

The proof of the claim is as follows. Since u is bounded, it is easy to verify that $u_0(x) \equiv -\int_{\mathbf{M}} \Gamma(x,y)V(y)u(y)\,dy$ satisfies

$$\Delta u_0 = Vu.$$

Hence $\Delta(u-u_0)=0$. Moreover $u-u_0$ is bounded. By S. T. Yau's Liouville theorem for the free Laplacian on $\mathbf{M}$, we know that $u-u_0=C$. This proves the claim.

Next we prove that the only bounded solution to

$$u(x)=-\int_{\mathbf{M}}\Gamma_0(x,y)V(y)u(y)\,dy \tag{4.2}$$

is zero. Let u be a bounded solution to (4.2), then

$$|u(x)|\le C\int_{\mathbf{M}}\Gamma_0(x,y)|V(y)|\,dy.$$

By our assumption on V and the estimate in [LY], we have

$$|u(x)|\le C\int_{\mathbf{M}}\frac{1}{d(x,y)^{n-2}(1+d(y,x_0)^a)}\,dy.$$

Since $a>2$ and $\mathbf{M}$ has maximum growth, we can find a constant $b>0$ such that

$$|u(x)|\le\frac{C}{1+d(x,x_0)^b}. \tag{4.3}$$

Since u is a solution to (4.1), it is also a solution to the corresponding heat equation, i.e.,

$$\Delta u(x)-V(x)u(x)-u_t(x)=0\qquad\text{in } \mathbf{M}\times(0,\infty)$$

with u itself as the initial value.

As before, let G be the heat kernel of $-\Delta+V$. We have

$$u(x)=\int_{\mathbf{M}}G(x,t;y,0)u(y)\,dy.$$

By assumption, G has global Gaussian upper bound. This, together with (4.3), implies

$$|u(x)|\le C\int_{\mathbf{M}}\frac{1}{t^{n/2}}e^{-c\frac{d(x,y)^2}{t}}\frac{1}{1+d(y,x_0)^b}\,dy. \tag{4.4}$$

Direct computations show that, for any x,

$$\lim_{R\to\infty}|B(x,R)|^{-1}\int_{B(x,R)}\frac{1}{1+d(y,x_0)^b}\,dy=0.$$

By Theorem 3 in [Li], we know that the righthand side of (4.4) converges to zero when $t\to\infty$. Hence $u=0$.

Let u_1 and u_2 be two bounded nontrivial solutions to (4.1). According to the above claim we know that

$$u_i(x)=C_i-\int_{\mathbf{M}}\Gamma(x,y)V(y)u_i(y)\,dy,$$

where $i = 1, 2$ and C_i are constants. Since C_i cannot be zero by the last paragraph, we can find a constant c such that $C_1 = cC_2$ and hence

$$u_1(x) - cu_2(x) = -\int_{\mathbf{M}} \Gamma(x, y)V(y)(u_1 - cu_2)(y)\,dy.$$

By the last paragraph again, $u_1 - cu_2 = 0$. □

Remark 4.1. If $-\Delta + V$ is not subcritical, then the above Liouville type theorem does not hold in general. For example, consider the Helmholtz operator $H = -\Delta - 1$ in $\mathbf{R}^3$. It is well-known that $Hu = 0$ has a bounded nontrivial solution. By symmetry, every translation of a solution to $Hu = 0$ is also a solution. Obviously they are not constant multiples of each other.

Using Theorem B, we derive an improved version of the trace formula obtained in [SZ]. Note that we have eliminated the restriction that the potential has superexponential decay and is smooth.

PROPOSITION 4.1. *Let $V \in L^1(\mathbf{R}^n) \cap K_n$, where K_n is the Kato class. Suppose that $-\Delta + V$ is subcritical. Then there exists $C(V) > 0$ such that*

$$\left|Tr\left(e^{-t(-\Delta+V)} - e^{-t(-\Delta)}\right)\right| \le C(V)t^{1-\frac{n}{2}}$$

for all $t > 0$.

Proof. We observe that if $V \in L^1(\mathbf{R}^n) \cap K_n$, then V is Green bound. Indeed, fixing $r > 0$, we have

$$\begin{aligned}\sup_x \int_{\mathbf{R}^n} \frac{|V(y)|}{|x-y|^{n-2}}\,dy &\le \sup_x \int_{|x-y|\le r} \frac{|V(y)|}{|x-y|^{n-2}}\,dy + \sup_x \int_{|x-y|\ge r} \frac{|V(y)|}{|x-y|^{n-2}}\,dy \\ &\le C + r^{-(n-2)}\|V\|_{L^1} < \infty.\end{aligned}$$

Now that we know V is Green bound and $-\Delta + V$ is subcritical, by Theorem A we know that the corresponding heat kernel has global Gaussian upper bound.

Once we have the Gaussian upper bound, the proof of the proposition is identical to that in [SZ]. Here we give a sketch of the proof while referring the reader to Proposition 3.1 in [SZ] for details. Indeed, by Duhamel's principle and Theorem A, there are $c, C > 0$ such that

$$\begin{aligned}|\,Tr(e^{-t(-\Delta+V)} - e^{-t(-\Delta)})| &= \left|\int_{\mathbf{R}^n} [G(x,t;x,0) - G_0(x,t;x,0)]\,dx\right| \\ &\le \int_0^t \int_{\mathbf{R}^n} G_0(x,t;z,s)G(x,s;z,0)|V(z)|\,dz\,dx\,ds \\ &\le C\int_0^t \int_{\mathbf{R}^n}\int_{\mathbf{R}^n} G_0(x,t;z,s)G_c(x,s;z,0)|V(z)|\,dz\,dx\,ds \\ &\le Ct^{1-\frac{n}{2}} \int_{\mathbf{R}^n} |V(z)|\,dz.\end{aligned}$$

□

Next we give examples of Schrödinger operators whose heat kernels do not have global Gaussian bounds. Let $L = -\Delta + \frac{1}{1+|x|^2}$. Since

$$\int_{\mathbf{R}^n} \frac{1}{|y|^{n-2}(1+|y|^2)} dy = c \int_0^\infty \frac{r}{1+r^2} dr = \infty,$$

we know that $V = \frac{1}{1+|x|^2}$ is not Green bound. By Corollary A, the corresponding heat kernel does not have global Gaussian lower bound. But Corollary B shows that the heat kernel will still have a polynomial decay on diagonal. By Corollary A again we know that the heat kernel of the operator $-\Delta - \frac{1}{1+|x|^2}$ does not have global Gaussian upper bound.

In contrast, Theorem A shows that the heat kernel of the operator

$$-\Delta + \frac{1}{(1+|x|^2)\ln(2+|x|^\alpha)}$$

with $\alpha > 1$ has global Gaussian bounds. This is because $V = \frac{1}{(2+|x|^2)\ln(1+|x|^\alpha)}$ is Green bound (see [Zo1]).

We have assumed that the local singularities of the potentials are in the Kato class K_n. This includes local singularity in the form of $\frac{1}{|x|^2|\ln|x||^\alpha}$ with $\alpha > 1$. Even though K_n (the Kato class) is already a natural class for Schrödinger equations (see [Si2]), one may still wonder whether α can take values in $[0, 1]$. The answer is no. In fact by (3.11) in the proof of Theorem B (iii), if the heat kernel of $-\Delta - \frac{1}{|x|^2|\ln|x||^\alpha}$ had global Gaussian lower and upper bound, then

$$\sup_{y\in\mathbf{R}^n} \int_{\mathbf{R}^n} \frac{1}{|x|^2|\ln|x||^\alpha|x-y|^{n-2}} dx \le C < \infty,$$

which is not true if $\alpha \in [0, 1]$. Here we remind the reader that in order to use Theorem B, an approximation argument like that in [BG] is needed. This is because the integral on the right hand side of the Duhamel's principle may not converge if V is an arbitrary measurable function.

As a final example, we recall the equation

$$\begin{cases} u_t - \Delta u - \frac{C}{|x|^2} u = 0, & (x,t) \in \mathbf{R}^n \times (0,\infty) \\ u(x,0) = u_0(x), & x \in \mathbf{R}^n. \end{cases}$$

By [BG], there exists $C^* > 0$ such that the above problem has no positive solution if $C > C^*$ and $u_0 (\geq 0)$ is not zero. The heat kernel is even undefined in this case.

Remark 4.2. Theorems A and B still hold if Δ is replaced by any time-independent uniformly elliptic operators in $\mathbf{R}^n$. Only minor modifications are needed for the proof.

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