

Note on Gradient Estimate of Heat Kernel for Schrödinger Operators

Shijun Zheng

Department of Mathematical Sciences, Georgia Southern University, Statesboro, USA

E-mail: szheng@georgiasouthern.edu

Received August 27, 2010; revised September 24, 2010; accepted September 27, 2010

Abstract

Let $H = -\Delta + V$ be a Schrödinger operator on \mathbb{R}^n . We show that gradient estimates for the heat kernel of H with upper Gaussian bounds imply polynomial decay for the kernels of certain smooth dyadic spectral operators. The latter decay property has been known to play an important role in the Littlewood-Paley theory for L^p and Sobolev spaces. We are able to establish the result by modifying Hebisch and the author's recent proofs. We give a counterexample in one dimension to show that there exists V in the Schwartz class such that the long time gradient heat kernel estimate fails.

Keywords: Heat Kernel, Schrödinger Operator, Functional Calculus

1. Introduction

Consider a Schrödinger operator $H = -\Delta + V$ on \mathbb{R}^n , where V is a real-valued potential in $L^1_{loc}(\mathbb{R}^n)$. It is noted in [1,2] that for positive V , if H admits the following gradient estimates for its heat kernel $p_t(x, y) = e^{-tH}(x, y)$: for all $x, y \in \mathbb{R}^n$ and $t > 0$,

$$|p_t(x, y)| \leq c_n t^{-n/2} e^{-c|x-y|^2/t}, \quad (1)$$

$$|\nabla_x p_t(x, y)| \leq c_n t^{-(n+1)/2} e^{-c|x-y|^2/t}, \quad (2)$$

then the kernel of $\Phi_j(H)$ and its derivatives satisfy a polynomial decay as in (4), where Φ_j is a function in certain Sobolev space with support in $[-2^j, 2^j]$. As is well-known, the decay estimate in (4) implies the Littlewood-Paley inequality for $L^p(\mathbb{R}^n)$ [3-6].

For positive V , based on heat kernel estimates one can show (4) by a scaling argument [2]. In this paper we will prove the general case, namely Theorem 1, by modifying the proofs in [7,8] and [2].

However, in general the gradient estimates (1), (2) do not hold for all t . This situation may occur when H is a Schrödinger operator with negative potential, or the sub-Laplacian on a Lie group of polynomial growth, cf. [9-12]. A second part of this paper is to show such a counterexample, based on Theorem 1.

Recall that for a Borel measurable function $\phi: \mathbb{R} \rightarrow \mathbb{C}$, one can define the spectral operator $\phi(H)$ by functional calculus $\phi(H) = \int_{-\infty}^{\infty} \phi(\lambda) dE_\lambda$, where dE_λ

is the spectral measure of H . The kernel of $\phi(H)$ is denoted $\phi(H)(x, y)$ in the following sense. Let A be an operator on a measure space $(M, d\mu)$, $d\mu$ being a Borel measure on M . If there exists a locally integrable function $K_A: M \times M \rightarrow \mathbb{C}$ such that

$$\begin{aligned} \langle Af, g \rangle &= \int_M (Af)g d\mu \\ &= \int_{M \times M} K_A(x, y) f(y)g(x) d\mu(x)d\mu(y) \end{aligned}$$

for all f, g in $C_0(M)$ with $\text{supp} f$ and $\text{supp} g$ being disjoint, where $C_0(M)$ is the set of continuous functions on M with compact supports, then A is said to have the kernel $A(x, y) := K_A(x, y)$. Throughout this paper, c or C will denote an absolute positive constant.

The main result is the following theorem for $V \in L^1_{loc}(\mathbb{R}^n)$.

Theorem 1 *Suppose that the kernel of e^{-tH} satisfies the upper Gaussian bound for $\alpha = 0, 1$*

$$|\nabla_x^\alpha e^{-tH}(x, y)| \leq c_n t^{-(n+\alpha)/2} e^{-c|x-y|^2/t}, \quad \forall t > 0. \quad (3)$$

Let Φ be supported in $[-1, 1]$ and belong to

$H^{\frac{n+1}{2}+N+\delta}(\mathbb{R})$ for some fixed $N \geq 0$ and $\delta > 0$. Then for each $N \geq 0$, there exists a constant c_N independent of Φ such that for all $j \in \mathbb{Z}$

$$\begin{aligned} &|\nabla_x^\alpha \Phi_j(H)(x, y)| \\ &\leq c_N 2^{j(n+\alpha)/2} (1 + 2^{j/2} |x - y|)^{-N} \|\Phi\|_{H^{\frac{n+1}{2}+N+\delta}}, \end{aligned} \quad (4)$$

where $\Phi_j(x) = \Phi(2^{-j}x)$ and $H^s := H^s(\mathbb{R})$ denotes the usual Sobolev space with norm

$$\|f\|_{H^s} = \|(1 - d^2 / dx^2)^{s/2} f\|_{L^2}.$$

When V is positive, a result of the above type was proved and applied to the cases for the Hermite and Laguerre operators [1]. The observation was that if $V \geq 0$, then the constants corresponding to Lemma 2 do not change for $H_\alpha = -\Delta + V_\alpha$ with $V_\alpha(x) = \alpha^2 V(\alpha x)$ (called *scaling-invariance* in what follows), according to the Feynman-Kac path integral formula [13]

$$e^{-tH} f(x) = E_x \left(f(\omega(t)) e^{-\int_0^t V(\omega(s)) ds} \right),$$

here E_x is the integral over the path space Ω with respect to the Wiener measure μ_x , $x \in \mathbb{R}^n$ and $\omega(t)$ stands for a brownian motion (generic path).

For general V the technical difficulty is that we do not have such a scaling-invariance. We are able to overcome this difficulty by establishing Lemma 6, a scaling version of the weighted L^1 inequality for $\Phi_j(H)(x, y)$ with $\Phi \in H^s$, for which we directly use the scaling information indicated by the time variable appearing in Lemma 2. Thus this leads to the proof of the main theorem by combining methods of Hebisch and the author's in [7,2].

In Section 3 we give a counterexample to show that for $V_\nu(x) = -\nu(\nu+1)(\cosh x)^{-2}$, $\nu \in \mathbb{N}$, the estimates in (1) and (2) fail for $t \rightarrow \infty$.

Note that under the condition in Theorem 1, (4) is valid for all $\varphi_j \in C_0^\infty(\mathbb{R})$, $j \in \mathbb{Z}$ satisfying (i) $\text{supp } \varphi_j \subset \{x : |x| \leq 2^j\}$ and (ii) $|\varphi_j^{(k)}(x)| \leq c_k 2^{-kj}$, $k \in \mathbb{N}_0 = \{0\} \cup \mathbb{N}$. A corollary is that (3) implies the Littlewood-Paley inequality

$$\|f\|_{L^p(\mathbb{R}^n)} \approx \left\| \left(\sum_j |\varphi_j(H)f(\cdot)|^2 \right)^{1/2} \right\|_{L^p(\mathbb{R}^n)}, \quad 1 < p < \infty \tag{5}$$

for both homogeneous and inhomogeneous systems $\{\varphi_j\}$, according to [1, Theorem 1.5], see also [2,3].

2. Heat Kernel Having Upper Gaussian Bound Implies Rapid Decay for Spectral Kernels

In this section we prove Theorem 1. Following [7] we begin with a simple lemma.

Lemma 2 *Suppose that (1) holds. Then*

$$\int |e^{-tH}(x, y)|^2 dx \leq ct^{-n/2} =: \tilde{C}(t)$$

$$\int |e^{-tH}(x, y)| e^{s|x-y|} dx \leq ce^{cs^2 t} =: C(s, t).$$

The next lemma can be easily proved by a duality argument and we omit the details.

Lemma 3 *Let L be a selfadjoint operator on $L^2(\mathbb{R}^n)$ and $\rho, \nu \in L^\infty(\mathbb{R})$. Then for each y ,*

$$\|(\rho\nu)(L)(\cdot, y)\|_{L^2} \leq \|\rho(L)\|_{2 \rightarrow 2} \|\nu(L)(\cdot, y)\|_{L^2}.$$

If in addition $\rho(L)$ is unitary, then the equality holds.

Let w be a submultiplicative weight on $\mathbb{R}^n \times \mathbb{R}^n$, i.e., $0 \leq w(x, y) \leq w(x, z)w(z, y)$, $\forall x, y, z \in \mathbb{R}^n$. For simplicity we also assume $w(x, y) = w(y, x)$. Define the norm for $k \in L^1_{loc}(\mathbb{R}^{2n})$ as follows:

$$\|k(x, y)\|_w = \sup_{y \in \mathbb{R}^n} \int_{\mathbb{R}^n} |k(x, y)| w(x, y) dx.$$

Then given two operators L_1, L_2 , it holds that

$$\|(L_1 L_2)(x, y)\|_w \leq \|L_1(x, y)\|_w \|L_2(x, y)\|_w. \tag{6}$$

The following lemma is a scaling version of [8, Theorem 3.1] for $V \in L^1_{loc}(\mathbb{R}^n)$.

Lemma 4 *Suppose that (1) holds. Let $L_j = e^{-2^{-j}H}$. Then for each $a \geq 0$, there exists a constant $c = c(n, a)$ depending on n, a only such that for all $j \in \mathbb{Z}$ and $k \in \mathbb{R}$,*

$$\int |e^{ikL_j} L_j(x, y)| (1 + 2^{j/2} |x - y|)^a dx \leq c(n, a)(1 + |k|)^{n/2+a}. \tag{7}$$

Proof. (a) First we show the case $j = 0$. For notational convenience write $L = L_0$, then by Lemma 2 we have, with $t = 1$,

$$\sup_y \|L(x, y)\|_{L^2_x} \leq \tilde{C}(1) = c$$

$$\sup_y \int |L(x, y)| e^{s|x-y|} dx \leq C(s, 1) =: C(s) = ce^{cs^2}.$$

Let $\phi(x, y) = e^{\beta|x-y|} (1 + |x - y|)^a$, $0 < \beta < s$. Then

$$\|L(x, y)\|_\phi = \int |L(x, y)| e^{s|x-y|} e^{-(s-\beta)|x-y|} (1 + |x - y|)^a dx$$

$$\leq C(s) \sup_{x, y} e^{-(s-\beta)|x-y|} (1 + |x - y|)^a =: C(s) c_{s, \beta, a}.$$

In view of Lemma 3, setting $\ell = \beta^{-1} |k| \|L(x, y)\|_\phi$, we have

$$\int |e^{ikL} L(x, y)| (1 + |x - y|)^a dx = \int_{|x-y| \leq \ell} + \int_{|x-y| > \ell}$$

$$\leq (1 + \ell)^{n/2+a} \|L(\cdot, y)\|_{L^2_x} + \|L(x, y)\|_\phi e^{-\beta\ell} e^{|k| \|L(x, y)\|_\phi}$$

$$\leq \tilde{C}(1)(1 + \beta^{-1} |k| C(s) c_{s, \beta, a})^{\frac{n}{2}+a} + C(s) c_{s, \beta, a},$$

where we note that by (6)

$$\|e^{ikL}(x, y)\|_{\phi} \leq \sum_{n=0}^{\infty} \frac{\|(ikL)^n(x, y)\|_{\phi}}{n!}$$

$$\leq \sum_{n=0}^{\infty} \frac{|k|^n}{n!} \|L(x, y)\|_{\phi}^n = e^{k\|L(x, y)\|_{\phi}}.$$

It is easy to calculate that

$$c_{s, \beta, a} = \begin{cases} 1 & 0 \leq a \leq s - \beta \\ e^{-(a-s+\beta)} \left(\frac{a}{s-\beta}\right)^a & a > s - \beta. \end{cases}$$

Hence taking $\beta = s/2$ and fixing $s = s_0 > 0$ give that

$$\int |e^{ikL}(x, y)| (1 + |x - y|)^a dx \leq c(s_0, n, a) (1 + |k|)^{\frac{n}{2} + a}.$$

(b) Similarly we show the case for all $j \in \mathbb{Z}$. If $L = e^{-2^{-j}H}$, then Lemma 2 tells that with $t = 2^{-j}$

$$\int |e^{-2^{-j}H}(x, y)|^2 dx \leq c2^{jn/2}$$

$$\int |e^{-2^{-j}H}(x, y)| e^{s|x-y|} dx \leq ce^{c2^{-j}s^2}.$$

For $j \in \mathbb{Z}$ let $\phi_j(x, y) = e^{\beta 2^{j/2}|x-y|} (1 + 2^{j/2}|x-y|)^a$, $0 < \beta < s$. Then similar to (a) we obtain

$$\|L_j(x, y)\|_{\phi_j} = \int |L_j(x, y)| e^{\beta 2^{j/2}|x-y|} (1 + 2^{j/2}|x-y|)^a dx$$

$$\leq C(s) \sup_x e^{-(s-\beta)|x|} (1 + |x|)^a = C(s) c_{s, \beta, a}.$$

It follows that, with $\beta = s/2$ and $s = s_0 > 0$ fixed,

$$\int |e^{ikL_j} L_j(x, y)| (1 + 2^{j/2}|x-y|)^a dx = \int_{|x-y| \leq \ell} + \int_{|x-y| > \ell}$$

$$\leq c_n \ell^{n/2} (1 + 2^{j/2} \ell)^a \|L_j(\cdot, y)\|_{L^2_{\ell}}$$

$$+ \|L_j(x, y)\|_{\phi_j} e^{-\beta 2^{j/2} \ell} e^{k\|L_j(x, y)\|_{\phi_j}}$$

$$\leq c(n, a) (1 + |k|)^{n/2 + a},$$

where we set $\ell = 2^{-j/2} \beta^{-1} |k| \|L_j(x, y)\|_{\phi_j}$.

We also need a basic property on the weighted ℓ^2 norm of Fourier coefficients of a compactly supported function in Sobolev space, which can be proved by elementary Fourier expansions.

Lemma 5 *Let $s \geq 0$, $T > 0$ and*

$H_0^s([0, T]) = C_0^\infty([0, T])$ *denote the subspace of Sobolev space $H^s(\mathbb{R})$. Then we have for all $g \in H_0^s([0, T])$,*

$$\sqrt{T} \|\hat{g}(n)\|_{\ell^2_s} \leq c \|g\|_{H_0^s}, \quad (8)$$

where $\|\{\alpha_n\}\|_{\ell^2_s} = (\sum_{n \in \mathbb{Z}} |\alpha(n)|^2 \langle n/T \rangle^{2s})^{1/2}$ and $\hat{g}(n)$ are the Fourier coefficients of g over the interval $[0, T]$.

The inequality in (8) can be replaced by equality (however we will not use this improvement), which is a special case of the general norm characterization for periodic functions in $H^s([0, T])$, see e.g. [14].

It follows from Lemma 4 and Lemma 5 the following weighted L^1 estimates for $\Phi_j(H)(x, y)$, which is an improved version of [2, Lemma 3.1], where the restriction $V \geq 0$ is removed.

Lemma 6 *Suppose $V \in L^1_{loc}(\mathbb{R}^n)$ and the kernel of e^{-tH} satisfies for all $t > 0$*

$$|e^{-tH}(x, y)| \leq c_n t^{-n/2} e^{-c|x-y|^2/t}. \quad (9)$$

If $s > (n+1)/2 + N$, $N \geq 0$ and $\text{supp } \Phi \subset [-10, 10]$, then

$$\sup_{j \in \mathbb{Z}, y \in \mathbb{R}^n} \|\Phi(2^{-j}H)(\cdot, y) \langle 2^{j/2}(\cdot - y) \rangle^N\|_{L^1(\mathbb{R}^n)} \leq c_n \|\Phi\|_{H^s(\mathbb{R})},$$

here $\langle x \rangle := 1 + |x|$.

Proof. Let $\Phi \subset [-1, 1]$. If $\text{supp } g \subset I := [0, 2\pi]$, then g has the Fourier series expansion on I

$$g(x) = \sum_k \hat{g}(k) e^{ikx},$$

where $\hat{g}(k) = \frac{1}{2\pi} \int_0^{2\pi} g(x) e^{-ikx} dx$. Let

$\Phi(\lambda) = g(e^{-\lambda}) e^{-\lambda}$ and $f_k(\lambda) = \lambda e^{ik\lambda}$. Then

$g(y) = \Phi(-\log y)/y$ with $\text{supp } g \subset [e^{-1}, e]$, and so

$$\Phi(2^{-j}H) = \sum_k \hat{g}(k) e^{ike^{-2^{-j}H}} e^{-2^{-j}H} = \sum_k \hat{g}(k) f_k(e^{-2^{-j}H}). \quad (10)$$

It follows from Lemma 4, (10) and Lemma 5 that for each y

$$\int |\Phi_j(H)(x, y)| \langle 2^{j/2}(x-y) \rangle^N dx \leq c \sum_k |\hat{g}(k)| (1 + |k|)^{n/2 + N}$$

$$= c \sum_k |\hat{g}(k)| (1 + |k|)^{n/2 + N + (1+\delta)/2} (1 + |k|)^{-(\delta+1)/2}$$

$$\leq c \left(\sum_k |\hat{g}(k)|^2 (1 + |k|)^{n+2N+1+\delta} \right)^{1/2} \left(\sum_k (1 + |k|)^{-\delta-1} \right)^{1/2}$$

$$\leq c \|g\|_{H_0^{n/2+N+(1+\delta)/2}([0, 2\pi])} \delta^{-1/2}$$

$$\leq c \delta^{-1/2} \|\Phi\|_{H_0^\delta([-1, 1])},$$

where $\delta = s - N - (n+1)/2$ and the last inequality follows from a change of variable and interpolation.

Remark 7 *Let $V = V_+ - V_-$, $V_{\pm} \geq 0$ on \mathbb{R}^n , $n \geq 3$. Then the heat kernel estimate in (9) holds if V_+ is in Kato class and $\|V_-\|_K$, the global Kato norm of V_- , is less than $\kappa_n := \pi^{n/2} / \Gamma(\frac{n}{2} - 1)$, see [15]. Also (9) holds*

whenever $V \geq 0$ is locally integrable on \mathbb{R}^n , $n \geq 1$.

2.1. Proof of Theorem 1

With (3) and Lemma 6 we are in a position to prove (4). The proof is similar to that of Proposition 3.3 in [2] in the case of positive V . For completeness, we present the details here.

$$\nabla_x^\alpha \Phi_j(H)(x, y) = \int_z \nabla_x^\alpha e^{-tH}(x, z)(e^{tH} \Phi_j(H))(z, y) dz.$$

By (3) we have

$$\begin{aligned} & |\nabla_x^\alpha \Phi_j(H)(x, y)| \\ & \leq c_n t^{-(n+\alpha)/2} \int e^{-c|x-z|^2/t} \langle (x-z)/\sqrt{t} \rangle^N \langle (x-z)/\sqrt{t} \rangle^{-N} \\ & \quad \langle (z-y)/\sqrt{t} \rangle^{-N} \\ & \quad \cdot \langle (z-y)/\sqrt{t} \rangle^N |(e^{tH} \Phi_j(H))(z, y)| dz \\ & \leq c_n t^{-(n+\alpha)/2} \langle (x-y)/\sqrt{t} \rangle^{-N} \int \langle (z-y)/\sqrt{t} \rangle^N \\ & \quad |(e^{tH} \Phi(2^{-j}H))(z, y)| dz. \end{aligned}$$

Applying Lemma 6 with $t = 2^{-j}$, we obtain

$$\begin{aligned} & |\nabla_x^\alpha \Phi_j(H)(x, y)| \\ & \leq c_n t^{-(n+\alpha)/2} \langle (x-y)/\sqrt{t} \rangle^{-N} \|e^\lambda \Phi(\lambda)\|_H^{\frac{n+1}{2}+N+\delta} \\ & \leq c_n t^{-(n+\alpha)/2} \langle (x-y)/\sqrt{t} \rangle^{-N} \|\Phi\|_H^{\frac{n+1}{2}+N+\delta}, \quad \delta > 0. \end{aligned}$$

Remark 8 In the following section we will show that there exists $V \in \mathcal{S}$, the Schwartz class, such that (4) does not hold for $j \rightarrow \pm\infty$. By Theorem 1, this means that for such V the gradient upper Gaussian bound (3) does not hold for all t .

3. A Counterexample to the Gradient Heat Kernel Estimate

Consider the solvable model $H_\nu = -d^2/dx^2 + V_\nu$, $\nu \in \mathbb{N}$, where

$$V_\nu(x) = -\nu(\nu+1)\text{sech}^2 x.$$

We know from [5] that solving the Helmholtz equation for $k \in \mathbb{R} \setminus \{0\}$

$$H_\nu e(x, k) = k^2 e(x, k),$$

yields the following formula for the continuum eigenfunctions:

$$e(x, k) = (\text{sign}(k))^\nu \left(\prod_{j=1}^\nu \frac{1}{j+i|k|} \right) P_\nu(x, k) e^{ikx},$$

where $P_\nu(x, k) = p_\nu(\tanh x, ik)$ is defined by the recursion formula

$$\begin{aligned} & p_\nu(\tanh x, ik) \\ & = \frac{d}{dx} (p_{\nu-1}(\tanh x, ik)) + (ik - \nu \tanh x) p_{\nu-1}(\tanh x, ik), \end{aligned}$$

with $p_0 \equiv 1$. Note that $e(x, -k) = e(-x, k)$ and the function

$$\begin{aligned} & (x, y, k) \mapsto e(x, k) \overline{e(y, k)} \\ & = \left(\prod_{j=1}^\nu \frac{1}{j^2 + k^2} \right) P_\nu(x, k) P_\nu(y, -k) e^{ik(x-y)} \end{aligned} \tag{11}$$

is real analytic on \mathbb{R}^3 . Moreover, H_ν has only absolutely continuous spectrum $\sigma_{ac} = [0, \infty)$ and point spectrum $\sigma_{pp} = \{-1, -4, \dots, -\nu^2\}$. The corresponding eigenfunctions $\{e_n\}_{n=1}^\nu$ in L^2 are Schwartz functions that are linear combinations of $\text{sech}^m x \tanh^\ell x$, $m \in \mathbb{N}$, $\ell \in \mathbb{N}_0$. Let $H_{ac} = H_\nu E_{ac}$ denote the absolutely continuous part of H_ν and $E_{ac} = E_{(0, \infty)}$ the corresponding orthogonal projection. If $\phi \in C_0(\mathbb{R})$, then we have for all $f \in L^1 \cap L^2$,

$$\phi(H_\nu) f(x) = \int K(x, y) f(y) dy + \sum_{n=1}^\nu \phi(-n^2) (f, e_n) e_n,$$

where $(f, e_n) = \int f(x) \bar{e}_n(x) dx$ and

$$K(x, y) = (2\pi)^{-1} \int \phi(k^2) e(x, k) \bar{e}(y, k) dk \tag{12}$$

is the kernel of $\phi(H_{ac}) = \phi(H) E_{ac}$, cf. [16]. Since H_ν has eigenfunctions in $\mathcal{S}(\mathbb{R})$ and σ_{pp} is finite, from now on it is essential to check the kernel $\phi(H_{ac})(x, y) = K(x, y)$ instead of the kernel of $\phi(H_\nu)$.

3.1. Decay for the Kernel of $\Phi_j(H) E_{ac}$

Let $\{\varphi_j\}_{j=-\infty}^\infty \subset C_0^\infty(\mathbb{R})$ satisfy

- (i') $\text{supp } \varphi_j \subset \{x : 2^{j-2} \leq |x| \leq 2^j\}$ and
- (ii') $|\varphi_j^{(k)}(x)| \leq c_k 2^{-kj}$, $\forall j \in \mathbb{Z}$, $k \in \mathbb{N}_0$. Let

$\kappa_j(x, y) = \varphi_j(H_{ac})(x, y)$. In [5] we showed that for each N

$$|\kappa_j(x, y)| \leq c_N 2^{j/2} (1 + 2^{j/2} |x-y|)^{-N}, \quad \forall j \in \mathbb{Z}, \tag{13}$$

but (with $\alpha = 1$)

$$|\partial_x^\alpha \kappa_j(x, y)| \leq c_N 2^{j/2(1+|\alpha|)} (1 + 2^{j/2} |x-y|)^{-N} \tag{14}$$

only holds for $j \geq 0$ and does not hold for all $j < 0$. This suggests that (3) fails for $\alpha = 1$ and $t > 1$ (or more precisely $t \rightarrow \infty$), according to Theorem 1.

Now consider the system $\{\Phi_j\}_{j \in \mathbb{Z}}$ which satisfy (i), (ii) as in Section 1. We may assume $\Phi_j(x) = \Phi(2^{-j}x)$ for a fixed Φ in $C^\infty([-1, 1])$ with $\Phi(x) = 1$ on $[-\frac{1}{2}, \frac{1}{2}]$. Let f^\wedge and f^\vee be the Fourier transform and its inverse of f on \mathbb{R} . The following lemma

shows that (13) does not hold for $\Phi_j(H_{ac})(x, y)$ when $j \rightarrow \infty$.

Lemma 9 Let $K_j(x, y)$ be the kernel of $\Phi_j(H)E_{ac}$.
 a) For each $N \in \mathbb{N}_0$ there exists c_N such that for all $j \leq 0$,

$$|K_j(x, y)| \leq c_N 2^{j/2} (1 + 2^{j/2} |x - y|)^{-N}. \quad (15)$$

b) For each $N \in \mathbb{N}_0$ there exists c_N such that for all $j > 0$, precisely

$$|K_j(x, y)| \leq c_N 2^{j/2} (1 + 2^{j/2} |x - y|)^{-1}. \quad (16)$$

In particular, the decay in (15) does not hold for all $j > 0$ with $N > 1$.

c) There exist positive constants C and c such that for all $j \in \mathbb{Z}$,

$$|K_j(x, y)| \leq C |\Psi_j^\vee(x - y)| + C \int_{-\infty}^{\infty} |\Psi_j^\vee(u)| e^{-c|x-y-u|} du,$$

where $\Psi_j(k) = \Phi_j(k^2)$ and it is easily to see that for each N , there exists c_N such that for all j

$$|\Psi_j^\vee(x - y)| \leq c_N 2^{j/2} (1 + 2^{j/2} |x - y|)^{-N}.$$

Proof. (a) Let $\lambda = 2^{-j/2}$. By (12), (11) and integration by parts we have

$$2\pi(i(x - y))^N K_j(x, y) = (-1)^N \int e^{ik(x-y)}.$$

$$\partial_k^N [\Phi_j(k^2) \prod_{j=1}^{\nu} (j^2 + k^2)^{-1} P_\nu(x, k) P_\nu(y, -k)] dk,$$

which can be written as a finite sum of

$$\begin{aligned} & (\tanh x)^\ell (\tanh y)^m \\ & [(\Phi_j(k^2))^{(i)} (\prod_{t=1}^{\nu} (t^2 + k^2)^{-1})^{(r)} (q_{2\nu}(k))^{(s)}]^\vee (x - y) \end{aligned} \quad (17)$$

$0 \leq \ell, m \leq \nu$, $i + r + s = N$, $q_{2\nu}(k)$ are polynomials of degree $\leq 2\nu$. We obtain for each N and all $j \leq 0$

$$|(x - y)^N K_j(x, y)| = O(\lambda^{i-1}) = O(\lambda^{N-1}) = O(2^{-j/2(N-1)}),$$

using

$$\begin{cases} (\Phi_j(k^2))^{(i)} = O(\lambda^i) \\ (\prod_{t=1}^{\nu} (t^2 + k^2)^{-1})^{(r)} = O(\langle k \rangle^{-2\nu-r}) \\ q_{2\nu}^{(s)} = O(\langle k \rangle^{2\nu-s}). \end{cases}$$

This proves (15) for $j \leq 0$.

In order to show part (c) for $j \in \mathbb{Z}$, using partial fractions we write $K_j(x, y)$ as a finite sum of

$$(\tanh x)^\ell (\tanh y)^m \left[\Phi_j(k^2) \prod_{t=1}^{\nu} (t^2 + k^2)^{-1} q_{2\nu}(k) \right]^\vee (x - y), \quad (18)$$

which is bounded by (up to a constant multiple)

$$|[\Psi_j(k)]^\vee(x - y)| + \sum_{t=1}^{\nu} |[\Psi_j(k) \frac{a_t + b_t k}{t^2 + k^2}]^\vee(x - y)|,$$

where $a_t, b_t \in \mathbb{R}$. The general term in the sum is estimated by

$$|[\Psi_j(k) \frac{a_t + b_t k}{t^2 + k^2}]^\vee(x - y)| \leq C \int |\Psi_j^\vee(u)| e^{-c|x-y-u|} du,$$

in terms of the identities

$$(e^{-|x|})^\wedge(k) = \frac{2}{1 + k^2} \quad (19)$$

$$(\text{sign}(x)e^{-|x|})^\wedge(k) = \frac{-2ik}{1 + k^2}. \quad (20)$$

(b) Finally we prove the sharp estimate in (16). For $j > 0$, (15) does not hold for $N \geq 2$, instead we have only, with $N = 0, 1$,

$$|K_j(x, y)| \leq c 2^{j/2} (1 + 2^{j/2} |x - y|)^{-N},$$

by using similar argument and noting (17), (19), (20). Indeed, let $J > 0$, $N \geq 2$. It is easy to find $\{\phi_j\}$ satisfying (i') and (ii') such that

$$\Phi_j(x) = 1 - \sum_J \phi_j(x).$$

We have by (13)

$$\sum_J (x - y)^N |\phi_j(H_{ac})(x, y)| \leq c_N \sum_J 2^{-j/2(N-1)} \sim 2^{-J/2(N-1)}.$$

On the other hand, from (18) and the relevant steps in part (c) we observe that if $N > 1$,

$$\begin{aligned} & (x - y)^N \mathbf{1}_{[0, \infty)}(H_\nu)(x, y) \\ &= (x - y)^N \int_{-\infty}^{\infty} e_\nu(x, k) \bar{e}_\nu(y, k) dk \\ &= \text{finite sum of } (x - y)^N \cdot \\ & \sum_t \left(\alpha_t e^{-c_t|x-y|} + \text{sign}(x - y) \beta_t e^{-c_t|x-y|} \right), \end{aligned} \quad (21)$$

where $\alpha_t, \beta_t \neq 0$ are of the form $c \tanh^\ell x \tanh^m y$. This shows that the term $(x - y)^N \Phi_j(H_{ac})(x, y)$ cannot admit a decay of $2^{-J/2(N-1)}$ for all $J > 0$, otherwise one would have $|(x - y)^N \mathbf{1}_{[0, \infty)}(H_\nu)(x, y)| \lesssim 2^{-J/2(N-1)}$, which leads to a contradiction that the sum of those functions in (21) must vanish, by letting $J \rightarrow \infty$.

Remark 10 The argument in the proof of part (b) can be made rigorous by replacing $\mathbf{1}_{[0, \infty)}(H_\nu)$ with $\Phi_L(H_\nu)$, and then let $L \rightarrow \infty$ to get the same contradiction.

3.2. The Derivative of the Kernel of $\Phi_j(H)E_{ac}$

Similar argument shows that

$$|\partial_x K_j(x, y)| \leq c_N 2^{-j/2(N-2)} / |x-y|^N$$

holds for all $j > 0$ but does not hold for all $j < 0$. Therefore the inequality in (4) does not hold for general $V \in L^1_{loc}$.

4. Acknowledgements

The author gratefully thanks the hospitality and support of Department of Mathematics, University of California, Riverside during his visit in November 2008. In particular he would like to thank Professor Qi S. Zhang for the kind invitation and discussions. The author also wishes to thank the referee for careful reading of the original manuscript, whose comments have improved the presentation of this article.

5. References

- [1] G. Ólafsson and S. Zheng, "Harmonic Analysis Related to Schrödinger Operators," *Contemporary Mathematics*, Vol. 464, 2008, pp. 213-230.
- [2] S. Zheng, "Littlewood-Paley Theorem for Schrödinger Operators," *Analysis in Theory and Applications*, Vol. 22, No. 4, 2006, pp. 353-361.
- [3] J. Epperson, "Triebel-Lizorkin Spaces for Hermite Expansions," *Studia Mathematica*, Vol. 114, No. 1, 1995, pp. 87-103.
- [4] J. Dziubański, "Triebel-Lizorkin Spaces Associated with Laguerre and Hermite Expansions," *Proceedings of the American Mathematical Society*, Vol. 125, No. 12, 1997, pp. 3547-3554.
- [5] G. Ólafsson and S. Zheng, "Function Spaces Associated with Schrödinger Operators: The Pöschl-Teller Potential," *Journal of Fourier Analysis and Application*, Vol. 12, No. 6, 2006, pp. 653-674.
- [6] J. Benedetto and S. Zheng, "Besov Spaces for the Schrödinger Operator with Barrier Potential," to appear in *Complex Analysis and Operator Theory*, Birkhäuser.
- [7] W. Hebisch, "A Multiplier Theorem for Schrödinger Operators," *Colloquium Mathematicum*, Vol. 60-61, No. 2, 1990, pp. 659-664.
- [8] W. Hebisch, "Almost Everywhere Summability of Eigenfunction Expansions Associated to Elliptic Operators," *Studia Mathematica*, Vol. 96, No. 3, 1990, pp. 263-275.
- [9] E. Ouhabaz, "Sharp Gaussian Bounds and L^p -Growth of Semigroups Associated with Elliptic and Schrödinger Operators," *Proceedings of the American Mathematical Society*, Vol. 134, No. 12, 2006, pp. 3567-3575.
- [10] G. Furioli, C. Melzi and A. Veneruso, "Littlewood-Paley Decompositions and Besov Spaces on Lie Groups of Polynomial Growth," *Mathematische Nachrichten*, Vol. 279, No. 9-10, 2006, pp. 1028-1040.
- [11] A. Grigor'yan, "Upper Bounds of Derivatives of the Heat Kernel on an Arbitrary Complete Manifold," *Journal of Functional Analysis*, Vol. 127, No. 2, 1995, pp. 363-389.
- [12] Q. Zhang, "Global Bounds of Schrödinger Heat Kernels with Negative Potentials," *Journal of Functional Analysis*, Vol. 182, No. 2, 2001, pp. 344-370.
- [13] B. Simon, "Schrödinger Semigroups," *Bulletin of the American Mathematical Society*, Vol. 7, No. 3, 1982, pp. 447-526.
- [14] H.-J. Schmeisser and H. Triebel, "Topics in Fourier Analysis and Function Spaces," Wiley-Interscience, Chichester, 1987.
- [15] P. D'Ancona and V. Pierfelice, "On the Wave Equation with a Large Rough Potential," *Journal of Functional Analysis*, Vol. 227, No. 1, 2005, pp. 30-77.
- [16] S. Zheng, "A Representation Formula Related to Schrödinger Operators," *Analysis in Theory and Applications*, Vol. 20, No. 3, 2004, pp. 294-296.