OPERATOR KERNEL ESTIMATES FOR FUNCTIONS OF GENERALIZED SCHRÖDINGER OPERATORS

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Abstract. We study the decay at large distances of operator kernels of functions of generalized Schrödinger operators, a class of semibounded second order partial differential operators of Mathematical Physics, which includes the Schrödinger operator, the magnetic Schrödinger operator, and the classical wave operators (i.e., acoustic operator, Maxwell operator, and other second order partial differential operators associated with classical wave equations). We derive an improved Combes-Thomas estimate, obtaining an explicit lower bound on the rate of exponential decay of the operator kernel of the resolvent. We prove that for slowly decreasing smooth functions the operator kernels decay faster than any polynomial.

1. Introduction

In this article we establish decay estimates on operator kernels of functions of generalized Schrödinger operators, a class of semibounded second order partial differential operators of Mathematical Physics, which includes the Schrödinger operator, magnetic Schrödinger operator, and the classical wave operators (i.e., acoustic operator, Maxwell operator, and other second order partial differential operators associated with classical wave equations).

We fix the dimension d. For each $k = 1, 2, \dots$ we set

$$\mathcal{H}^{(k)} = \mathrm{L}^2(\mathbb{R}^d, \mathrm{d}x; \mathbb{C}^k)\,.$$

The spectrum and the domain of an operator B will be denoted by $\sigma(B)$ and $\mathcal{D}(B)$, respectively. If B is a semibounded operator we will denote the corresponding quadratic form by $B[\psi]$, with $\psi \in \mathcal{Q}(B)$, its form domain. ($B[\psi] = \langle \psi, B\psi \rangle$ for $\psi \in \mathcal{D}(B)$.)

A *generalized Schrödinger operator* is of the form

$$H = W + V \quad \text{on} \quad \mathcal{H}^{(n)}, \tag{1}$$

with

$$W = \sqrt{\mathcal{K}}(\mathbf{D} - \mathcal{A})^* \mathcal{R} (\mathbf{D} - \mathcal{A})\sqrt{\mathcal{K}}, \tag{2}$$

where:

- $\mathbf{D}$ is a first order constant coefficient partial differential operator from $\mathcal{H}^{(n)}$ to $\mathcal{H}^{(m)}$; it is given by multiplication by an $m \times n$ matrix $D(-i\nabla)$, where,

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for a d-component vector k, $D(k)$ is an $m \times n$ matrix with entries of the form $D(k)_{r,s} = a_{r,s} \cdot k$ with $a_{r,s} \in \mathbb{C}^d$, for $r = 1, \ldots, m,\ s = 1, \ldots, n$. We set

$$D_+ = \sup\{\|D(k)\|;\ \ k \in \mathbb{C}^d,\ |k| = 1\} < \infty\,, \tag{3}$$

note $\|D(k)\| \le D_+|k|$ for all $k \in \mathbb{C}^d$.

- $\mathcal{A}$ is the operator from $\mathcal{H}^{(n)}$ to $\mathcal{H}^{(m)}$ given by multiplication by the $m \times n$ matrix-valued measurable function $\mathcal{A}(x)$. We require $\mathcal{A}(x)$ to be locally in L^2.
- $\mathcal{K}$ and $\mathcal{R}$ are coefficients operators on $\mathcal{H}^{(n)}$ and $\mathcal{H}^{(m)}$, respectively. A coefficient operator $\mathcal{S}$ on $\mathcal{H}^{(k)}$ is a bounded, invertible operator given by multiplication by a coefficient matrix: an $k \times k$ matrix -valued measurable function $\mathcal{S}(x)$ on $\mathbb{R}^d$, satisfying

$$S_- I_k \le \mathcal{S}(x) \le S_+ I_k\ ,\ \ \text{with}\ \ 0 < S_- \le S_+ < \infty\ . \tag{4}$$

(I_k is the $k \times k$ identity matrix.)

- V is a potential, an operator given by multiplication by a real-valued measurable function $V(x)$. We write $V = V^+ - V^-$, with $V^\pm \ge 0$, and require V^+ to be locally in L^1 and V^- to be W-form bounded with relative bound < 1, i.e., there exist constants $0 \le \Theta_1, \Theta_2 < \infty$, with $\Theta_1 < 1$, such that

$$\langle \psi, V^- \psi \rangle \le \Theta_1 \langle \psi, W\psi \rangle + \Theta_2 \|\psi\|^2\ \ \text{for all}\ \ \ \psi \in \mathcal{Q}(W)\,. \tag{5}$$

A generalized Schrödinger operator is well defined as a semibounded self-adjoint operator. To see that, note that $\mathbf{D} - \mathcal{A}$, initially defined on infinitely differentiable functions with compact support from $\mathcal{H}^{(n)}$ to $\mathcal{H}^{(m)}$, extends to a closed, densely defined operator. We set (as in [13, 15])

$$A = \sqrt{\mathcal{R}}(\mathbf{D} - \mathcal{A})\sqrt{\mathcal{K}}\ \ \text{on}\ \ \mathcal{D}(A) = \sqrt{\mathcal{K}}\,\mathcal{D}(\mathbf{D} - \mathcal{A}), \tag{6}$$

a closed, densely defined operator from $\mathcal{H}^{(n)}$ to $\mathcal{H}^{(m)}$, and define W by

$$W = A^* A, \tag{7}$$

a positive self-adjoint operator with $\mathcal{Q}(W) = \mathcal{D}(A)$. It follows from the conditions on $V^\pm$ that $H = W + V$ is a semibounded self-adjoint operator on $\mathcal{H}^{(n)}$, with

$$H \ge (1 - \Theta_1)W - \Theta_2\ \ \ \text{and}\ \ \ \mathcal{Q}(H) = \mathcal{Q}(W) \cap \mathcal{Q}(V^+). \tag{8}$$

Our estimates will be stated in terms of the constants Θ_1, Θ_2, and

$$\Xi = D_+\sqrt{R_+ K_+}\,. \tag{9}$$

Note that while Ξ depends only on W, Θ_1 and Θ_2 depend on both W and V.

Examples include the *Schrödinger operator* (e.g., [16])

$$H = -\Delta + V\ \ \text{on}\ \ L^2(\mathbb{R}^d, \mathrm{d}x),\ \ \text{where}\ \ \Xi = 1\,, \tag{10}$$

where Δ is the d-dimensional Laplacian operator, the *magnetic field Schrödinger operator*

$$H = (-i\nabla - \mathbf{a}) \cdot (-i\nabla - \mathbf{a}) + V\ \ \text{on}\ \ L^2(\mathbb{R}^d, \mathrm{d}x),\ \ \text{where}\ \ \Xi = 1\,, \tag{11}$$

where $\mathbf{a}$ is a vector potential, an operator from $\mathcal{H}^{(1)}$ to $\mathcal{H}^{(d)}$ given by multiplication by the vector-valued function $\mathbf{a}(x) \in L^2_{\mathrm{loc}}(\mathbb{R}^d, \mathrm{d}x; \mathbb{R}^d)$, and the *classical wave operator* W given by (2) with $\mathcal{A} = 0$ (see [13, 15]). Examples of classical wave operators include the *acoustic operator*

$$W = -\frac{1}{\sqrt{\kappa}}\nabla\cdot\frac{1}{\rho}\nabla\frac{1}{\sqrt{\kappa}} \quad on \quad L^2(\mathbb{R}^d, \mathrm{d}x), \tag{12}$$

where ∇ is the d-dimensional gradient, $\kappa(x)$ is the compressibility, and $\varrho(x)$ is the mass density, and the *Maxwell operator*

$$W = \frac{1}{\sqrt{\mu}}\nabla\times\frac{1}{\varepsilon}\nabla\times\frac{1}{\sqrt{\mu}} \quad on \quad L^2(\mathbb{R}^3, \mathrm{d}x; \mathbb{C}^3), \tag{13}$$

where $\nabla\times$ is the curl, $\mu(x)$ is the magnetic permeability, and $\varepsilon(x)$ is the dielectric constant.

Definition 1. The *operator kernel* of a bounded operator B on $\mathcal{H}^{(n)}$ is defined by

$$K_B(x,y) = \chi_x B \chi_y \quad for\ all \quad x, y \in \mathbb{R}^d, \tag{14}$$

where χ_x denotes the operator given by multiplication by the characteristic function of a cube of side 1 centered at x.

A bounded operator B may or may not have an integral kernel, but it always has an operator kernel. (The choice of a cube of side 1 is arbitrary, one may fix a scale L and replace the characteristic functions in (14) by characteristic functions of cubes of side L.) Note that $\|K_B(x,y)\| \le \|B\|$, and

$$(B\psi)_x = \sum_{y\in x+\mathbb{Z}^d} K_B(x,y)\psi_y \quad \text{in} \quad \mathrm{L}^2(\mathbb{R}^d, \mathrm{d}x; \mathbb{C}^n)\,, \tag{15}$$

for all $\psi \in \mathrm{L}^2(\mathbb{R}^d, \mathrm{d}x; \mathbb{C}^n)$, where $\phi_x = \chi_x\phi$. Operator kernels avoid many technical problems associated with integral kernels; they have proved very useful in the study of Anderson localization of random Schrödinger operators and classical wave operators [2, 7, 8, 9, 13, 14].

Schrödinger operators and classical wave operators satisfy a resolvent decay estimate, commonly called the Combes-Thomas estimate in the Mathematical Physics literature. The proofs are based on an argument of Combes and Thomas [3]. (For Schrödinger operators see [16, 1]; for classical wave operators see [7, 8, 13].) In the following theorem we state and prove a Combes-Thomas estimate for generalized Schrödinger operators, using ideas from [7, Lemma 12] and [13, Theorem 3.5]. Our proof does not use analyticity. We give explicit estimates on the constants, valid for all energies z. This will be of importance in Theorem 2.

Theorem 1. *Let H be a generalized Schrödinger operator, let $R(z) = (H-z)^{-1}$, $z \notin \sigma(H)$, be its resolvent, and let $K_{n,z}(x,y)$ be the operator kernel of $R(z)^n$, $n = 1, 2, \ldots$. Then for any $0 < \gamma < 1$ we have*

$$\|K_{n,z}(x,y)\| \le \left(\left(\tfrac{1+\gamma}{1-\gamma}\right)^2 \tfrac{1}{\eta_z}\right)^n \mathrm{e}^{\gamma m_z\sqrt{d}}\,\mathrm{e}^{-\gamma m_z|x-y|} \tag{16}$$

for all $x, y \in \mathbb{R}^d$, where $\eta_z = \operatorname{dist}(z, \sigma(H))$, and

$$m_z = \Gamma\frac{\eta_z}{\sqrt{\Theta_2 + \eta_z + |z|}}\ , \tag{17}$$

with

$$\Gamma = \frac{3\sqrt{7}\,\sqrt{1-\Theta_1}}{32\,\Xi}\,. \tag{18}$$

If $\operatorname{Re} z < \Sigma = \inf \sigma(H)$ *we also have*

$$\|K_{n,z}(x,y)\| \le \left(\tfrac{1}{(1-\gamma^2)(\Sigma - Re\, z)} \right)^n \mathrm{e}^{\gamma \frac{\sqrt{\Sigma - Re\, z}\,\sqrt{d}}{\Xi}} \,\mathrm{e}^{-\gamma \frac{\sqrt{\Sigma - Re\, z}}{\Xi}\,|x-y|} \tag{19}$$

for all $x, y \in \mathbb{R}^d$.

Theorem 1 is the basic tool in our derivation of estimates on operator kernels of functions of generalized Schrödinger operators. The proof is given in Section 2.

If the energy z is real and sits in a spectral gap of the operator H, one can obtain estimates where the rate of the exponential decay is proportional to the product of the square roots of the distances from z to the edges of the gap, similarly to (19); see [1, 13].

Note that m_z grows as $\sqrt{\eta_z}$ as $\eta_z \to \infty$, so the the constant in (16) grows as $\mathrm{e}^{c\sqrt{\eta_z}}$. This can be avoided by picking $\gamma = (2 + \sqrt{\eta_z})^{-1}$. The resulting estimate, which will be used in the proof of Theorem 2, is given in the following corollary.

Corollary 1. *Let* H *be a generalized Schrödinger operator. Then, with the notation of Theorem 1,*

$$\|K_{n,z}(x,y)\| \le \left(\tfrac{9}{\eta_z} \right)^n \mathrm{e}^{\Gamma\sqrt{d}}\, \mathrm{e}^{-\frac{m_z}{2+\sqrt{\eta_z}}|x-y|} \tag{20}$$

for all $x, y \in \mathbb{R}^d$.

If $f \in C_0(\mathbb{R})$ (the continuous functions vanishing at infinity), it follows from the Stone-Weierstrass theorem and Corollary 1 that the operator kernel $K_f(x,y)$ of $f(H)$ goes to 0 as $|x-y| \to \infty$. But this soft argument gives no estimate on the rate of decay. In fact, it is known that for $H = -\Delta$ the kernel of $f(H)$ will not have rapid decay as $|x-y| \to \infty$ if f is not smooth [16, Remark 3 on p. 476].

In this article we combine Corollary 1 with the Helffer-Sjöstrand formula [11] to derive estimates on the decay of operator kernels of functions of generalized Schrödinger operators. The existing literature derives estimates on integral kernels from the heat kernel estimate [16, 4, 5]. But heat kernels estimates are only available for Schrödinger operators [16] and acoustic operators with constant compressibility [5]; they are not available for Maxwell operators, for example. We show that a Combes-Thomas estimate as in Corollary 1 is a natural tool to obtain kernel estimates for a large class of operators. Even for Schrödinger operators polynomial decay for the (integral or operator) kernel of $f(H)$ with f an arbitrary function in $C_0^\infty(\mathbb{R})$ is an open question (see [16, p. 476]). In the case when there is a heat kernel estimate, Davies [5, Theorem 3.4.10] proved polynomial decay of any order for $f \in \mathcal{S}(\mathbb{R})$. In Theorem 2 we allow any generalized Schrödinger operator and prove polynomial decay of any order if f belongs to the much larger class of slowly decreasing smooth functions (see Definition 2). A particular example of interest [10] is $f(u) = \frac{1-\mathcal{X}_I(u)}{u-E}$, where $I \subset \sigma(H)$ is a bounded open interval, $E \in I$, and $\mathcal{X}_I$ is a smooth charateristic function for the interval I. Note that in this case we have $f(H) = (1 - \mathcal{X}_I(H))R(E)$ with $E \in \sigma(H)$.

If $w \in \mathbb{R}^n$ we write

$$\langle w \rangle = \sqrt{1 + |w|^2}\,.$$

Definition 2. $f\colon \mathbb{R} \to \mathbb{C}$ is called a *slowly decreasing smooth function* if it is infinitely differentiable and there exists $\gamma > 0$ such that

$$|f^{(n)}(u)| \le \frac{c_n}{\langle u \rangle^{\gamma + n}}\,, \tag{21}$$

for some constants $c_n < \infty$, all $u \in \mathbb{R}$, and all $n = 0, 1, 2, \ldots$.

If f is a slowly decreasing smooth function, we define the norms [6, eq. (2.1.3)]:

$$\| f \|_n = \sum_{r=0}^{n} \int_{\mathbb{R}} |f^{(r)}(u)| \langle u \rangle^{r-1} \mathrm{d}x \quad , \quad n = 1, 2, \ldots . \tag{22}$$

Theorem 2. *Let H be a generalized Schrödinger operator and let f be a slowly decreasing smooth function. Then the operator kernel $K_f(x,y)$ of $f(H)$ decays faster than any polynomial as $|x-y| \to \infty$. More precisely, there is a finite constant $\widetilde{C}$, independent of f and H, such that for all $k = 1, 2, \ldots$ we have*

$$\| K_f(x,y) \| \le \widetilde{C}\, \mathrm{e}^{\Gamma \sqrt{d}} \| f \|_{k+2} \frac{\left\langle 3k(\Theta_2 + 8)\Gamma^{-1} \right\rangle^k}{\langle x - y \rangle^k} \tag{23}$$

for all $x, y \in \mathbb{R}^d$.

Theorem 2 is proved in Section 3. The proof is based on the estimate (20) and the Helffer-Sjöstrand formula. Theorem 2 provides a crucial ingredient for the results in [10].

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2. The Combes-Thomas estimate

In this section we prove Theorem 1. We start by defining the operators formally given by

$$H_\alpha = \mathrm{e}^{\alpha \cdot x} H \mathrm{e}^{-\alpha \cdot x} \text{ and } W_\alpha = \mathrm{e}^{\alpha \cdot x} W \mathrm{e}^{-\alpha \cdot x}, \text{ where } \alpha \in \mathbb{R}^d ; \tag{24}$$

note that

$$H_\alpha = W_\alpha + V. \tag{25}$$

To do so, let us consider the bounded operator G_α, defined as

$$G_\alpha = \sqrt{\mathcal{R}} D(\alpha) \sqrt{\mathcal{K}}, \text{ so } \| G_\alpha \| \le |\alpha|\, \Xi , \tag{26}$$

as in [13, Theorem 3.5]. Then

$$A_\alpha = \mathrm{e}^{\alpha \cdot x} A \mathrm{e}^{-\alpha \cdot x} = A + iG_\alpha \text{ on } \mathcal{D}(A), \tag{27}$$

$$(A^*)_\alpha = \mathrm{e}^{\alpha \cdot x} A^* \mathrm{e}^{-\alpha \cdot x} = A^* + iG_\alpha^* \text{ on } \mathcal{D}(A^*), \tag{28}$$

are closed, densely defined operators. (Note $(A^*)_\alpha \ne (A_\alpha)^*$.) We now define $W_\alpha = (A^*)_\alpha A_\alpha$ as a quadratic form with form domain $\mathcal{D}(A) = \mathcal{Q}(W)$, i.e., for each $\alpha \in \mathbb{R}^d$,

$$W_\alpha [\psi] = \langle (A^*)_\alpha^* \psi, A_\alpha \psi \rangle , \quad \psi \in \mathcal{D}(A). \tag{29}$$

If $\alpha = 0$, W_0 is the closed, nonegative quadratic form associated to the operator W. We also define the quadratic form $H_\alpha = W_\alpha + V$ on $\mathcal{Q}(W) \cap \mathcal{Q}(V^+)$.

It follows from (27) and (28) that

$$H_\alpha [\psi] - H [\psi] = W_\alpha [\psi] - W [\psi] = 2i \operatorname{Re} \langle A\psi, G_\alpha \psi \rangle - \langle G_\alpha \psi, G_\alpha \psi \rangle , \tag{30}$$

so, using (26) and (8), we get

$$
\begin{aligned}
(31)\quad |H_\alpha[\psi] - H[\psi]| &= \left(4\left(\operatorname{Re}\langle A\psi, G_\alpha\psi\rangle\right)^2 + \|G_\alpha\psi\|^4\right)^{\frac{1}{2}} \\
&\leq \|G_\alpha\psi\|\left(4\|A\psi\|^2 + \|G_\alpha\psi\|^2\right)^{\frac{1}{2}} \leq 2sW[\psi] + \tfrac{1}{2}(\tfrac{1}{s}+s)|\alpha|^2\Xi^2\|\psi\|^2 \\
&\leq \tfrac{2s}{1-\Theta_1}H[\psi] + \left(\tfrac{2s\Theta_2}{1-\Theta_1} + \tfrac{1}{2}(\tfrac{1}{s}+s)|\alpha|^2\Xi^2\right)\|\psi\|^2\,,
\end{aligned}
$$

for any $s > 0$. It follows [12, Theorem VI.1.33] that H_α is a closed sectorial form on the form domain of H. We define H_α as the unique m-sectorial operator associated with it [12, Theorem VI.2.1].

Let $z \notin \sigma(H)$, if $0 < \gamma < 1$ and

$$
(32)\qquad \Omega = 2\|(a+bH)R(z)\| \leq \gamma\,,
$$

where

$$
(33)\qquad a = \tfrac{2s\Theta_2}{1-\Theta_1} + \tfrac{1}{2}(\tfrac{1}{s}+s)|\alpha|^2\Xi^2\,, \quad b = \tfrac{2s}{1-\Theta_1}\,,
$$

it follows from [12, Theorem VI.3.9] that $z \notin \sigma(H_\alpha)$ and

$$
(34)\qquad \|R(z) - R_\alpha(z)\| \leq \frac{4\Omega}{(1-\Omega)^2}\|R(z)\| \leq \frac{4\gamma}{(1-\gamma)^2\,\eta_z}\,,
$$

where $R_\alpha(z) = (H_\alpha - z)^{-1}$ and $\eta_z = \operatorname{dist}(z, \sigma(H))$, so

$$
(35)\qquad \|R_\alpha(z)\| \leq \left(\frac{1+\gamma}{1-\gamma}\right)^2 \frac{1}{\eta_z}\,.
$$

Since

$$
(36)\qquad \Omega \leq \frac{2}{\eta_z}\left(a + b(\eta_z + |z|)\right),
$$

(32) will be satisfied if

$$
(37)\qquad As + (\tfrac{1}{s}+s)|\alpha|^2 \leq B,
$$

with

$$
(38)\qquad A = \frac{4}{(1-\Theta_1)\Xi_2^2}(\Theta_2 + \eta_z + |z|)\,, \quad B = \frac{\gamma\eta_z}{\Xi^2}\,.
$$

The left hand side of (37) is minimized by the choice

$$
(39)\qquad s = \frac{|\alpha|}{\sqrt{A + |\alpha|^2}}\,,
$$

in which case (37) becomes

$$
(40)\qquad 2|\alpha|\sqrt{A + |\alpha|^2} \leq B\,,
$$

i.e.,

$$
(41)\qquad 4|\alpha|^4 + 4A|\alpha|^2 - B^2 \leq 0\,,
$$

so it suffices to require

$$
(42)\qquad |\alpha|^2 \leq \tfrac{1}{2}\left(-A + \sqrt{A^2 + B^2}\right) = \frac{A}{2}\left(\sqrt{1 + \frac{B^2}{A^2}} - 1\right) \equiv \beta.
$$

Since $\sqrt{1+x} \geq 1 + \frac{x}{2} - \frac{x^2}{8}$ for $x \geq 0$, we have

$$\begin{aligned}(43)\qquad \beta &\geq \frac{B^2}{4A}\left(1 - \frac{B^2}{4A^2}\right) \geq \frac{B^2}{4A}\left(1 - \frac{\gamma^2(1-\Theta_1)^2}{64}\right) \\ &\geq \frac{63B^2}{256A} = \frac{63\,(1-\Theta_1)\gamma^2\eta_z^2}{1024\,\Xi^2(\Theta_2+\eta_z+|z|)} = \gamma^2 m_z^2\,,\end{aligned}$$

with m_z as in (17).

Thus, if we take $|\alpha| \leq \gamma m_z$, we satisfy (32) and obtain (35).

Now let $x_0, y_0 \in \mathbb{R}^d$, $n \in \mathbb{N}$, and take $\alpha = \gamma \frac{m_z}{|x_0-y_0|}(x_0 - y_0)$. We have

$$\begin{aligned}(44)\qquad K_{n,z}(x_0,y_0) &= \chi_{x_0} R(z)^n \chi_{y_0} = \chi_{x_0} \mathrm{e}^{-\alpha\cdot x} R_\alpha(z)^n \mathrm{e}^{\alpha\cdot x}\chi_{y_0} \\ &= \mathrm{e}^{-\gamma m_z|x_0-y_0|}\chi_{x_0}\mathrm{e}^{-\alpha\cdot(x-x_0)}R_\alpha(z)^n\mathrm{e}^{\alpha\cdot(x-y_0)}\chi_{y_0},\end{aligned}$$

so

$$(45)\qquad \|K_{n,z}(x_0,y_0)\| \leq \left(\left(\tfrac{1+\gamma}{1-\gamma}\right)^2 \tfrac{1}{\eta_z}\right)^n \|\chi_{x_0}\mathrm{e}^{-\alpha\cdot(x-x_0)}\|_\infty \|\chi_{y_0}\mathrm{e}^{\alpha\cdot(x-y_0)}\|_\infty \mathrm{e}^{-\gamma m_z|x_0-y_0|}\,.$$

Since

$$(46)\qquad \|\chi_{x_0}\mathrm{e}^{\pm\alpha\cdot(x-x_0)}\|_\infty \leq \mathrm{e}^{\frac{\sqrt{d}}{2}|\alpha|} = \mathrm{e}^{\frac{\sqrt{d}}{2}\gamma m_z},$$

(16) follows.

Now let $\mathrm{Re}\, z < \Sigma = \inf\sigma(H)$. It follows from (30) and (26) that

$$(47)\qquad Re\, H_\alpha[\psi] = H[\psi] - \langle G_\alpha\psi, G_\alpha\psi\rangle \geq \Sigma - |\alpha|^2\Xi^2.$$

As H_α is an m-sectorial operator, it follows that $z \notin \sigma(H_\alpha)$ as long as we have $|\alpha|^2\Xi^2 < \Sigma - \mathrm{Re}\, z$ (see [12, p. 279]). Moreover, if $0 < \gamma < 1$ and

$$(48)\qquad |\alpha| \leq \gamma\,\frac{\sqrt{\Sigma - Re\, z}}{\Xi}\,,$$

we have

$$(49)\qquad \|R_\alpha(z)\| \leq \frac{1}{(1-\gamma^2)(\Sigma - Re\, z)}\,.$$

Proceeding as in (44), we conclude that (19) follows from (48) and (49).

Theorem 1 is proven.

3. Kernel estimates for slowly decreasing smooth functions

In this section we prove Theorem 2. Let f be a slowly decreasing smooth function satisfying (21). We recall the Helffer-Sjöstrand formula [11] (see also [6, Section 2.2]):

$$(50)\qquad f(H) = \frac{1}{\pi}\int_{\mathbb{R}^2} \frac{\partial \tilde{f}_n(z)}{\partial \bar{z}}\, R(z)\,\mathrm{d}u\mathrm{d}v\,,$$

where $z = u + iv$, $n = 1, 2, \ldots$, and

$$(51)\qquad \tilde{f}_n(z) = \left\{\sum_{r=0}^{n} \frac{1}{r!} f^{(r)}(u)(iv)^r\right\}\sigma(u,v)\,,$$

called a quasi-analytic extension of f of order n, with $\sigma(u,v) = \tau\left(\frac{v}{\langle u\rangle}\right)$ for some infinitely differentiable function $\tau(s)$ on the real line, which equals 1 if $|s| < 1$ and equals 0 if $|s| > 2$. We have

$$\begin{aligned} \frac{\partial \tilde{f}_n(z)}{\partial \bar{z}} &= \frac{1}{2}\left\{\frac{\partial \tilde{f}_n(z)}{\partial u} + i\frac{\partial \tilde{f}_n(z)}{\partial v}\right\} \\ &= \frac{1}{2}\left\{\sum_{r=0}^{n} \frac{1}{r!} f^{(r)}(u)(iv)^r\right\}\left\{\frac{\partial \sigma(u,v)}{\partial u} + i\frac{\partial \sigma(u,v)}{\partial v}\right\} \\ &\qquad + \frac{1}{2n!} f^{(n+1)}(u)(iv)^n \sigma(u,v)\,. \end{aligned} \tag{52}$$

The integral in (50) converges in operator norm, The identity (50) holds for any $n = 1, 2, \ldots$ and any choice of the function $\tau(s)$ (we choose $\tau(s)$ once for all, with $0 \le \tau(s) \le 1$). We also have the following bound [6, p. 25]:

$$\begin{aligned} &\left|\frac{\partial \tilde{f}_n(z)}{\partial \bar{z}}\right| \le \\ &\qquad C\left\{\sum_{r=0}^{n} \frac{1}{r!}|f^{(r)}(u)|\frac{|v|^r}{\langle u\rangle}\right\}\chi_A(u,v) + \frac{1}{2n!}|f^{(n+1)}(u)||v|^n \chi_B(u,v)\,, \end{aligned} \tag{53}$$

where $A = \{\langle u\rangle < |v| < 2\langle u\rangle\}$, $B = \{0 < |v| < 2\langle u\rangle\}$, χ_A and χ_B are the corresponding characteristic functions, and C is some constant depending only on our choice of $\tau(s)$. Thus there is a finite constant c, independent of f and n, such that [6, Lemma 2.2.1]

$$\|f(H)\| \le c|\!|\!|f|\!|\!|_{n+1} \quad \text{for all } n = 1, 2, \ldots. \tag{54}$$

It follows that the operator kernel $K_f(x,y)$ of $f(H)$ is given by

$$K_f(x,y) = \frac{1}{\pi}\int_{\mathbb{R}^2} \frac{\partial \tilde{f}_n(z)}{\partial \bar{z}}\, K_z(x,y)\mathrm{d}u\mathrm{d}v\,, \tag{55}$$

for any $n = 1, 2, \ldots$, where $K_z(x,y) = K_{1,z}(x,y)$ is the operator kernel of the resolvent $R(z)$. To estimate $\|K_f(x,y)\|$ we use (53) and (20), and make use in (56) and (57) of the fact that the function $g(s) = \frac{s}{(a+\sqrt{s})\sqrt{b+s}}$, with $a, b \ge 0$, is increasing for $s \ge 0$. Note that $\eta_z \ge |v|$ and hence

$$\frac{m_z}{2+\sqrt{\eta_z}} \ge \frac{\Gamma\,|v|}{\left(2+\sqrt{|v|}\right)\sqrt{\Theta_2 + |v| + |z|}}\,. \tag{56}$$

Thus, if $(u,v) \in A$, we have $|v| \ge 1$ and $|z| \le \sqrt{2}|v|$, hence

$$\frac{m_z}{2+\sqrt{\eta_z}} \ge \frac{\Gamma}{3\sqrt{\Theta_2 + 1 + \sqrt{2}}} \ge \frac{\Gamma}{3\sqrt{\Theta_2 + 3}}\,, \tag{57}$$

so for any $r = 0, 1, 2, \ldots$ it follows that

$$\begin{aligned}
(58)\qquad & \int_{\mathbb{R}^2} |f^{(r)}(u)| \frac{|v|^r}{\langle u\rangle} \chi_A(u,v) \|K_z(x,y)\| \mathrm{d}u\mathrm{d}v \\
& \leq 9\mathrm{e}^{\Gamma\sqrt{d}} \left[\int_{\mathbb{R}^2} |f^{(r)}(u)| \frac{|v|^{r-1}}{\langle u\rangle} \chi_A(u,v) \mathrm{d}u\mathrm{d}v \right] \mathrm{e}^{-\frac{\Gamma}{3\sqrt{\Theta_2+3}}|x-y|} \\
& \leq 9\mathrm{e}^{\Gamma\sqrt{d}} \left[t_r \int_{\mathbb{R}} |f^{(r)}(u)| \langle u\rangle^{r-1} \mathrm{d}u \right] \mathrm{e}^{-\frac{\Gamma}{3\sqrt{\Theta_2+3}}|x-y|} ,
\end{aligned}$$

where $t_0 = 2\log 2$, $t_r = \frac{2^{r+1}}{r}$ for $r = 1, 2 \ldots, n$. We can thus conclude that

$$\begin{aligned}
(59)\qquad & C \int_{\mathbb{R}^2} \left\{ \sum_{r=0}^{n} \frac{1}{r!} |f^{(r)}(u)| \frac{|v|^r}{\langle u\rangle} \right\} \chi_A(u,v) \|K_z(x,y)\| \mathrm{d}u\mathrm{d}v \\
& \qquad \leq \widehat{C}_1 \, \mathrm{e}^{\Gamma\sqrt{d}} \, |\!|\!| f |\!|\!|_n \, \mathrm{e}^{-\frac{\Gamma}{3\sqrt{\Theta_2+3}}|x-y|} ,
\end{aligned}$$

where $\widehat{C}_1 = C \max_r \frac{t_r}{r!} < \infty$.

When $(u, v) \in B$, we have $|v| \leq 2\langle u\rangle$ and $|z| \leq \sqrt{5}\langle u\rangle \leq 3\langle u\rangle$. Using these inequalities in (56), we get (using $2ab \leq a^2 + b^2$ in the third inequality)

$$\begin{aligned}
(60)\qquad \frac{m_z}{2+\sqrt{\eta_z}} & \geq \frac{\Gamma\,|v|}{\left(2+\sqrt{2\langle u\rangle}\right)\sqrt{\Theta_2+5\langle u\rangle}} \geq \frac{\Gamma\,|v|}{2\sqrt{(2+\langle u\rangle)\,(\Theta_2+5\langle u\rangle)}} \\
& \geq \frac{\Gamma\,|v|}{\Theta_2+2+6\langle u\rangle} \geq \frac{\Gamma\,|v|}{(\Theta_2+8)\langle u\rangle} .
\end{aligned}$$

If k is a positive integer, we recall that for all $t \geq 0$ we have

$$(61)\qquad \mathrm{e}^{-t} \leq \frac{b_k}{t^k} , \quad \text{where} \quad b_k = \mathrm{e}^{-k} k^k .$$

Thus, if $n \geq k+1$, we have

$$\begin{aligned}
(62)\qquad & \frac{1}{2n!} \int_{\mathbb{R}^2} |f^{(n+1)}(u)| |v|^n \chi_B(u,v) \|K_z(x,y)\| \mathrm{d}u\mathrm{d}v \\
& \leq \frac{9\,\mathrm{e}^{\Gamma\sqrt{d}}(\Theta_2+8)^k b_k}{2n!\,\Gamma^k |x-y|^k} \int_{\mathbb{R}^2} |f^{(n+1)}(u)| |v|^{n-k-1} \langle u\rangle^k \chi_B(u,v) \mathrm{d}u\mathrm{d}v \\
& \leq \frac{9\mathrm{e}^{\Gamma\sqrt{d}}(\Theta_2+8)^k b_k}{n!\Gamma^k |x-y|^k} \frac{2^{n-k}}{n-k} \int_{\mathbb{R}} |f^{(n+1)}(u)| \langle u\rangle^n \mathrm{d}u .
\end{aligned}$$

If we now pick $n = k+1$, it follows that for any $k = 1, 2, \ldots$ we have

$$\begin{aligned}
(63)\qquad & \frac{1}{2(k+1)!} \int_{\mathbb{R}^2} |f^{(k+2)}(u)| |v|^{k+1} \chi_B(u,v) \|K_z(x,y)\| \mathrm{d}u\mathrm{d}v \\
& \qquad \leq \widehat{C}_2 \frac{\mathrm{e}^{\Gamma\sqrt{d}}(\Theta_2+8)^k}{\Gamma^k |x-y|^k} \int_{\mathbb{R}} |f^{(k+2)}(u)| \langle u\rangle^{k+1} \mathrm{d}u ,
\end{aligned}$$

with $\widehat{C}_2 = 18 \max_k \frac{b_k}{(k+1)!} < \infty$.

It now follows from (55), (53), (59), (63) , (22), and (61), that we have

$$\begin{aligned}
(64)\qquad \|K_f(x,y)\| & \leq \widetilde{C}\,\mathrm{e}^{\Gamma\sqrt{d}} |\!|\!| f |\!|\!|_{k+2} \left(\mathrm{e}^{-\frac{\Gamma}{3\sqrt{\Theta_2+3}}|x-y|} + \frac{(\Theta_2+8)^k}{\Gamma^k |x-y|^k} \right) \\
(65)\qquad & \leq 2\,\widetilde{C}\,\mathrm{e}^{\Gamma\sqrt{d}} |\!|\!| f |\!|\!|_{k+2} \frac{\left(3k(\Theta_2+8)\Gamma^{-1}\right)^k}{|x-y|^k}
\end{aligned}$$

for any $k = 1, 2, \ldots$, where $\widetilde{C} < \infty$ is some constant independent of k, f, and H. Since we have $\|K_f(x,y)\| \leq c|\!|\!|f|\!|\!|_{k+2}$ by (54), and $\min\left\{1, \left|\frac{a}{b}\right|\right\} \leq \frac{\langle a \rangle}{\langle b \rangle}$, the estimate (23) follows with some different constant $\widetilde{C}$.

Theorem 2 is proven.

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