

## Heat kernel estimates for pseudodifferential operators, fractional Laplacians and Dirichlet-to-Neumann operators

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*Abstract.* The purpose of this article is to establish upper and lower estimates for the integral kernel of the semigroup  $\exp(-tP)$  associated with a classical, strongly elliptic pseudodifferential operator  $P$  of positive order on a closed manifold. The Poissonian bounds generalize those obtained for perturbations of fractional powers of the Laplacian. In the selfadjoint case, extensions to  $t \in \mathbb{C}_+$  are studied. In particular, our results apply to the Dirichlet-to-Neumann semigroup.

### 0. Introduction

Let  $M$  be a compact  $n$ -dimensional Riemannian  $C^\infty$ -manifold and  $P$  a classical, strongly elliptic pseudodifferential operator ( $\psi$ do) on  $M$  of order  $d > 0$ . We consider upper and lower estimates for the integral kernel  $\mathcal{K}_V(x, y, t)$  of the generalized heat semigroup  $V(t) = e^{-tP}$ . Semigroups generated by such nonlocal operators have been of recent interest in different settings.

- (1) For a Riemannian manifold  $\tilde{M}$  with boundary  $M$ , the Dirichlet-to-Neumann operator is a first-order pseudodifferential operator on  $M$  with principal symbol  $|\xi|$ . Arendt and Mazzeo [3,4], initiated the study of the associated semigroup and its relation to eigenvalue inequalities, motivating later studies, e.g., by Gesztesy and Mitrea [12] and Safarov [21].
- (2) The heat kernel generated by fractional powers of the Laplacian  $\Delta^{d/2}$  and their perturbations provides another example. Sharp estimates for  $e^{-t\Delta^{d/2}}$ ,  $0 < d < 2$ , can be obtained from those for  $e^{-t\Delta}$  by subordination formulas. For perturbations on bounded domains in  $\mathbb{R}^n$ , recent work on estimates includes Chen et al. [8] and other works by these authors, and Bogdan et al. [6].

In this article, we generalize the Poissonian estimates obtained in the second case to sectorially elliptic operators  $P$  of all positive orders on closed manifolds, by pseudodifferential methods. In particular, we allow nonselfadjoint operators and systems. A main result for such systems  $P$  is as follows:

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**THEOREM 1.** *The kernel of the semigroup satisfies*

$$|\mathcal{K}_V(x, y, t)| \leq C e^{-c_1 t} (d(x, y) + t^{1/d})^{-n-d}, \quad \text{for all } x, y \in M, t \geq 0, \quad (*)$$

for any  $c_1$  smaller than the infimum  $\gamma(P)$  of the real part of the spectrum of  $P$ .

If  $P$  is selfadjoint  $\geq 0$ , the estimates extend to the complex  $t = e^{i\theta}|t|$  with  $|\theta| < \frac{\pi}{2}$ , with uniform estimates

$$|\mathcal{K}_V(x, y, t)| \leq C (\cos \theta)^{-N} e^{-\gamma(P) \operatorname{Re} t} \frac{|t|}{(d(x, y) + |t|^{1/d})^d} ((d(x, y) + |t|^{1/d})^{-n} + 1), \quad (**)$$

where  $N = \max\{\frac{n}{d}, \frac{7n}{2} + 4d + 7\}$ .

Here,  $d(x, y)$  denotes the distance between  $x$  and  $y$ . If  $P$  is a system, it suffices that  $P$  is sectorially elliptic, having the spectrum of the principal symbol in a sector  $\{\lambda \neq 0 \mid |\arg \lambda| \leq \theta_0\}$  with  $\theta_0 < \frac{\pi}{2}$ . Extending (\*), also derivatives of the kernel, and, if further spectral information is available, a refined description of the long-time behavior, are obtained in the paper. Moreover, for the expansion of the kernel in quasi-homogeneous terms in local coordinates, we show estimates of each term.

For the Dirichlet-to-Neumann operator, as well as for the perturbations of fractional powers of the Laplacian of orders  $0 < d < 2$ , we get not only upper estimates but also similar lower estimates at small distances.

The estimate (\*) exhibits a large class of operators which satisfy upper estimates closely related to those studied abstractly, e.g., in Duong and Robinson [10] and Coulhon and Duong [9]. They have implications for the maximal regularity of the associated evolution equation in  $L_p$ , the  $L_p$ -independence of the spectrum as well as the functional calculus.

As a simple application of (\*\*) and Hölder’s inequality, one can obtain ultracontractive estimates

$$\|e^{-tP}\|_{\mathcal{L}(L_p, L_q)} \leq C (\cos \theta)^{-N} \left\| \frac{|t|}{(d(x, y) + |t|^{1/d})^d} ((d(x, y) + |t|^{1/d})^{-n} + 1) \right\|_{L_{q, y} L_{p', x}},$$

uniformly for all  $t \in \mathbb{C}$  with  $\operatorname{Re} t > 0$ . In the case of operators with Gaussian heat kernel estimates, a rich spectral theory has been developed (see e.g., Arendt [2], Ouhabaz [20]).

With the help of comparison principles, our result implies Poissonian estimates, e.g., for boundary problems in an open subset  $\Omega$  of  $M$ : If  $P$  is the variational operator associated with a Dirichlet form  $a$  with domain  $\mathcal{D} \subset L_2(M)$ , we consider the abstract Dirichlet realization  $P_\Omega$  associated with the closure of  $a|_{\mathcal{D} \cap C_0(\Omega)}$ . In the case where  $a$  is Markovian, one obtains  $0 \leq \mathcal{K}_{e^{-tP_\Omega}} \leq \mathcal{K}_{e^{-tP}}$  on  $\Omega$ . See Grigor’yan and Hu [14] for more refined comparison principles.

*Outline.* Section 1 collects some known facts. In Sect. 2, we treat semigroups generated by nonselfadjoint  $P$  for  $t \geq 0$ , by pseudodifferential methods based on [16]. Section 3 extends the estimates to complex  $t$  for selfadjoint  $P$ . Section 4 includes lower estimates for perturbations of fractional powers of the Laplacian and for the Dirichlet-to-Neumann operator.

**1. Preliminaries**

*Notation:*  $\langle \xi \rangle = \sqrt{\xi^2 + 1}$ . The indication  $\lesssim$  means “ $\leq$  a constant times,”  $\gtrsim$  means “ $\geq$  a constant times,” and  $\doteq$  means that both hold.

Let  $P$  be a classical  $\psi$ do of order  $d \in \mathbb{R}_+$ , acting in a Hermitian  $N$ -dimensional  $C^\infty$  vector bundle  $E$  over a closed, compact Riemannian  $n$ -dimensional manifold  $M$ .

We assume that the principal symbol  $p^0(x, \xi)$  of  $P$  has its spectrum (for  $\xi \neq 0$ ) in a sector  $\{\lambda \neq 0 \mid |\arg \lambda| \leq \varphi_0\}$  for some  $\varphi_0 < \frac{\pi}{2}$ . (In the notation of the book [16],  $P - \lambda$  is parameter-elliptic on the rays in the complementing sector; according to Seeley [23], the latter are “rays of minimal growth” of the resolvent.) From  $P$ , one can define the generalized heat operator  $V(t) = e^{-tP}$ ,  $t \geq 0$ , a holomorphic semigroup generated by  $P$ , as explained in detail, e.g., in [16, Sect. 4.2]. The kernel  $\mathcal{K}_V(x, y, t)$  ( $C^\infty$  for  $t > 0$ ) was analyzed there in its dependence on  $t$ , but mainly with a view to sup-norm estimates over all  $x, y$ , allowing an analysis of the diagonal behavior, that of  $\mathcal{K}_V(x, x, t)$ . We shall expand the analysis here to give more information on  $\mathcal{K}_V(x, y, t)$ .

For convenience of the reader, we recall the definitions of symbol spaces that are used. For  $d \in \mathbb{R}$ , the symbol space  $S^d_{1,0}(\mathbb{R}^n \times \mathbb{R}^n)$  consists of the  $C^\infty$ -functions  $a(x, \xi)$  ( $x, \xi \in \mathbb{R}^n$ ) such that for all  $\alpha, \beta \in \mathbb{N}^n_0$ ,

$$|D_x^\beta D_\xi^\alpha a(x, \xi)| \lesssim \langle \xi \rangle^{d-|\alpha|}; \tag{1.1}$$

it is a Fréchet space provided with the seminorms  $\sup_{x,\xi} |\langle \xi \rangle^{-d+|\alpha|} D_x^\beta D_\xi^\alpha a|$ . The symbols define operators  $A = \text{Op}(a(x, \xi))$  of order  $d$  by

$$\text{Op}(a(x, \xi))u = \mathcal{F}^{-1}a(x, \xi)\mathcal{F}u = \int_{\mathbb{R}^n} e^{ix \cdot \xi} a(x, \xi) \hat{u}(\xi) d\xi,$$

where  $\mathcal{F}u = \hat{u}$  denotes the Fourier transform and  $d\xi = (2\pi)^{-n}d\xi$ . The operator maps from  $\mathcal{S}(\mathbb{R}^n)$  to  $\mathcal{S}(\mathbb{R}^n)$ , extending to suitable spaces of distributions and Sobolev spaces, and obeying various composition rules.

The space of *classical symbols* of order  $d$ ,  $S^d(\mathbb{R}^n \times \mathbb{R}^n)$ , is the subset of  $S^d_{1,0}(\mathbb{R}^n \times \mathbb{R}^n)$  where  $a(x, \xi)$  moreover has an asymptotic expansion  $a \sim \sum_{l \in \mathbb{N}_0} a_{d-l}$  in terms  $a_{d-l}(x, \xi)$  homogeneous in  $\xi$  of degree  $d - l$  for  $|\xi| \geq 1$ , such that  $a'_M = a - \sum_{l < M} a_{d-l} \in S^{d-M}_{1,0}$  for all  $M \in \mathbb{N}_0$ . The principal symbol  $a_d$  is often denoted  $a^0$ . (The homogeneity need only hold for  $|\xi| \geq R$ , some  $R > 0$ .)

It should be noted that we here use the globally estimated symbols of Hörmander [17, Section 18.1], which have the advantage that remainders are kept inside the calculus.

Operators on manifolds are defined by use of local coordinates and rules for change of variables, composition with cut-off functions etc.; we refer to the quoted works for details.

The book [16] moreover includes parameter-dependent symbols  $a(x, \xi, \lambda)$  for  $\lambda$  in a sector of  $\mathbb{C}$ , with special symbol estimates involving the parameter (also operators on manifolds with boundary are treated there).

Consider a localized situation where the symbol  $p(x, \xi)$  of  $P$  is defined in a bounded open subset of  $\mathbb{R}^n$ —we can assume that it is extended to  $\mathbb{R}^n$ , with symbol estimates valid uniformly in  $x$ . The principal symbol  $p^0(x, \xi)$  is an  $N \times N$ -matrix with spectrum in the sector  $\{\lambda \neq 0 \mid |\arg \lambda| \leq \varphi_0\}$ , when  $|\xi| \geq 1$ . This holds in particular when  $P$  is strongly elliptic, for then

$$\operatorname{Re}(p^0(x, \xi)v, v) \geq c|\xi|^d|v|^2, \quad \text{for } |\xi| \geq 1, v \in \mathbb{C}^N, \text{ with } c > 0, \quad (1.2)$$

and hence since

$$|\operatorname{Im}(p^0v, v)| \leq |(p^0v, v)| \leq C|\xi|^d|v|^2 \leq c^{-1}C \operatorname{Re}(p^0v, v), \quad \text{for } |\xi| \geq 1, v \in \mathbb{C}^N, \quad (1.3)$$

the sectorial ellipticity holds with  $\varphi_0 = \arctan(c^{-1}C) \in [0, \frac{\pi}{2}[$ . When  $P$  is scalar, the two ellipticity properties are equivalent, but for systems, strong ellipticity is more restrictive than the mentioned sectorial ellipticity (also called parabolicity of  $\partial_t + P$ ).

When working in a localized situation, we assume (as we may) that the sectorial ellipticity holds uniformly for the symbols extended to  $\mathbb{R}^n$ . The estimates in the following are valid in particular for operators given on  $\mathbb{R}^n$  with global symbol estimates.

The spectrum  $\sigma(P)$  of  $P$  lies in a right half plane and has a finite lower bound  $\gamma(P) = \inf\{\operatorname{Re} \lambda \mid \lambda \in \sigma(P)\}$ . We can modify  $p^0$  for small  $\xi$  such that  $\sigma(p^0(x, \xi))$  has a positive lower bound for all  $(x, \xi)$  and lies in  $\{\lambda = re^{i\varphi} \mid r > 0, |\varphi| \leq \varphi_0\}$ .

The information in the following is taken from [16, Section 3.3].

The resolvent  $Q_\lambda = (P - \lambda)^{-1}$  exists and is holomorphic in  $\lambda$  on a neighborhood of a set

$$W_{r_0, \varepsilon} = \{\lambda \in \mathbb{C} \mid |\lambda| \geq r_0, \arg \lambda \in [\varphi_0 + \varepsilon, 2\pi - \varphi_0 - \varepsilon],\} \cup \{\operatorname{Re} \lambda \leq \gamma(P) - \varepsilon\}. \quad (1.4)$$

(with  $\varepsilon > 0$ ). There exists a parametrix  $Q'_\lambda$  on a neighborhood of a possibly larger set (with  $\delta > 0, \varepsilon > 0$ )

$$V_{\delta, \varepsilon} = \{\lambda \in \mathbb{C} \mid |\lambda| \geq \delta \text{ or } \arg \lambda \in [\varphi_0 + \varepsilon, 2\pi - \varphi_0 - \varepsilon]\} \cup \{\operatorname{Re} \lambda < \inf_{x, \xi} \gamma(p^0(x, \xi))\};$$

such that this parametrix coincides with  $(P - \lambda)^{-1}$  on the intersection. Its symbol  $q(x, \xi, \lambda)$  in local coordinates is holomorphic in  $\lambda$  there and has the form

$$q(x, \xi, \lambda) \sim \sum_{l \geq 0} q_{-d-l}(x, \xi, \lambda), \quad \text{where } q_{-d} = (p^0(x, \xi) - \lambda)^{-1}. \quad (1.5)$$

Here, when  $P$  is scalar,

$$q_{-d-1} = b_{1,1}(x, \xi)q_{-d}^2, \dots, q_{-d-l} = \sum_{k=1}^{2l} b_{l,k}(x, \xi)q_{-d}^{k+1}, \dots; \quad (1.6)$$

with symbols  $b_{l,k}$  independent of  $\lambda$  and homogeneous of degree  $dk - l$  in  $\xi$  for  $|\xi| \geq 1$ . When  $P$  is a system, each  $q_{-d-l}$  is for  $l \geq 1$  a finite sum of terms with the structure

$$r(x, \xi, \lambda) = b_1 q_{-d}^{v_1} b_2 q_{-d}^{v_2} \cdots b_M q_{-d}^{v_M} b_{M+1}, \tag{1.7}$$

where the  $b_k$  are homogeneous  $\psi$ do symbols of order  $s_k$  independent of  $\lambda$ , the  $v_k$  are positive integers with  $\sum_{k=1}^M v_k \in [2, 2l+1]$ , and  $s_1 + \cdots + s_{M+1} - d(v_1 + \cdots + v_M) = -d - l$ . (Further information and references in Remark 3.3.7.) Moreover (cf. Theorems 3.3.2, 3.3.5.), the remainder  $q'_M = q - \sum_{l < M} q_{-d-l}$  satisfies for  $\lambda$  on the rays in  $W_{r_0, \varepsilon}$ :

$$|D_x^\beta D_\xi^\alpha q'_M(x, \xi, \lambda)| \leq \langle \xi \rangle^{d-|\alpha|-M} (1 + |\xi| + |\lambda|^{1/d})^{-2d}, \text{ when } M + |\alpha| > d. \tag{1.8}$$

**2. Semigroups generated by sectorially elliptic pseudodifferential operators**

As explained in [16, Section 4.2], the semigroup  $V(t) = e^{-tP}$  can be defined from  $P$  by the Cauchy integral formula

$$V(t) = \frac{i}{2\pi} \int_{\mathcal{C}} e^{-t\lambda} (P - \lambda)^{-1} d\lambda, \tag{2.1}$$

where  $\mathcal{C}$  is a suitable curve going in the positive direction around the spectrum of  $P$ ; it can be taken as the boundary of  $W_{r_0, \varepsilon}$  for a small  $\varepsilon$ . In the local coordinate patch, the symbol is (for any  $M \in \mathbb{N}_0$ )

$$v(x, \xi, t) = v_{-d} + \cdots + v_{-d-M+1} + v'_M \sim \sum_{l \geq 0} v_{-d-l}(x, \xi, t), \text{ where} \\ v_{-d-l} = \frac{i}{2\pi} \int_{\mathcal{C}} e^{-t\lambda} q_{-d-l}(x, \xi, \lambda) d\lambda, \quad v'_M = \frac{i}{2\pi} \int_{\mathcal{C}} e^{-t\lambda} q'_M d\lambda. \tag{2.2}$$

A prominent example is  $e^{-t\sqrt{\Delta}}$  where  $\Delta$  denotes the (nonnegative) Laplace–Beltrami operator on  $M$ . This is a Poisson operator from  $M$  to  $M \times \mathbb{R}_+$  as defined in the Boutet de Monvel calculus ([7], cf. also [16]), when  $t$  is identified with  $x_{n+1}$ . When  $M$  is replaced by  $\mathbb{R}^n$ , its kernel is the well-known Poisson kernel

$$\mathcal{K}(x, y, t) = c_n \frac{t}{(|x - y|^2 + t^2)^{(n+1)/2}} \tag{2.3}$$

for the operator solving the Dirichlet problem for  $\Delta$  on  $\mathbb{R}_+^{n+1}$ .

Also, more general operator families  $V(t) = e^{-tP}$  with  $P$  of order 1 are sometimes spoken of as Poisson operators (e.g., by Taylor [24]), and indeed, we can show that for  $P$  of any order  $d \in \mathbb{R}_+$ ,  $V(t)$  identifies with a Poisson operator in the Boutet de Monvel calculus. This will be taken up in detail elsewhere. In order to match the conventions for Poisson symbol-kernels, the indexation in (2.2) is chosen slightly differently from that in [16, Section 4.2], where  $v_{-d-l}$  would be denoted  $v_{-l}$ . We define

$V_{-d-l}(t)$  and  $V'_M(t)$  in local coordinates to be the  $\psi$ do's with symbol  $v_{-d-l}(x, \xi, t)$  resp.  $v'_M(x, \xi, t)$ . The kernel  $\mathcal{K}_V(x, y, t)$  is in local coordinates expanded according to the symbol expansion:

$$\mathcal{K}_V(x, y, t) = \sum_{0 \leq l < M} \mathcal{K}_{V_{-d-l}}(x, y, t) + \mathcal{K}_{V'_M}(x, y, t). \quad (2.4)$$

The following result follows from [16].

**THEOREM 2.1.**  $1^\circ$  In local coordinates, the kernel terms satisfy for some  $c' > 0$ :

$$|\mathcal{K}_{V_{-d-l}}(x, y, t)| \leq e^{-c't} \begin{cases} t^{(l-n)/d} & \text{if } d-l > -n, \\ t(|\log t| + 1) & \text{if } d-l = -n, \\ t & \text{if } d-l < -n. \end{cases} \quad (2.5)$$

For a given  $c_0 > 0$  we can modify  $p^0$  to satisfy  $\inf_{x, \xi} \gamma(p^0(x, \xi)) \geq c_0$ ; then  $c'$  can be any number in  $]0, c_0[$ .

$2^\circ$  Moreover, with the modification in  $1^\circ$  used with  $c_0 = \gamma(P)$  if  $\gamma(P) > 0$ , the remainder satisfies

$$|\mathcal{K}_{V'_M}(x, y, t)| \leq e^{-c_1 t} \begin{cases} t^{(M-n)/d} & \text{if } d-M > -n, \\ t(|\log t| + 1) & \text{if } d-M = -n, \\ t & \text{if } d-M < -n, \end{cases} \quad (2.6)$$

for any  $c_1 < \gamma(P)$ . In particular,

$$|\mathcal{K}_V(x, y, t)| \leq e^{-c_1 t} t^{-n/d}. \quad (2.7)$$

*Proof.* The theorem was shown with slightly less precision on the constants  $c', c_1$  in [16, Theorems 4.2.2 and 4.2.5]. It was there aimed toward applications where  $d$  is integer. The estimates of resolvent symbols in Sect. 3.3 are still valid when  $d \in \mathbb{R}_+$ , but the replacement of  $P$  by  $P + a$  ( $a \in \mathbb{R}$ ) in the beginning of Sect. 4.2 on heat operators only gives a classical  $\psi$ do when  $d$  is integer, so we need another device to take the value of  $\gamma(P)$  into account for general  $d \in \mathbb{R}_+$ . We shall now explain the needed modifications, with reference to [16].

For  $1^\circ$ , the proof in Theorem 4.2.2 shows the validity of (2.5) with a small positive  $c' < \inf_{x, \xi} \gamma(p^0(x, \xi))$ . For a given  $c_0 > 0$ , the proof goes through to allow any  $c' < c_0$ , when  $p^0(x, \xi)$  is modified for  $|\xi| \leq R$  (for a possibly large  $R$ ) to satisfy  $\inf \gamma(p^0(x, \xi)) \geq c_0$ .

For  $2^\circ$ , the remainder symbol  $q'_M$  is holomorphic on  $W_{r_0, \varepsilon}$ ; here, if  $\gamma(P) > 0$  we define the terms  $q_{-d-l}$  as under  $1^\circ$ , with  $c_0 = \gamma(P)$ . For large  $M$ ,  $q'_M$  is  $\leq \langle \lambda \rangle^{-2}$ . The proof of Th. 4.2.2 gives an estimate of  $\mathcal{K}_{V'_M}$  by  $e^{-c_1 t} t(1 + |\log t|)$ , and the proof of Theorem 4.2.5 shows how to remove the logarithm. The estimates of  $\mathcal{K}_{V'_M}$  for lower values of  $M$  follow by addition of the estimates of finitely many  $\mathcal{K}_{V_{-d-l}}$ -terms.  $\square$

We shall improve this to give information on the dependence on  $|x - y|$  also. This will rely on the following result on kernels of  $S'_{1,0}$ - $\psi$ do's, found, e.g., in Taylor [24, Lemma XII 3.1] or [25, Proposition VII 2.2].

**PROPOSITION 2.2.** *Let  $a \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n)$  be such that for some  $r \in \mathbb{R}$ , some  $N \in \mathbb{N}_0$  with  $N > n + r$ , and all  $0 \leq |\alpha| \leq N$ ,*

$$\sup_{x,\xi} \langle \xi \rangle^{-r+|\alpha|} |D_\xi^\alpha a(x, \xi)| \leq C_0 < \infty. \tag{2.8}$$

*Then the inverse Fourier transform  $\mathcal{K}_A(x, y) = \mathcal{F}_{\xi \rightarrow z}^{-1} a(x, \xi)|_{z=x-y}$  is  $O(|x - y|^{-N})$  for  $|x - y| \rightarrow \infty$ , and satisfies for all  $|x - y| > 0$ :*

$$|\mathcal{K}_A(x, y)| \leq C_0 \begin{cases} |x - y|^{-r-n} & \text{if } r > -n, \\ |\log |x - y|| + 1 & \text{if } r = -n, \\ 1 & \text{if } r < -n. \end{cases} \tag{2.9}$$

*In particular, if  $a \in S'_{1,0}(\mathbb{R}^n \times \mathbb{R}^n)$  defining the  $\psi$ do  $A$ , the estimates hold for its kernel  $\mathcal{K}_A(x, y)$  for all  $N > n + r$ , each estimate depending only on the listed symbol seminorms.*

The dependence of the kernel norms on  $C_0$  is seen from an inspection of the proof.

In the scalar case, the kernel study can be based on nice explicit formulas that we think are worth explaining. Consider the contribution from one of the terms in (1.6). As integration curve, we can here use  $C_\varphi$  consisting of the two rays  $re^{i\varphi}$  and  $re^{-i\varphi}$ ,  $\varphi = \varphi_0 + \varepsilon$ . For  $t > 0$ , a replacement of  $t\lambda$  by  $\varrho$  gives the following:

$$\begin{aligned} w_{l,k}(x, \xi, t) &= \frac{i}{2\pi} \int_{C_\varphi} e^{-t\lambda} \frac{b_{l,k}(x, \xi)}{(p^0(x, \xi) - \lambda)^{k+1}} d\lambda = \frac{i}{2\pi} \int_{C_\varphi} e^{-\varrho} \frac{t^k b_{l,k}}{(tp^0 - \varrho)^{k+1}} d\varrho \\ &= \frac{i}{2\pi} t^k b_{l,k} \int_{C_{\varphi,R}} \frac{e^{-\varrho}}{(tp^0 - \varrho)^{k+1}} d\varrho = \frac{1}{k!} t^k b_{l,k} e^{-tp^0}; \end{aligned} \tag{2.10}$$

here, we have replaced the integration curve by a closed curve  $C_{\varphi,R}$  connecting the two rays by a circular piece in the right half plane with radius  $R \geq 2t|p^0(x, \xi)|$  and applied the Cauchy integral formula for derivatives of holomorphic functions. This shows the following:

$$v_{-d} = e^{-tp^0}, \quad v_{-d-l}(x, \xi, t) = \sum_{k=1}^{2l} \frac{1}{k!} t^k b_{l,k}(x, \xi) e^{-tp^0(x, \xi)} \quad \text{for } l \geq 1. \tag{2.11}$$

Then, the kernels of the  $V_{-d-l}(t)$  can be estimated by the following observations.

**PROPOSITION 2.3.** *Let  $p^0(x, \xi)$  be the principal symbol of a classical scalar strongly elliptic  $\psi$ do  $P$  on  $\mathbb{R}^n$  of order  $d \in \mathbb{R}_+$ , chosen such that  $\text{Re } p^0(x, \xi) \geq c_0 > 0$ .*

*1° Let  $c' \in [0, c_0[$ . For any  $j \in \mathbb{N}_0$ ,  $(t(p^0(x, \xi) - c'))^j e^{-t(p^0(x, \xi) - c')}$  is in  $S'_{1,0}(\mathbb{R}^n \times \mathbb{R}^n)$  uniformly in  $t \geq 0$ .*

2° Let

$$w(x, \xi, t) = \frac{i}{2\pi} \int_{C_\varphi} e^{-t\lambda} \frac{b(x, \xi)}{(p^0(x, \xi) - \lambda)^{k+1}} d\lambda, \tag{2.12}$$

where  $k \geq 1$  and  $b \in S_{1,0}^{dk-l}(\mathbb{R}^n \times \mathbb{R}^n)$ . Then

$$w(x, \xi, t) = \frac{1}{k!} t^k b(x, \xi) e^{-tp^0(x, \xi)} = e^{-c't} t w'(x, \xi, t), \tag{2.13}$$

where  $w'(x, \xi, t) \in S_{1,0}^{d-l}(\mathbb{R}^n \times \mathbb{R}^n)$ , uniformly for  $t \geq 0$ .

Moreover,  $\tilde{w}(x, z, t) = \mathcal{F}_{\xi \rightarrow z}^{-1} w$  satisfies for any  $c' \in ]0, c_0[$ :

$$|\tilde{w}(x, z, t)| \leq e^{-c't} \begin{cases} t |z|^{l-d-n} & \text{if } d-l > -n, \\ t (|\log |z|| + 1) & \text{if } d-l = -n, \\ t & \text{if } d-l < -n. \end{cases} \tag{2.14}$$

It follows that for  $l \geq 1$ ,  $\mathcal{K}_{V_{-d-l}}(x, y, t) = \mathcal{F}_{\xi \rightarrow z}^{-1} v_{-d-l}(x, \xi, t)|_{z=x-y}$  satisfies the estimates

$$|\mathcal{K}_{V_{-d-l}}(x, y, t)| \leq e^{-c't} \begin{cases} t |x-y|^{l-d-n} & \text{if } d-l > -n, \\ t (|\log |x-y|| + 1) & \text{if } d-l = -n, \\ t & \text{if } d-l < -n. \end{cases} \tag{2.15}$$

Moreover,  $\mathcal{K}_{V_{-d-l}}(x, y, t)$  is  $O(e^{-c't} t |x-y|^{-N})$  for  $|x-y| \rightarrow \infty$ , any  $N$ .

*Proof.* 1°. For each fixed  $t > 0$ ,  $e^{-tp^0(x, \xi)}$  is rapidly decreasing in  $\xi$ , hence is in  $S_{1,0}^{-\infty}$ . But for our purposes we need estimates that hold uniformly in  $t$  for  $t \rightarrow 0$ . Let

$$M_{j,k,l} = \sup_{s \geq 0} s^l \partial_s^k (s^j e^{-s}).$$

Then, for all  $t \geq 0$ ,  $\xi \in \mathbb{R}^n$ ,

$$\begin{aligned} |(tp^0(x, \xi))^j e^{-tp^0(x, \xi)}| &\leq M_{j,0,0}, \\ |\partial_{\xi_i}^{\alpha} ((tp^0)^j e^{-tp^0})| &= |\partial_s (s^j e^{-s})|_{s=tp^0} t \partial_{\xi_i} p^0 \leq M_{j,k,1} |(p^0)^{-1} \partial_{\xi_i} p^0| \leq (\xi)^{-1}, \dots \\ |\partial_{\xi}^{\alpha} ((tp^0)^j e^{-tp^0})| &\leq (\xi)^{-|\alpha|}, \dots \end{aligned} \tag{2.16}$$

showing the assertion for  $c' = 0$ . (2.16) holds also if  $p^0$  is replaced by  $p^0 - c'$  throughout, when  $c' \in ]0, c_0[$ .

2°. The first identity in (2.13) was shown in (2.10). We can also write

$$w(x, \xi, t) = \frac{1}{k!} t b(p^0 - c')^{1-k} (t(p^0 - c'))^{k-1} e^{-c't} e^{-t(p^0 - c')} = e^{-c't} t w'(x, \xi, t).$$

Here,  $b(p^0 - c')^{1-k}$  is in  $S_{1,0}^{d-l}$ , independent of  $t$ , and by 1°,  $(t(p^0 - c'))^{k-1} e^{-t(p^0 - c')}$  is uniformly in  $S_{1,0}^0$ , so it follows that  $w'$  is uniformly in  $S_{1,0}^{d-l}$ . We can now apply Proposition 2.2 to draw the conclusion (2.14).

Since  $v_{-d-l}(x, \xi, t)$  is a sum of such terms when  $l \geq 1$ , the estimates (2.15) follow. □



For systems  $P$ , we can use systematic estimates from [16]. We find for general  $P$ :

**THEOREM 2.4.**  $1^\circ$  In local coordinates,  $\mathcal{K}_{V-d}$  satisfies for some  $c' > 0$ :

$$|\mathcal{K}_{V-d}(x, y, t)| \leq e^{-c't} t |x - y|^{-d-n}. \tag{2.17}$$

For  $l \geq 1$ , the kernels  $\mathcal{K}_{V-d-l}$  satisfy (2.15). For all  $l$ , the kernels are  $O(e^{-c't} t |x - y|^{-N})$  for  $|x - y| \rightarrow \infty$ , any  $N$ . If  $\gamma(P) > 0$ , we modify  $p^0$  to satisfy  $\inf_{x, \xi} \gamma(p^0(x, \xi)) \geq \gamma(P)$ , then  $c'$  can be any number in  $]0, \gamma(P)[$ .

$2^\circ$  Moreover, with  $p^0$  chosen as in  $1^\circ$ ,

$$|\mathcal{K}_{V'_M}(x, y, t)| \leq e^{-c_1 t} \begin{cases} t |x - y|^{M-d-n} & \text{if } d - M > -n, \\ t (|\log |x - y|| + 1) & \text{if } d - M = -n, \\ t & \text{if } d - M < -n, \end{cases} \tag{2.18}$$

for any  $c_1 < \gamma(P)$ . In particular,

$$|\mathcal{K}_V(x, y, t)| \leq e^{-c_1 t} t |x - y|^{-d-n}. \tag{2.19}$$

*Proof.*  $1^\circ$ . When  $P$  is scalar, the estimates in (2.15) for  $l \geq 1$  are shown in Proposition 2.3, when we take  $c_0 = \gamma(P)$  if  $\gamma(P) > 0$ . For general systems  $P$ , the symbols  $q_{-d-l}$  are sums of symbols as in (1.7), and we apply [16, Lemma 4.2.3]. Here, (4.2.35) with  $k = -d - l$  shows that

$$|D_x^\beta D_\xi^\alpha v_{-d-l}(x, \xi, t)| \leq \langle \xi \rangle^{d-l-|\alpha|} t e^{-c't},$$

for all  $\alpha, \beta$ . Actually, the estimate (4.2.35) has  $e^{-ct \langle \xi \rangle^d}$  with a positive  $c$  as the last factor, but an inspection of the proof (the location of integral contours) shows that  $e^{-ct \langle \xi \rangle^d}$  can be replaced by  $e^{-c't}$ , if  $c' < \inf \gamma(p^0(x, \xi))$ . This shows that  $e^{c't} t^{-1} v_{-d-l}$  is in  $S_{1,0}^{d-l}$  uniformly in  $t$ , so the estimates of the  $\mathcal{K}_{V-d-l}$  follow by use of Proposition 2.2.

For  $l = 0$ , we can argue as follows in the scalar case: For each  $j = 1, \dots, n$ ,

$$\partial_{\xi_j} v_{-d} = \partial_{\xi_j} e^{-t p^0} = -t (\partial_{\xi_j} p^0) e^{-t p^0},$$

where  $\partial_{\xi_j} p^0 \in S_{1,0}^{d-1}$ . Now, as in Proposition 2.3,  $e^{-c't} \partial_{\xi_j} p^0 e^{-t(p^0 - c')}$  is in  $S_{1,0}^{d-1}$  uniformly in  $t$ , and hence  $\tilde{v}_{-d} = \mathcal{F}_{\xi \rightarrow z}^{-1} v_{-d}$  satisfies, since  $d - 1 > -n$ ,

$$|z_j \tilde{v}_{-d}| \leq e^{-c't} t |z|^{-d+1-n}. \tag{2.20}$$

Taking the square root of the sum of squares for  $j = 1, \dots, n$ , we find after division by  $|z|$  that

$$|\tilde{v}_{-d}| \leq e^{-c't} t |z|^{-d-n}. \tag{2.21}$$

In the systems case, we note that

$$\partial_{\xi_j} q_{-d} = -q_{-d} (\partial_{\xi_j} p^0) q_{-d}, \tag{2.22}$$

since  $\partial_{\xi_j} [(p^0 - \lambda)(p^0 - \lambda)^{-1}] = 0$ . Lemma 4.2.3 applies to this in the same way as above, showing that

$$|D_x^\beta D_\xi^\alpha \partial_{\xi_j} v_{-d}(x, \xi, t)| \leq \langle \xi \rangle^{d-1-|\alpha|} t e^{-c't},$$

so  $e^{c't} t \partial_{\xi_j} v_{-d}$  is uniformly in  $S_{1,0}^{d-1}$ . We conclude (2.20), from which (2.21) follows, implying (2.17).

2°. Here, the estimate in (2.18) has already been shown for large  $M$  in Theorem 2.1. For lower values of  $M$ , we can add the estimates of the entering homogeneous terms  $\mathcal{K}_{V_{-d-l}}$  with  $l \geq M$ ; the top term gives the weakest estimate.  $\square$

Theorems 2.1 and 2.4 together lead to Poisson-like kernel estimates:

THEOREM 2.5. 1° *One has in local coordinates:*

$$|\mathcal{K}_{V_{-d-l}}(x, y, t)| \leq e^{-c't} \begin{cases} t (|x - y| + t^{1/d})^{l-d-n} & \text{if } d - l > -n, \\ t (|\log(|x - y| + t^{1/d})| + 1) & \text{if } d - l = -n, \\ t & \text{if } d - l < -n, \end{cases} \quad (2.23)$$

for some  $c' > 0$ . If  $\gamma(P) > 0$ , we modify  $p^0$  to satisfy  $\inf_{x,\xi} \gamma(p^0(x, \xi)) \geq \gamma(P)$ ; then  $c'$  can be any number in  $]0, \gamma(P)[$ .

2° Moreover, with  $p^0$  chosen as in 1°,

$$|\mathcal{K}_{V'_M}(x, y, t)| \leq e^{-c_1 t} \begin{cases} t (|x - y| + t^{1/d})^{M-d-n} & \text{if } d - M > -n, \\ t (|\log(|x - y| + t^{1/d})| + 1) & \text{if } d - M = -n, \\ t & \text{if } d - M < -n, \end{cases} \quad (2.24)$$

for any  $c_1 < \gamma(P)$ . In particular,

$$\begin{aligned} |\mathcal{K}_V(x, y, t)| &\leq e^{-c_1 t} t (|x - y| + t^{1/d})^{-d-n}, \\ |\mathcal{K}_{V'_1}(x, y, t)| &\leq e^{-c_1 t} t (|x - y| + t^{1/d})^{1-d-n}. \end{aligned} \quad (2.25)$$

3° For the operators defined on  $M$ , one has (with  $d(x, y)$  denoting the distance between  $x$  and  $y$ )

$$|\mathcal{K}_V(x, y, t)| \leq e^{-c_1 t} t (d(x, y) + t^{1/d})^{-d-n}, \quad (2.26)$$

for any  $c_1 < \gamma(P)$ .

*Proof.* 1°–2°. In the region where  $|x - y| \geq t^{1/d}$ ,

$$|x - y| \leq |x - y| + t^{1/d} \leq 2|x - y|,$$

in other words,  $|x - y| \doteq |x - y| + t^{1/d}$ . Then, the estimates in Theorem 2.4 imply the validity of the above estimates on this region.

In the region where  $|x - y| \leq t^{1/d}$ , we have instead that  $t^{1/d} \doteq |x - y| + t^{1/d}$ . Then the estimates in Theorem 2.1 imply the above estimates on that region; for example

$$t^{-n/d} = t (t^{1/d})^{-d-n} \doteq t (|x - y| + t^{1/d})^{-d-n}$$

there. For the two regions together, this shows (2.23)–(2.25).

3°. This follows from the estimates in local coordinates. □

The operator  $P$  on  $M$  has compact resolvent. When the eigenvalues with real part equal to  $\gamma(P)$  (necessarily finitely many) are semisimple (i.e., the algebraic multiplicity equals the geometric multiplicity), we can sharpen the information on the behavior for  $t \rightarrow \infty$ :

**COROLLARY 2.6.** *Assume that all eigenvalues of  $P$  with real part  $\gamma(P)$  are semisimple (it holds in particular when  $P$  is selfadjoint). Then*

$$|\mathcal{K}_{e^{-tP}}(x, y, t)| \lesssim e^{-\gamma(P)t} \frac{t}{(d(x, y) + t^{1/d})^d} \left( (d(x, y) + t^{1/d})^{-n} + 1 \right). \quad (2.27)$$

*Proof.* The spectral projections  $\Pi_j = \frac{i}{2\pi} \int_{C_j} (P - \lambda)^{-1} d\lambda$  onto the eigenspaces  $X_j$  for the eigenvalues  $\{\lambda_1, \dots, \lambda_k\}$  with real part  $\gamma(P)$  (where  $C_j$  is a small circle around the eigenvalue) are pseudodifferential operators of order  $-\infty$ , and their kernels  $\mathcal{K}_{\Pi_j}(x, y)$  are bounded. If  $\varepsilon > 0$ , the operator  $P' = P + \varepsilon \sum_{j=1}^k \Pi_j$  satisfies  $\gamma(P') > \gamma(P)$ . By Theorem 2.5 applied to  $P'$ ,

$$|\mathcal{K}_{e^{-tP'}}(x, y, t)| \lesssim e^{-\gamma(P')t} t (d(x, y) + t^{1/d})^{-d-n}.$$

On the other hand,  $V(t) = e^{-tP'} + (1 - e^{-\varepsilon t}) \sum_{j=1}^k e^{-t\lambda_j} \Pi_j$ , so

$$\mathcal{K}_{e^{-tP}}(x, y, t) = \mathcal{K}_{e^{-tP'}}(x, y, t) + (1 - e^{-\varepsilon t}) \sum_{j=1}^k e^{-t\lambda_j} \mathcal{K}_{\Pi_j}(x, y).$$

From

$$1 - e^{-\varepsilon t} \leq \min\{1, \varepsilon t\} \lesssim \frac{t}{(\text{diam}(M) + t^{1/d})^d} \leq \frac{t}{(d(x, y) + t^{1/d})^d},$$

we conclude that  $(1 - e^{-\varepsilon t})|\mathcal{K}_{\Pi_j}(x, y)| \lesssim \frac{t}{(d(x, y) + t^{1/d})^d}$ , and (2.27) follows since  $|e^{-t\lambda_j}| = e^{-t\gamma(P)}$  for each  $j$ . □

**REMARK 2.7.** The proof of Corollary 2.6 allows to sharpen the estimates in Theorem 2.5 and Theorem 2.9 below also in the general case where the eigenvalues with real part  $\gamma(P)$  are not all semisimple. Denote by  $r$  the dimension of the largest irreducible  $P$ -invariant subspace of any eigenspace  $X_j$  associated with an eigenvalue with real part  $\gamma(P)$ . Then, in Theorems 2.5 and 2.9, we may replace the upper bound  $e^{-c't} t (d(x, y) + t^{1/d})^{-d-n-k}$  by

$$e^{-\gamma(P)t} (1 + t^{r-1}) \frac{t}{(d(x, y) + t^{1/d})^d} \left( (d(x, y) + t^{1/d})^{-n-k} + 1 \right). \quad (2.28)$$

It is not hard to extend the estimates to complex  $t$  in convenient sectors around  $\mathbb{R}_+$ . Namely, since  $p^0$  has its spectrum in the sector  $\{|\arg \lambda| \leq \varphi_0\}$ ,  $e^{i\theta}P$  has the sectorial ellipticity property when  $|\theta| < \theta_0 = \frac{\pi}{2} - \varphi_0$ . For each  $\theta$ , it generates a semigroup  $e^{-te^{i\theta}P}$ , and these operator families coincide with the holomorphic extension of  $V(t)$  to the rays  $\{re^{i\theta}\}$  in the sector  $V_{\theta_0} = \{t \in \mathbb{C} \mid |\arg t| < \theta_0\}$ . On each ray, we have the estimates in Theorem 2.5, and they hold uniformly in closed subsectors of  $V_{\theta_0}$ . We have hereby obtained the following:

**THEOREM 2.8.** *With  $\varphi_0$  defined as in the beginning of Sect. 1 and  $\theta_0 = \frac{\pi}{2} - \varphi_0$ , the semigroup generated by  $P$  extends holomorphically to the sector  $\{|\arg t| < \theta_0\}$ , and the estimates in Theorem 2.5 hold in terms of  $|t|$  on any closed sector  $\{|\arg t| \leq \theta\}$  with  $0 < \theta < \theta_0$ , taking  $c_1 < \min_{|\theta'| \leq \theta} \gamma(e^{i\theta'}P)$ .*

For the case where  $P$  is selfadjoint, global estimates on the open sector  $\{|\arg t| < \frac{\pi}{2}\}$  will be given in Sect. 3.

Also, the derivatives of the kernels can be estimated by use of the symbol estimates in [16].

**THEOREM 2.9.** *1° One has in local coordinates:*

$$\begin{aligned} & |D_x^\beta D_y^\gamma D_t^j \mathcal{K}_{V_{-d-l}}(x, y, t)| \\ & \leq e^{-c't} \begin{cases} t (|x - y| + t^{1/d})^{l-(j+1)d-|\gamma|-n} & \text{if } (j+1)d + |\gamma| - l > -n, \\ t (|\log(|x - y| + t^{1/d})| + 1) & \text{if } (j+1)d + |\gamma| - l = -n, \\ t & \text{if } (j+1)d + |\gamma| - l < -n, \end{cases} \end{aligned} \quad (2.29)$$

for some  $c' > 0$ . If  $\gamma(P) > 0$ , we modify  $p^0$  to satisfy  $\inf_{x,\xi} \gamma(p^0(x, \xi)) \geq \gamma(P)$ ; then  $c'$  can be any number in  $]0, \gamma(P)[$ .

2° Moreover, with  $p^0$  chosen as in 1°,

$$\begin{aligned} & |D_x^\beta D_y^\gamma D_t^j \mathcal{K}_{V'_M}(x, y, t)| \\ & \leq e^{-c_1 t} \begin{cases} t (|x - y| + t^{1/d})^{M-(j+1)d-|\gamma|-n} & \text{if } (j+1)d + |\gamma| - M > -n, \\ t (|\log(|x - y| + t^{1/d})| + 1) & \text{if } (j+1)d + |\gamma| - M = -n, \\ t & \text{if } (j+1)d + |\gamma| - M < -n, \end{cases} \end{aligned} \quad (2.30)$$

for any  $c_1 < \gamma(P)$ .

3° The estimates of derivatives of  $\mathcal{K}_V$  hold for the operator defined on  $M$  with  $|x - y|$  replaced by  $d(x, y)$ .

*Proof.* As in Theorem 2.5, the estimates are pieced together from estimates generalizing those in Theorem 2.1 resp. Theorem 2.4 to include derivatives. We use that

$$\begin{aligned} & |D_x^\beta D_y^\gamma D_t^j \mathcal{K}_{V_{-d-l}}(x, y, t)| = |D_x^\beta D_z^\gamma D_t^j \tilde{v}_{-d-l}(x, z, t)|_{z=x-y}| \\ & = |\mathcal{F}_{\xi \rightarrow z}^{-1}(\xi^\gamma D_x^\beta D_t^j v_{-d-l}(x, \xi, t))|_{z=x-y}|. \end{aligned}$$

To generalize Theorem 2.1 to allow  $x$ - and  $y$ -derivatives, we just have to apply the arguments of [16, Theorems 4.2.2 and 4.2.5], to the modified symbols  $\xi^\gamma D_x^\beta v_{-d-l}$ , to get the estimates (2.29) with  $|x - y|$  replaced by 0. Derivatives with respect to  $t$  alone are explained in Theorem 4.2.5; finally, this is combined with  $x$ - and  $y$ -derivatives in a straightforward way. Similar considerations work for remainders; here, we can in fact refer directly to (4.2.60) for large  $M$ , and the statements for lower  $M$  follow by addition of the appropriate set of estimates of  $\mathcal{K}_{V_{-d-l}}$ -terms. This gives the expected generalization of Theorem 2.1, namely (2.29)–(2.30) with  $|x - y|$  replaced by 0.

For the generalization of Theorem 2.4, we note that estimates

$$|\xi^\gamma D_x^\beta D_\xi^\alpha D_t^j v_{-d-l}(x, \xi, t)| \leq \langle \xi \rangle^{(j+1)d+|\gamma|-|\alpha|-l} t e^{-c't}$$

for  $|\alpha| + l > 0$ , all  $\beta, j$ , follow from [16, Lemma 4.2.3] (see the remarks around (4.2.40) for how to include  $t$ -derivatives, as done also in Theorem 4.2.5). Thus,  $e^{c't} t^{-1} \xi^\gamma D_x^\beta D_t^j v_{-d-l}$  is in  $S_{1,0}^{(j+1)d+|\gamma|-l}$  uniformly in  $t$ , and it follows by Proposition 2.2 that

$$|D_z^\gamma D_x^\beta D_t^j \tilde{v}_{-d-l}(x, z, t)| \leq e^{-c't} \begin{cases} t|z|^{-(j+1)d-|\gamma|+l-n}, & \text{if } (j+1)d + |\gamma| - l > -n, \\ t(|\log(|z| + t^{1/d})| + 1) & \text{if } (j+1)d + |\gamma| - l = -n, \\ t & \text{if } (j+1)d + |\gamma| - l < -n. \end{cases}$$

This implies estimates as in (2.29) with  $|x - y| + t^{1/d}$  replaced by  $|x - y|$ . The conclusion is immediate for  $l \geq 1$ , and for  $l = 0$ , we use the estimates of  $D_{\xi_j} v$  as in the proof of Theorem 2.4. Again for remainder estimates, we can appeal to (4.2.60) for large  $M$ .

The proof is now completed as in Theorem 2.5. □

*REMARK 2.10.* As an example of a nonselfadjoint strongly elliptic case of interest to which the results apply, let us mention the first-order operator  $P = \Delta^{\frac{1}{2}} + L$ , where  $L$  is a first-order differential operator with real coefficients (in the situation on  $\mathbb{R}^n$ ,  $L = b(x) \cdot \nabla + c(x)$ ,  $b$  and  $c$  real smooth with all derivatives bounded). Since the principal symbol  $b(x) \cdot i\xi$  of  $L$  is purely imaginary,  $\text{Re } p^0(x, \xi) = |\xi|$ , so  $p^0(x, \xi)$  for  $\xi \neq 0$  ranges in a sector  $\{\lambda \neq 0 \mid |\arg \lambda| \leq \varphi_0\}$ ,  $\varphi_0 < \frac{\pi}{2}$ . This case is treated by other methods in Xie and Zhang [26].

### 3. Estimates in the complex plane for selfadjoint operators

In this section, we shall derive some uniform kernel estimates for the extension of the semigroup into the region  $\mathbb{C}_+ = \{t \in \mathbb{C} \mid \text{Re } t > 0\}$ , when  $P$  is selfadjoint. We assume for simplicity that  $P$  is  $\geq 0$ . As noted in Theorem 2.8,  $V(t)$  exists for all  $t \in \mathbb{C}_+$ , and the estimates worked out in Sect. 2 hold uniformly on closed subsectors  $\{t \in \mathbb{C}_+ \mid |\arg t| \leq \theta\}$ ,  $0 \leq \theta < \frac{\pi}{2}$ . For the analysis of the behavior for  $\theta \rightarrow \frac{\pi}{2}$ , additional efforts are needed. We shall rely on a theorem of Agmon [1]:

**PROPOSITION 3.1.** *Let  $\Omega$  be an open set having the cone property. Let  $T$  be a bounded operator in  $L_2(\Omega)$  such that the ranges of  $T$  and  $T^*$  are contained in  $H^m(\Omega)$  for an  $m > n$  ( $m$  can be noninteger if  $\Omega = \mathbb{R}^n$  or is suitably smooth). Then  $T$  is an integral operator with a continuous and bounded kernel  $\mathcal{K}_T(x, y)$  on  $\Omega \times \Omega$  satisfying*

$$|\mathcal{K}_T(x, y)| \leq C(\|T\|_{0,m} + \|T^*\|_{0,m})^{n/m} \|T\|_{0,0}^{1-n/m},$$

with a constant depending only on  $\Omega$  and  $m$ .

Here,  $\|T\|_{a,b}$  stands for the norm of  $T$  as an operator from  $H^a(\Omega)$  to  $H^b(\Omega)$ . The theorem holds in particular when  $\Omega$  is replaced by our manifold  $M$  or by  $\mathbb{R}^n$ .

We note first that there is an easy estimate of the kernel in terms of  $t$  alone that can be obtained essentially by functional analysis.

**THEOREM 3.2.** *The full kernel satisfies for  $t = e^{i\theta}|t| \in \mathbb{C}_+$ :*

$$|\mathcal{K}_V(x, y, t)| \leq 1 + (\cos \theta)^{-n/d} |t|^{-n/d}.$$

*Proof.* Note that  $\|V(t)\|_{0,m} \doteq \|(1 + P^{m/d})V(t)\|_{0,0}$  because  $P \geq 0$  is strongly elliptic and of order  $d$ . By the standard theory of analytic semigroups (see e.g., Lunardi [18, Proposition 2.1.1]) or functional calculus, and  $((\operatorname{Re} t)P)^M V(t)$  is uniformly bounded for  $M \in \mathbb{N}_0$ . This extends to  $M \geq 0$  by interpolation. Hence, we obtain for  $m \geq 0$ :

$$\|V(t)\|_{0,m} \doteq \|(1 + P^{m/d})V(t)\|_{0,0} \leq 1 + (\operatorname{Re} t)^{-m/d}.$$

The estimates likewise hold for  $V(t)^* = V(\bar{t})$ . Proposition 3.1, therefore, yields for any  $m > n$

$$\begin{aligned} |\mathcal{K}_V(x, y, t)| &\leq (\|V(t)\|_{0,m} + \|V(\bar{t})\|_{0,m})^{n/m} \|V(t)\|_{0,0}^{1-n/m} \leq 1 + (\operatorname{Re} t)^{-n/d} \\ &\doteq 1 + (\cos \theta |t|)^{-n/d}, \end{aligned}$$

as was to be shown. □

Extensions to  $\mathbb{C}_+$  of the other estimates in Sect. 2 are more costly in negative powers of  $\cos \theta$ . We first consider the homogeneous terms in the symbol of  $Q_\lambda$ , showing how the estimates of symbols like (1.5)–(1.7) depend on  $\arg \lambda$ , when  $\lambda$  is close to the spectrum of  $P$ .

As in [16], we denote  $|\lambda|^{1/d} = \mu$  and write  $\langle(\xi, \mu)\rangle = (1 + |\xi|^2 + \mu^2)^{1/2}$  for short as  $\langle\xi, \mu\rangle$ ; it is  $\doteq (1 + |\xi| + |\lambda|^{1/d})$ .

**PROPOSITION 3.3.** *Let  $p^0(x, \xi)$  be symmetric with lower bound  $\geq c\langle\xi\rangle^d$ , and let  $\lambda \in \mathbb{C}$  with  $\arg \lambda = \varphi$ ,  $0 < |\varphi| \leq \frac{\pi}{2}$ . Then*

$$\begin{aligned} |q_{-d}(x, \xi, \lambda)| &= |(p^0(x, \xi) - \lambda)^{-1}| \leq |\sin \varphi|^{-1} \langle\xi, \mu\rangle^{-d}, \\ |D_x^\beta D_\xi^\alpha q_{-d}(x, \xi, \lambda)| &\leq |\sin \varphi|^{-1-|\alpha|-|\beta|} \langle\xi\rangle^{d-|\alpha|} \langle\xi, \mu\rangle^{-2d}, \text{ when } |\alpha| + |\beta| > 0. \end{aligned} \tag{3.1}$$

For all  $l, \alpha, \beta$  with  $l > 0$ ,

$$|D_x^\beta D_\xi^\alpha q_{-d-l}(x, \xi, \lambda)| \leq |\sin \varphi|^{-2l-1-|\alpha|-|\beta|} \langle\xi\rangle^{d-l-|\alpha|} \langle\xi, \mu\rangle^{-2d}. \tag{3.2}$$

*Proof.* We have for  $\lambda = e^{i\varphi}|\lambda|$  with  $0 < |\varphi| \leq \frac{\pi}{2}$ , and  $v \in \mathbb{C}^N$ :

$$\begin{aligned} |(p^0 v, v) - \lambda|v|^2| &\geq |\operatorname{Im}((p^0 v, v) - \lambda|e^{i\varphi}|v|^2)| = |\lambda| |\sin \varphi| |v|^2, \\ |(p^0 v, v) - \lambda|v|^2| &= |e^{-i\varphi}(p^0 v, v) - |\lambda||v|^2| \geq |\operatorname{Im} e^{-i\varphi}(p^0 v, v)| \\ &= |\sin \varphi|(p^0 v, v) \geq |\sin \varphi| c \langle \xi \rangle^d |v|^2, \end{aligned}$$

from which follows

$$|(p^0 - \lambda)v||v| \geq |((p^0 - \lambda)v, v)| \geq |\sin \varphi| (|\lambda| + \langle \xi \rangle^d) |v|^2.$$

This implies that  $|(p^0 - \lambda)^{-1}| \leq |\sin \varphi|^{-1} (\langle \xi \rangle^d + |\lambda|)^{-1} \doteq |\sin \varphi|^{-1} \langle \xi, \mu \rangle^{-d}$ , showing (3.1).

The other estimates follow as in [16] from the structure of the terms in the parametrix, using (3.1):  $q_{-d-l}$  is for  $l \geq 1$  a finite sum of terms, where  $\nu_1 + \dots + \nu_M \geq 2$  takes values up to  $2l + 1$ ,

$$r(x, \xi, \lambda) = b_1 q_{-d}^{\nu_1} b_2 q_{-d}^{\nu_2} \dots b_M q_{-d}^{\nu_M} b_{M+1},$$

cf. (1.7). Each  $q_{-d}$  contributes to the estimates with a factor  $|\sin \varphi|^{-1}$ , and there are up to  $2l + 1$  such factors; this shows (3.2) for  $\alpha = \beta = 0$ . Each differentiation may hit a factor  $q_{-d}$  giving an extra  $|\sin \varphi|^{-1}$  in view of (2.22); this leads to the estimates (3.2) by the Leibniz formula.  $\square$

The symbol terms  $v_{-d-l}(x, \xi, t)$  are defined from the  $q_{-d-l}(x, \xi, \lambda)$  as in (2.2). When  $t \in \mathbb{C}_+$ , with argument  $\arg t = \theta \in ]-\frac{\pi}{2}, \frac{\pi}{2}[$ , we must assure that  $\operatorname{Re}(\lambda t) \rightarrow \infty$  when  $|\lambda| \rightarrow \infty$  on the integral curve  $\mathcal{C}$ . This holds if  $\lambda$  runs on a contour formed of the rays  $\lambda = r e^{\pm i\varphi_0}$ , where  $\varphi_0 = \frac{1}{2}(\frac{\pi}{2} - |\theta|)$ , connected near 0 by a circle of radius  $\varepsilon' < \inf \gamma(p^0(x, \xi))$  passing to the right of 0:

$$\begin{aligned} \mathcal{C} &= \{r e^{i\varphi_0} \mid \infty > r > \varepsilon'\} \cup \{\varepsilon' e^{i\varphi} \mid \varphi_0 > \varphi > -\varphi_0\} \cup \{r e^{-i\varphi_0} \mid \varepsilon' < r < \infty\}, \\ \varphi_0 &= \frac{1}{2}(\frac{\pi}{2} - |\theta|). \end{aligned} \tag{3.3}$$

Here,  $\inf_{\lambda \in \mathcal{C}} \operatorname{Re}(\lambda) = c_1 > 0$ .

*REMARK 3.4.* Note that  $|\theta| = \frac{\pi}{2} - 2\varphi_0$  belongs to  $[0, \frac{\pi}{2}[$  if and only if  $\varphi_0$  belongs to  $]0, \frac{\pi}{4}[$ . On this interval,  $\sin \varphi_0 \doteq \sin(2\varphi_0) = \cos \theta$ , so they can be used interchangeably in our estimates.

We shall need the following generalization of [16, Lemma 4.2.3].

*LEMMA 3.5.* Let  $t = e^{i\theta}|t|$ , and choose  $\varphi_0$  and  $\mathcal{C}$  as in (3.3).

Let  $M \in \mathbb{N}$ , let  $\sigma_1, \dots, \sigma_M$  be nonnegative integers with

$$\sigma = \sigma_1 + \dots + \sigma_M \geq 1, \tag{3.4}$$

and let  $f(x, \xi, \lambda)$  be a (matrix-formed) symbol of the form

$$f(x, \xi, \lambda) = f_1(p^0 - \lambda)^{-\sigma_1} f_2(p^0 - \lambda)^{-\sigma_2} \dots (p^0 - \lambda)^{-\sigma_M} f_{M+1}, \tag{3.5}$$

where the  $f_j(x, \xi)$  are  $\psi$ do symbols of order  $s_j \in \mathbb{R}$ , homogeneous for  $|\xi| \geq 1$ . Denote  $s_1 + \dots + s_{M+1} = s$ , then the order of  $f$  is  $k = s - \sigma d$ . Let  $F_\lambda = \text{Op}(f(x, \xi, \lambda))$  on  $\mathbb{R}^n$ , and let  $E(t)$  be the operator family defined from  $F_\lambda$  for  $\text{Re } t > 0$  by

$$E(t) = \frac{i}{2\pi} \int_C e^{-t\lambda} F_\lambda \, d\lambda. \tag{3.6}$$

Then  $E(t) = \text{Op}(e(x, t, \xi))$ , where the symbol

$$e(x, t, \xi) = \frac{i}{2\pi} \int_C e^{-t\lambda} f(x, \xi, \lambda) \, d\lambda \tag{3.7}$$

satisfies:

- (i)  $e(x, s^{-d}t, s\xi) = s^{d+k}e(x, t, \xi)$  for  $|\xi| \geq 1, s \geq 1$ ,
- (ii)  $|D_x^\beta D_\xi^\alpha e(x, t, \xi)| \leq (\sin \varphi_0)^{-\sigma - |\alpha| - |\beta|} \langle \xi \rangle^{d+k-|\alpha|} e^{-c \text{Re } t \langle \xi \rangle^d}$ . (3.8)

The kernel of  $E(t)$  satisfies for  $d + k > -n$

$$|\mathcal{K}_E(x, y, t)| \leq (\sin \varphi_0)^{-\sigma - (d+k+n)/d} e^{-c' \text{Re } t |t|^{-(d+k+n)/d}}, \tag{3.9}$$

with  $c' > 0$ .

If  $\sigma \geq 2$ ,

$$|D_x^\beta D_\xi^\alpha e(x, t, \xi)| \leq (\sin \varphi_0)^{-\sigma - |\alpha| - |\beta|} |t| \langle \xi \rangle^{2d+k-|\alpha|} e^{-c' \text{Re } t \langle \xi \rangle^d}. \tag{3.10}$$

In this case, the kernel satisfies for  $d + k \leq -n$

$$|\mathcal{K}_E(x, y, t)| \leq (\sin \varphi_0)^{-\sigma} e^{-c' \text{Re } t} \begin{cases} |t| (|\log \text{Re } t| + 1) & \text{if } d + k = -n, \\ |t| & \text{if } d + k < -n. \end{cases} \tag{3.11}$$

*Proof.* As in [16, Lemma 4.2.3], we can pass the operator definition through the integral. To estimate  $e$ , we first consider  $|\xi| \leq 1$ . We use the residue theorem and that  $p^0$  is selfadjoint to obtain

$$|e(t, x, \xi)| = \left| \frac{i}{2\pi} \int_C e^{-t\lambda} f(x, \xi, \lambda) \, d\lambda \right| \leq (1 + |t|^{\sigma-1}) e^{-c \text{Re } t}.$$

Here,  $c = \gamma(p^0(x, \xi))$ .

For  $|\xi| \geq 1$ , we replace  $\mathcal{C}$  by a closed, homogeneous curve  $\mathcal{C}_{c,C}$  around the spectrum of  $p^0(x, \xi)$ .  $\mathcal{C}_{c,C}$  coincides with  $\mathcal{C}$  on an annulus of inner radius  $c|\xi|^d$  and outer radius  $C|\xi|^d$  and is closed by the segments of the boundary of this annulus which lie to the right of  $\mathcal{C}$ . Then, by homogeneity,

$$|e(t, x, \xi)| = \left| \frac{i}{2\pi} \int_{\mathcal{C}_{c,C}} e^{-t\lambda} f(x, \xi, \lambda) \, d\lambda \right| \leq (\sin \varphi_0)^{-\sigma} \langle \xi \rangle^d \langle \xi \rangle^k e^{-\frac{c}{2} \text{Re } t |\xi|^d}.$$

Combining the two estimates, we conclude (3.8) for  $\alpha = \beta = 0$ . The derivatives  $D_x^\beta D_\xi^\alpha e(x, t, \xi)$  are sums of terms of a similar form, with  $k$  replaced by  $k - |\alpha|$  and  $\sigma$  replaced by numbers  $\leq \sigma + |\alpha| + |\beta|$ .



To show (3.9) for  $d+k > -n$ , we estimate  $\mathcal{K}_E$  by comparing  $e$  with its homogeneous extension  $e^h$ :

$$\mathcal{K}_E(x, y, t) = \int_{\mathbb{R}^n} e^{i(x-y)\cdot\xi} e^h(x, t, \xi) \, d\xi + \int_{|\xi| \leq 1} e^{i(x-y)\cdot\xi} (e - e^h) \, d\xi.$$

Using (3.8) and a homogeneous variant,

$$\begin{aligned} |\mathcal{K}_E(x, y, t)| &\leq (\sin \varphi_0)^{-\sigma} e^{-c_1 \operatorname{Re} t} \int_{\mathbb{R}^n} e^{-c_2 \operatorname{Re} t |\xi|^d} |\xi|^{d+k} \, d\xi \\ &\quad + (\sin \varphi_0)^{-\sigma} e^{-c_1 \operatorname{Re} t} \int_{|\xi| \leq 1} e^{-c_2 \operatorname{Re} t |\xi|^d} (|\xi|^{d+k} + |\xi|^{d+k}) \, d\xi. \end{aligned}$$

The first integral is  $\doteq (\operatorname{Re} t)^{-(d+k+n)/d} \doteq (\sin \varphi_0)^{-(d+k+n)/d} |t|^{-(d+k+n)/d}$ , while the second remains bounded as  $|t| \rightarrow 0$ .

Now, consider the case where  $\sigma \geq 2$ . As  $|f| \leq \langle \lambda \rangle^{-2}$  away from  $\mathbb{R}_+$ , the integral converges uniformly in  $t \geq 0$ . We may deform  $\mathcal{C}$  to a closed curve in the left half plane, where  $f$  is holomorphic, to conclude  $e(x, 0, \xi) = 0$ . Also, using  $(-\lambda)(p_d - \lambda)^{-1} = 1 - p_d(p_d - \lambda)^{-1}$ ,

$$\partial_t e(x, t, \xi) = \frac{i}{2\pi} \int_{\mathcal{C}} e^{-t\lambda} (-\lambda) f(x, \xi, \lambda) \, d\lambda$$

can be expressed in terms of  $e$  and a second term of the same form, with one of the  $s_j$  replaced by  $s_j + d$ . By (3.8)

$$|\partial_t e(x, t, \xi)| \leq (\sin \varphi_0)^{-\sigma} \langle \xi \rangle^{2d+k} e^{-c \operatorname{Re} t \langle \xi \rangle^d}$$

and hence, since the value at  $t = 0$  is 0,

$$|e(x, t, \xi)| \leq (\sin \varphi_0)^{-\sigma} |t| \langle \xi \rangle^{2d+k} e^{-c \operatorname{Re} t \langle \xi \rangle^d}.$$

This shows (3.10) for  $\alpha = \beta = 0$ . The proof for  $D_x^\beta D_\xi^\alpha e(x, t, \xi)$  is analogous. The estimate (3.11) is obtained similarly to (3.9), using (3.10) instead of (3.8).  $\square$

This leads to the estimates of homogeneous terms:

**THEOREM 3.6.** *Let  $t = e^{i\theta} |t| \in \mathbb{C}_+$ . In local coordinates, the homogeneous terms in the kernel of  $V(t)$  satisfy for some  $c' > 0$ :*

$$|\mathcal{K}_{V_{-d}}(x, y, t)| \leq (\cos \theta)^{-n/d} e^{-c' \operatorname{Re} t} |t|^{-n/d}, \tag{3.12}$$

$$|\mathcal{K}_{V_{-d-l}}(x, y, t)| \leq (\cos \theta)^{-2l-1} e^{-c' \operatorname{Re} t} \begin{cases} (\cos \theta)^{(l-n)/d} |t|^{(l-n)/d} & \text{if } d-l > -n, \\ |t| (|\log \operatorname{Re} t| + 1) & \text{if } d-l = -n, \\ |t| & \text{if } d-l < -n. \end{cases} \tag{3.13}$$

*Proof.* We choose  $\varphi_0$  and the curve  $\mathcal{C}$  as in (3.3), recalling that  $\cos \theta \doteq \sin \varphi_0$ . For  $l \geq 1$ , the assertion follows from Lemma 3.5, (3.9) resp. (3.11), using that in the terms of  $q_{-d-l}$ ,  $(d+k+n)/d = (n-l)/d$  and  $\sigma \leq 2l+1$ .

For  $l = 0$ , we explicitly compute

$$\begin{aligned} |\mathcal{K}_{V_{-d}}(x, y, t)| &= (2\pi)^{-n} \left| \int_{\mathbb{R}^n} e^{i(x-y)\cdot\xi} e^{-t p^0(x, \xi)} d\xi \right| \\ &\leq e^{-c_1 \operatorname{Re} t} \left( \int_{\mathbb{R}^n} e^{-c_2 \operatorname{Re} t |p_h^0(x, \xi)|} d\xi + \int_{|\xi| \leq 1} \left( e^{-c_2 \operatorname{Re} t |p^0(x, \xi)|} - e^{-c_2 \operatorname{Re} t |p_h^0(x, \xi)|} \right) d\xi \right) \\ &\leq e^{-c_1 \operatorname{Re} t} \left( \int_{\mathbb{R}^n} e^{-\operatorname{Re} t |\xi|^d} d\xi + 1 \right) \leq e^{-c' \operatorname{Re} t} (\operatorname{Re} t)^{-n/d}. \end{aligned}$$

The assertion follows, since  $\operatorname{Re} t = |t| \cos \theta$ .  $\square$

Moreover, estimates in terms of  $|t|$  and powers of  $|x-y|$  are obtained. For  $a \in \mathbb{R}$ , we denote by  $[a]$  the largest integer  $\leq a$ .

**THEOREM 3.7.** *1° In local coordinates,  $\mathcal{K}_{V_{-d}}$  satisfies for some  $c' > 0$ :*

$$|\mathcal{K}_{V_{-d}}(x, y, t)| \leq (\cos \theta)^{-[d-1+n]-3} e^{-c' \operatorname{Re} t} |t| |x-y|^{-d-n}. \quad (3.14)$$

For  $l \geq 1$ , the kernels  $\mathcal{K}_{V_{-d-l}}$  satisfy

$$\begin{aligned} |\mathcal{K}_{V_{-d-l}}(x, y, t)| &\leq (\cos \theta)^{-2l-1} e^{-c' \operatorname{Re} t} \\ &\times \begin{cases} (\cos \theta)^{-[d-l+n]-1} |t| |x-y|^{l-d-n} & \text{if } d-l > -n, \\ (\cos \theta)^{-1} |t| (|\log |x-y|| + 1) & \text{if } d-l = -n, \\ |t| & \text{if } d-l < -n. \end{cases} \end{aligned} \quad (3.15)$$

2° Moreover,

$$|\mathcal{K}_{V_{-d-l}}(x, y, t)| \leq e^{-c' \operatorname{Re} t} \begin{cases} (\cos \theta)^{-N_l} |t| (|x-y| + |t|^{1/d})^{l-d-n} & \text{if } d-l > -n, \\ (\cos \theta)^{-N_l} |t| (|\log(|x-y| + |t|^{1/d})| + 1) & \text{if } d-l = -n, \\ (\cos \theta)^{-N_l} |t| & \text{if } d-l < -n, \end{cases}$$

$$\text{where } N_l = \begin{cases} \max\{n/d, [d-1+n]+3\} & \text{if } l = 0, \\ \max\{2l+1+(n-l)/d, 2l+2+[d-1+n]\} & \text{if } l > 0, d-l > -n, \\ 2l+2 & \text{if } d-l = -n, \\ 2l+1 & \text{if } d-l < -n. \end{cases} \quad (3.16)$$

*Proof.* 1°. For  $l \geq 1$ , we obtain from Lemma 3.5, (3.10), that

$$|D_\xi^\alpha v_{-d-l}(x, t, \xi)| \leq (\cos \theta)^{-2l-1-|\alpha|} \langle \xi \rangle^{d-l-|\alpha|} |t| e^{-c' \operatorname{Re} t}.$$

Here, we apply Proposition 2.2 with  $r = d-l$ ; then, we need  $|\alpha| \leq N$  where  $N \in \mathbb{N}_0$ ,  $N > d-l+n$ . If  $d-l+n < 0$  we take  $N = 0$ , and if  $d-l+n \geq 0$ , we take  $N = [d-l+n] + 1$ . This shows (3.15).

For  $l = 0$ ,  $v_{-d}(x, t, \xi) = e^{-tP^0(x, \xi)}$ , and we pass via  $\partial_{\xi_j} v$  to show the estimate, as in Theorem 2.4. Here,  $\partial_{\xi_j} v$  enters by application of Lemma 3.5 to  $f(x, \xi, \lambda) = \partial_{\xi_j} q_{-d} = -q_{-d}(\partial_{\xi_j} P^0)q_{-d}$ ; it has  $\sigma = 2, k = -d - 1$ . Then (3.10) gives that

$$|D_{\xi}^{\alpha} \partial_{\xi_j} v_{-d}(x, t, \xi)| \leq (\cos \theta)^{-2-|\alpha|} \langle \xi \rangle^{d-1-|\alpha|} |t| e^{-c' \operatorname{Re} t},$$

so an application of Proposition 2.2 with  $N = [d - 1 + n] + 1$  gives that

$$|z_j \tilde{v}_{-d}| \leq (\cos \theta)^{-2-[d-1+n]-1} |t| e^{-c' \operatorname{Re} t} |z|^{-d+1-n}.$$

Using this for all  $j = 1, \dots, n$ , we find (3.14).

2°. We here combine the preceding estimates with those in Theorem 3.6 in the same way as in the proof of Theorem 2.5. □

Estimates of remainders  $V'_M$  are more difficult to work out, since they depend on the interplay between the exact resolvent  $Q_{\lambda}$  and the homogeneous symbol terms, and they will be more costly in powers of  $(\cos \theta)^{-1}$ , the larger  $M$  is taken. We shall here go directly to remainder *kernel* estimates.

Let us define the  $M$ th resolvent remainder operator

$$Q'_M = Q_{\lambda} - \sum_{l < M} Q_{-d-l},$$

where each  $Q_{-d-l}$  is an operator on the manifold  $M$  constructed from the symbols  $q_{-d-l}$  in local coordinates. For each  $\lambda$ ,  $Q'_M$  is a  $\psi$ do of order  $-d - M$ , but we do not know on beforehand how it is estimated in terms of  $\lambda$ , although we have such information on the terms  $Q_{-d-l}$ . Let us write

$$\begin{aligned} Q'_M &= Q'_M(P - \lambda)Q_{\lambda} = R_M Q_{\lambda}, \text{ where} \\ R_M &= Q'_M(P - \lambda) = 1 - \sum_{l < M} Q_{-d-l}(P - \lambda) \end{aligned} \tag{3.17}$$

is a  $\psi$ do of order  $-M$  constructed from known symbols. The idea is now that functional analysis gives us a certain control over operator norms of  $Q_{\lambda}$ , whereas  $\psi$ do calculus will allow us to estimate operator norms of  $R_M$ , and then Agmon's result Proposition 3.1 will lead to a kernel estimate of the composed operator. For  $\lambda$  with argument  $\varphi$  satisfying  $0 < |\varphi| \leq \frac{\pi}{2}$ ,

$$\begin{aligned} \|(P - \lambda)u\| \|u\| &\geq |((P - \lambda)u, u)| \geq |\operatorname{Im} \lambda| \|u\|^2 = |\sin \varphi| |\lambda| \|u\|^2; \text{ hence} \\ \|Q_{\lambda}\|_{0,0} &\leq |\sin \varphi|^{-1} |\lambda|^{-1}. \end{aligned} \tag{3.18}$$

We are aiming for an estimate of  $\mathcal{K}_{V'_M}$  by  $c|t|$ , and we know from Theorem 2.1 based on [16, Thm. 4.2.5] that to avoid logarithmic factors, it is better to use the resolvent formula

$$Q_{\lambda} = -\lambda^{-1} + \lambda^{-1} Q_{\lambda} P, \tag{3.19}$$

inserted in the integral (2.1) derived with respect to  $t$ .

First some details on how to handle the possible zero eigenspace of  $P$ . Similarly to Corollary 2.6, it will be convenient to write  $P = P^\varepsilon - \varepsilon \Pi_0$ , where  $\Pi_0$  is the orthogonal projection onto the zero eigenspace of  $P$ , and  $\varepsilon > 0$  is chosen  $\leq$  the lowest positive eigenvalue, whereby  $P^\varepsilon = P + \varepsilon \Pi_0$  is  $\geq \varepsilon$ . Here,  $\Pi_0$  is the  $\psi$ do of order 0 with kernel  $\sum_{j=1}^{\nu} \varphi_j(x) \varphi_j(y)^*$ , for an orthonormal basis  $\varphi_1, \dots, \varphi_\nu$  of the zero eigenspace. Then

$$V(t) = V^\varepsilon(t) + (1 - e^{-\varepsilon t})\Pi_0, \text{ where } V^\varepsilon(t) = e^{-tP^\varepsilon};$$

and it is the latter operator that needs investigation.  $V^\varepsilon(t)$  is defined from the resolvent  $Q_\lambda^\varepsilon = Q_\lambda - (\varepsilon - \lambda)^{-1} \Pi_0 = (P^\varepsilon - \lambda)^{-1}$  by

$$V^\varepsilon(t) = \frac{i}{2\pi} \int_C e^{-t\lambda} Q_\lambda^\varepsilon d\lambda. \tag{3.20}$$

For this integral, the contour can be chosen as in (3.3) with  $\varepsilon' < \varepsilon$ .

For simplicity of notation, we drop the  $\varepsilon$ -index in the next calculations and return to include the contribution from  $\Pi_0$  in the final formulations.

An application of (3.19) gives

$$\begin{aligned} V(t) &= \frac{i}{2\pi} \int_C e^{-t\lambda} (-\lambda^{-1} + \lambda^{-1} Q_\lambda P) d\lambda = \frac{i}{2\pi} \int_C e^{-t\lambda} \lambda^{-1} Q_\lambda P d\lambda, \\ \partial_t V(t) &= -\frac{i}{2\pi} \int_C e^{-t\lambda} Q_\lambda P d\lambda. \end{aligned} \tag{3.21}$$

Thus,  $\partial_t \mathcal{K}_{V'_M}$  is the kernel of the integral of the  $M$ th remainder  $-(Q_\lambda P)'_M$  of  $-Q_\lambda P$ . We know that  $\mathcal{K}_{V'_M}$  vanishes at  $t = 0$  and want to show boundedness of the last integral applied to the kernel of the  $M$ th remainder. Here, (cf. also (3.17))

$$Q_\lambda P = \left( \sum_{l < M} Q_{-d-l} + Q'_M \right) P = \sum_{l < M} Q_{-d-l} P + R_M Q_\lambda P = \sum_{l < M} Q_{-d-l} P + R_M P Q_\lambda.$$

Since  $R_M P Q_\lambda$  is already of order  $-M$ , the  $M$ th remainder of  $Q_\lambda P$  is

$$(Q_\lambda P)'_M = \tilde{R}_M + R_M P Q_\lambda, \text{ where } \tilde{R}_M = \left( \sum_{l < M} Q_{-d-l} P \right)'_M. \tag{3.22}$$

In preparation for the study of the symbols of  $R_M$  and  $\tilde{R}_M$ , we prove a lemma on composition formulas from the  $\psi$ do theory. In the general first two rules, it is important that the component to the right is  $\lambda$ -independent, to keep the introduction of factors  $|\sin \varphi|^{-1}$  as low as possible.

LEMMA 3.8. *Let  $b(x, \xi) \in S_{1,0}^{d_2}(\mathbb{R}^n \times \mathbb{R}^n)$ , and let  $a(x, \xi, \lambda) \in S_{1,0}^{d_1}(\mathbb{R}^n \times \mathbb{R}^n)$  with respect to  $(x, \xi)$ , with  $\lambda$  as in Proposition 3.3, such that for some  $d' \geq 0$ ,  $N \in \mathbb{R}$ , one has for all  $\alpha, \beta \in \mathbb{N}_0^n$ .*

$$|D_x^\beta D_\xi^\alpha a(x, \xi, \lambda)| \leq |\sin \varphi|^{-N-|\alpha|-|\beta|} \langle \xi \rangle^{d'+d_1-|\alpha|} \langle \xi, \mu \rangle^{-d'}. \tag{3.23}$$

1° There exists  $c(x, \xi, \lambda) \in S_{1,0}^{d_1+d_2}(\mathbb{R}^n \times \mathbb{R}^n)$  such that  $\text{Op}(a) \text{Op}(b) = \text{Op}(c)$ , and for every  $M \in \mathbb{N}_0$ ,

$$c(x, \xi, \lambda) = \sum_{|\alpha| < M} \frac{1}{\alpha!} D_\xi^\alpha a(x, \xi, \lambda) \partial_x^\alpha b(x, \xi) + c_M(a, b), \tag{3.24}$$

where

$$|D_x^\beta D_\xi^\alpha c_M(a, b)| \leq |\sin \varphi|^{-N-M-|\alpha|-|\beta|} \langle \xi \rangle^{d'+d_1+d_2-M-|\alpha|} \langle \xi, \mu \rangle^{-d'}. \tag{3.25}$$

2° If (3.23) for  $\alpha = \beta = 0$  is replaced by

$$|a(x, \xi, \lambda)| \leq |\sin \varphi|^{-N} \langle \xi \rangle^{d+d_1} \langle \xi, \mu \rangle^{-d}. \tag{3.26}$$

for some  $0 \leq d \leq d'$ , then (3.24) holds with (3.25) valid for  $M \geq 1$  and the estimates of  $c_0$  replaced by

$$|D_x^\beta D_\xi^\alpha c_0(a, b)| \leq |\sin \varphi|^{-N-|\alpha|-|\beta|} \langle \xi \rangle^{d+d_1+d_2-|\alpha|} \langle \xi, \mu \rangle^{-d}. \tag{3.27}$$

3° For  $\gamma \in \mathbb{N}_0^n$ ,  $D^\gamma \text{Op}(a) = \text{Op}(a^\gamma)$ , where

$$|D_x^\beta D_\xi^\alpha a^\gamma(x, \xi, \lambda)| \leq \sum_{k \leq |\gamma|} |\sin \varphi|^{-N-k-|\alpha|-|\beta|} \langle \xi \rangle^{d'+d_1+|\gamma|-k-|\alpha|} \langle \xi, \mu \rangle^{-d'}. \tag{3.28}$$

*Proof.* 1°. Let  $\chi(x, \xi)$  denote a  $C^\infty$ -function that is 1 for  $|x|^2 + |\xi|^2 \leq 1$  and vanishes for  $|x|^2 + |\xi|^2 \geq 2$ , then we can replace the given symbols by their products with  $\chi(\varepsilon x, \varepsilon \xi)$ , which makes all integrals calculated below convergent. It is known in the theory (by the technique of oscillatory integrals, cf. [17, Sect. 7.8]) that the resulting symbols converge to the given symbols for  $\varepsilon \rightarrow 0$  in all the seminorms that are involved. The modified symbols will again be denoted  $a, b$ . We can also assume that  $b$  has compact support in  $x$  (in a set containing the  $x$  for which we need the formula). Then  $\hat{b}(\eta, \xi) = \mathcal{F}_{x \rightarrow \eta} b(x, \xi)$  satisfies

$$|D_\xi^\alpha \hat{b}(\eta, \xi)| \leq \langle \eta \rangle^{-N'} \langle \xi \rangle^{d_2-|\alpha|}, \tag{3.29}$$

for all  $\alpha, N'$ . It follows from the  $\psi$ do defining formula that  $\text{Op}(a) \text{Op}(b) = \text{Op}(c)$ , where

$$\begin{aligned} c(x, \xi, \lambda) &= \int_{\mathbb{R}^{4n}} a(x, \eta, \lambda) b(y, \xi) e^{i(x-y)\cdot\eta} e^{i(y-z)\cdot\xi} dz d\xi dy d\eta \\ &= \int_{\mathbb{R}^n} a(x, \xi + \eta, \lambda) \hat{b}(\eta, \xi) e^{i x \cdot \eta} d\eta. \end{aligned} \tag{3.30}$$

If  $M > 0$ , we insert the Taylor expansion of  $a$  in  $\xi$  up to order  $M$ ,

$$\begin{aligned} a(x, \xi + \eta, \lambda) &= \sum_{|\alpha| < M} \frac{1}{\alpha!} \eta^\alpha \partial_\xi^\alpha a(x, \xi, \lambda) \\ &\quad + \sum_{|\alpha|=M} \frac{M}{\alpha!} \eta^\alpha \int_0^1 (1-h)^{M-1} \partial_\xi^\alpha a(x, \xi + h\eta, \lambda) dh, \end{aligned}$$

obtaining that  $c = c_{<M} + c_M$ , where

$$\begin{aligned} c_{<M} &= (2\pi)^{-n} \int_{\mathbb{R}^n} \sum_{|\alpha|<M} \frac{1}{\alpha!} \partial_\xi^\alpha a(x, \xi, \lambda) \eta^\alpha \hat{b}(\eta, \xi) e^{ix \cdot \eta} \, d\eta \\ &= \sum_{|\alpha|<M} \frac{1}{\alpha!} \partial_\xi^\alpha a(x, \xi, \lambda) D_x^\alpha b(x, \xi) = \sum_{|\alpha|<M} \frac{1}{\alpha!} D_\xi^\alpha a(x, \xi, \lambda) \partial_x^\alpha b(x, \xi), \\ c_M &= (2\pi)^{-n} \int_{\mathbb{R}^n} \sum_{|\alpha|=M} \frac{M}{\alpha!} \int_0^1 (1-h)^{M-1} \partial_\xi^\alpha a(x, \xi+h\eta, \lambda) \, dh \, \eta^\alpha \hat{b}(\eta, \xi) e^{ix \cdot \eta} \, d\eta. \end{aligned}$$

The sum over  $|\alpha| < M$  equals the sum in (3.24). For the last integral, we use that

$$\begin{aligned} |\partial_\xi^\alpha a(x, \xi+h\eta, \lambda)| &\leq |\sin \varphi|^{-N-M} \langle \xi+h\eta \rangle^{d'+d_1-M} \langle \xi+h\eta, \mu \rangle^{-d'} \\ &\leq |\sin \varphi|^{-N-M} \langle \xi \rangle^{d'+d_1-M} \langle \xi, \mu \rangle^{-d'} \langle \eta \rangle^{|d'+d_1-M|+d'}, \end{aligned}$$

by the Peetre inequality. Taking this together with the estimates (3.29) of  $\hat{b}$  (with a large  $N'$ ), we can conclude that

$$|c_M| \leq |\sin \varphi|^{-N-M} \langle \xi \rangle^{d'+d_1+d_2-M} \langle \xi, \mu \rangle^{-d'}.$$

For  $M = 0$ , we apply such considerations directly to  $c_0 = c(x, \xi, \lambda)$  in (3.30):

$$\begin{aligned} |c_0| &\leq |\sin \varphi|^{-N} \int \langle \xi+\eta \rangle^{d'+d_1} \langle \xi+\eta, \mu \rangle^{-d'} \langle \eta \rangle^{-N'} \langle \xi \rangle^{d_2} \, d\eta \\ &\leq |\sin \varphi|^{-N} \langle \xi \rangle^{d'+d_1+d_2} \langle \xi, \mu \rangle^{-d'}. \end{aligned}$$

Derivatives of  $c_M$  in  $x$  and  $\xi$  are treated in a similar way.

In the case  $2^\circ$ , the proof goes through in a similar way, except that  $d'$  is replaced by  $d$  in expressions containing undifferentiated factors  $a$ .

In  $3^\circ$ , the  $\lambda$ -independent factor is to the left, and (3.30) holds with integrand  $(\xi+\eta)^\gamma \mathcal{F}_{z \rightarrow \eta} a(z, \xi, \lambda) e^{ix \cdot \eta}$ . The Taylor expansion of  $(\xi+\eta)^\gamma$  is a finite binomial expansion  $\sum_{\kappa \leq \gamma} \binom{\gamma}{\kappa} \xi^{\gamma-\kappa} \eta^\kappa$  and leads to a finite composition formula where the estimates (3.28) of the terms can be read off directly.  $\square$

The composed symbol  $c = c_0(a, b)$  is also denoted  $a \circ b$  (used in [16]) or  $a \# b$ .

For the analysis of  $R_M$ , we denote  $P - \lambda = \tilde{P}$ , with the parameter-dependent symbol  $\tilde{p}(x, \xi, \lambda) = p(x, \xi) - \lambda$  in local coordinates; here, for any  $M \in \mathbb{N}_0$ ,

$$\begin{aligned} p &= \sum_{k < M} p_{d-k} + p'_M, \quad \tilde{p} = \sum_{k < M} \tilde{p}_{d-k} + \tilde{p}'_M, \quad \text{with} \\ \tilde{p}_d &= p - \lambda, \quad \tilde{p}_{d-k} = p_{d-k} \quad \text{for } k > 0, \quad \tilde{p}'_M = p'_M \quad \text{for } M > 0. \end{aligned} \tag{3.31}$$

$p_d$  is also denoted  $p^0$ . The  $p_{d-k}$  are homogeneous in  $|\xi|$  of degree  $d-k$  for  $|\xi| \geq 1$ , and  $p'_M \in S_{1,0}^{d-M}(\mathbb{R}^n \times \mathbb{R}^n)$ .

PROPOSITION 3.9. *Let  $M \geq 1$ . The symbol  $r_M(x, \xi, \lambda)$  of  $R_M$  (cf. (3.17)) satisfies in local coordinates:*

$$|D_x^\beta D_\xi^\alpha r_M(x, \xi, \lambda)| \leq |\sin \varphi|^{-2M-|\alpha|-|\beta|} \langle \xi \rangle^{d-M-|\alpha|} \langle \xi, \mu \rangle^{-d}. \tag{3.32}$$

We also have that  $R_M = R_M^{(1)} + R_M^{(2)}$  with symbols

$$r_M = r_M^{(1)} + r_M^{(2)}, \quad r_M^{(2)} = q_{-d} p'_M, \tag{3.33}$$

estimated by:

$$\begin{aligned} |D_x^\beta D_\xi^\alpha r_M^{(1)}(x, \xi, \lambda)| &\leq |\sin \varphi|^{-2M-|\alpha|-|\beta|} \langle \xi \rangle^{2d-M-|\alpha|} \langle \xi, \mu \rangle^{-2d}, \\ |D_x^\beta D_\xi^\alpha r_M^{(2)}(x, \xi, \lambda)| &\leq |\sin \varphi|^{-1-|\alpha|-|\beta|} \langle \xi \rangle^{d-M-|\alpha|} \langle \xi, \mu \rangle^{-d}. \end{aligned} \tag{3.34}$$

Moreover,  $\tilde{R}_M = -R_M$ .

*Proof.* We have that

$$r_M = 1 - \sum_{k < M} \sum_{l < M} q_{-d-l} \circ \tilde{p}_{d-k} - \sum_{l < M} q_{-d-l} \circ \tilde{p}'_M.$$

The terms in the parametrix symbol  $\sum_{l \geq 0} q_{-d-l}$  are constructed as solutions to the successive equations for  $m \in \mathbb{N}_0$ :

$$\sum_{|\alpha|+k+l=m} \frac{1}{\alpha!} D_\xi^\alpha q_{-d-l} \partial_x^\alpha \tilde{p}_{d-k} = \begin{cases} 1 & \text{for } m = 0, \\ 0 & \text{for } m = 1, 2, \dots, \end{cases} \tag{3.35}$$

cf. e.g., Seeley [23, (1)]. We use the truncated composition formula in Lemma 3.8 to compute the symbol  $r_M$  of  $R_M$  with expansions in up to  $M$  homogeneous terms:

$$\begin{aligned} r_M = 1 - \sum_{k < M} \sum_{l < M} &\left\{ \sum_{k+l+|\alpha| < M} \frac{1}{\alpha!} D_\xi^\alpha q_{-d-l} \partial_x^\alpha \tilde{p}_{d-k} + c_{M-k-l}(q_{-d-l}, \tilde{p}_{d-k}) \right\} \\ &- c_0 \left( \sum_{l < M} q_{-d-l}, \tilde{p}'_M \right). \end{aligned}$$

By (3.35),

$$\sum_{k < M} \sum_{l < M} \sum_{k+l+|\alpha| < M} \frac{1}{\alpha!} D_\xi^\alpha q_{-d-l} \partial_x^\alpha \tilde{p}_{d-k} = 1.$$

Thus,  $r_M$  consists of the following terms:

$$r_M = - \sum_{k < M} \sum_{l < M} c_{M-k-l}(q_{-d-l}, \tilde{p}_{d-k}) - c_0 \left( \sum_{l < M} q_{-d-l}, \tilde{p}'_M \right). \tag{3.36}$$

Using the estimates (3.1) and (3.2) together with  $|D_x^\beta D_\xi^\alpha \tilde{p}_{d-k}(x, \xi)| \leq \langle \xi \rangle^{d-k-|\alpha|}$ , we obtain from Lemma 3.8 with  $d' = 2d$ ,  $d_1 = -d-l$  and  $d_2 = d-k$  that for  $l \geq 1$  in the sum over  $k, l$ :

$$\begin{aligned} & |D_x^\beta D_\xi^\alpha c_{M-k-l}(q_{-d-l}, \tilde{p}_{d-k})| \\ & \leq |\sin \varphi|^{-M+k+l-1-2l-|\alpha|-|\beta|} \langle \xi \rangle^{2d-d-l+d-k-(M-k-l)-|\alpha|} \langle \xi, \mu \rangle^{-2d} \\ & \leq |\sin \varphi|^{-2M-|\alpha|-|\beta|} \langle \xi \rangle^{2d-M-|\alpha|} \langle \xi, \mu \rangle^{-2d}, \end{aligned} \quad (3.37)$$

since  $k-l \geq -M+1$ .

For  $l=0$ , we find in view of Lemma 3.8 2°, since  $k < M$ ,

$$\begin{aligned} & |D_x^\beta D_\xi^\alpha c_{M-k}(q_{-d}, \tilde{p}_{d-k})| \\ & \leq |\sin \varphi|^{-1-(M-k)-|\alpha|-|\beta|} \langle \xi \rangle^{2d-d+d-k-(M-k)-|\alpha|} \langle \xi, \mu \rangle^{-2d} \\ & \leq |\sin \varphi|^{-M-1-|\alpha|-|\beta|} \langle \xi \rangle^{2d-M-|\alpha|} \langle \xi, \mu \rangle^{-2d}. \end{aligned} \quad (3.38)$$

In the last term,

$$\begin{aligned} & \left| D_x^\beta D_\xi^\alpha c_0 \left( \sum_{1 \leq l < M} q_{-d-l}, \tilde{p}'_M \right) \right| \\ & \leq \sum_{1 \leq l < M} |\sin \varphi|^{-2l-1-|\alpha|-|\beta|} \langle \xi \rangle^{2d-d-l+(d-M)-|\alpha|} \langle \xi, \mu \rangle^{-2d} \\ & \leq |\sin \varphi|^{-2M-|\alpha|-|\beta|} \langle \xi \rangle^{2d-M-|\alpha|} \langle \xi, \mu \rangle^{-2d}, \end{aligned} \quad (3.39)$$

whereas

$$c_0(q_{-d}, p'_M) = q_{-d} p'_M + c_1(q_{-d}, p'_M),$$

with  $c_1(q_{-d}, p'_M)$  estimated as in (3.39) and

$$|D_x^\beta D_\xi^\alpha (q_{-d} p'_M)| \leq |\sin \varphi|^{-1-|\alpha|-|\beta|} \langle \xi \rangle^{d-M-|\alpha|} \langle \xi, \mu \rangle^{-d}. \quad (3.40)$$

An addition of the contributions (using that  $\langle \xi \rangle / \langle \xi, \mu \rangle \leq 1$ ) gives (3.32). We also have the representation (3.33), where all the contributions to  $r_M^{(1)}$  have  $O(\langle \xi, \mu \rangle^{-2d})$ , so that it satisfies (3.34), and  $r_M^{(2)}$  is estimated in (3.40).

For the analysis of  $\tilde{R}_M$ , we have by Lemma 3.8:

$$\begin{aligned} \sum_{l < M} q_{-d-l} \circ p &= \sum_{k < M} \sum_{l < M} q_{-d-l} \circ p_{d-k} + \sum_{l < M} q_{-d-l} \circ p'_M \\ &= \sum_{k < M} \sum_{l < M} \left\{ \sum_{k+l+|\alpha| < M} \frac{1}{\alpha!} D_\xi^\alpha q_{-d-l} \partial_x^\alpha p_{d-k} + c_{M-k-l}(q_{-d-l}, p_{d-k}) \right\} \\ &\quad + c_0 \left( \sum_{l < M} q_{-d-l}, p'_M \right), \end{aligned}$$

such that the  $M$ th remainder has symbol



$$\begin{aligned} \tilde{r}_M &= \sum_{k < M} \sum_{l < M} c_{M-k-l}(q_{-d-l}, p_{d-k}) + c_0 \left( \sum_{l < M} q_{-d-l}, p'_M \right) \\ &= \sum_{k < M} \sum_{l < M} c_{M-k-l}(q_{-d-l}, p_{d-k}) + c_0 \left( \sum_{1 \leq l < M} q_{-d-l}, p'_M \right) + q_{-d} p'_M + c_1(q_{-d}, p'_M). \end{aligned}$$

Here, we can observe that all the  $p$ -factors can be replaced by the corresponding  $\tilde{p}$ -factors, for they are the same when the index is  $\neq d$ , and  $p_d$  enters only in differentiated form since  $l < M$  (and  $\tilde{p}_d = p_d - \lambda$  and  $p_d$  have the same derivatives). Then, in view of the formula (3.36) for  $r_M$ , we have indeed  $\tilde{r}_M = -r_M$  and  $\tilde{R}_M = -R_M$ .  $\square$

Summing up, we now have (cf. (3.22) ff.), since  $\tilde{R}_M = -R_M$ ,

$$(Q_\lambda P)'_M = -R_M + R_M P Q_\lambda = -R_M^{(1)} - R_M^{(2)} + R_M^{(1)} P Q_\lambda + R_M^{(2)} P Q_\lambda.$$

These terms will enter in different ways in the integral defining  $V'_M(t)$ . Some further symbol estimates will be needed in the following:

**PROPOSITION 3.10.** *For  $\gamma \in \mathbb{N}_0^n$ ,  $k \in \mathbb{N}_0$ , the symbols of  $R_M^{(1)} \langle D \rangle^k$ ,  $D^\gamma R_M^{(1)}$ ,  $R_M^{(2)} P \langle D \rangle^k$  and  $D^\gamma R_M^{(2)} P$  satisfy:*

$$\begin{aligned} |D_x^\beta D_\xi^\alpha (r_M^{(1)} \circ \langle \xi \rangle^k)| &\leq |\sin \varphi|^{-2M-|\alpha|-|\beta|} \langle \xi \rangle^{2d-M-|\alpha|+k} \langle \xi, \mu \rangle^{-2d}, \\ |D_x^\beta D_\xi^\alpha (\xi^\gamma \circ r_M^{(1)})| &\leq |\sin \varphi|^{-2M-|\alpha|-|\beta|-|\gamma|} \langle \xi \rangle^{2d-M-|\alpha|+|\gamma|} \langle \xi, \mu \rangle^{-2d}, \\ |D_x^\beta D_\xi^\alpha (r_M^{(2)} \circ p \circ \langle \xi \rangle^k)| &\leq |\sin \varphi|^{-1-|\alpha|-|\beta|} \langle \xi \rangle^{2d-M-|\alpha|+k} \langle \xi, \mu \rangle^{-d}, \\ |D_x^\beta D_\xi^\alpha (\xi^\gamma \circ r_M^{(2)} \circ p)| &\leq |\sin \varphi|^{-1-|\alpha|-|\beta|-|\gamma|} \langle \xi \rangle^{2d-M-|\alpha|+|\gamma|} \langle \xi, \mu \rangle^{-d}. \end{aligned} \tag{3.41}$$

*Proof.* The composition with  $\langle D \rangle^k = \text{Op}(\langle \xi \rangle^k)$  to the right just corresponds to multiplying the symbol by  $\langle \xi \rangle^k$ , so the first line in (3.42) results directly from (3.34). For the second line, we use the composition rule in Lemma 3.8 3°. For the third line, we can for  $k = 0$  use the composition rule in Lemma 3.8 1°, which gives the result in view of (3.34). The third line with  $k \neq 0$  follows simply by multiplication by  $\langle \xi \rangle^k$ , and the fourth line follows by another application of Lemma 3.8 3°.  $\square$

To apply Agmon’s estimate Proposition 3.1 to obtain kernel estimates, we need an estimate of  $L_2$ -bounds in terms of symbol seminorms. Many variants are known, and we use the following, found in Marschall [19, Theorem 2.1].

**PROPOSITION 3.11.** *Let  $a \in S_{1,0}^0(\mathbb{R}^n \times \mathbb{R}^n)$  be such that for some  $C_0 > 0$ , some  $N \in \mathbb{N}_0$  with  $N > \frac{n}{2}$ , and all  $\alpha, \beta \in \mathbb{N}_0^n$  with  $0 \leq |\alpha| \leq N$ ,  $0 \leq |\beta| \leq 1$ ,*

$$\sup_{x, \xi} \langle \xi \rangle^{-|\alpha|} |D_x^\beta D_\xi^\alpha a(x, \xi)| \leq C_0 < \infty. \tag{3.42}$$

*Then the associated operator  $A = \text{Op}(a)$  is bounded on  $L_2(\mathbb{R}^n)$ , and  $\|A\|_{0,0} \leq C_0$ .*

The dependence of the operator norm on  $C_0$  follows from an inspection of the proof.

**THEOREM 3.12.** *The kernels of the operators  $-R_M^{(1)}$ ,  $R_M^{(1)}PQ_\lambda$  and  $R_M^{(2)}PQ_\lambda$  are estimated by*

$$\begin{aligned} |\mathcal{K}_{R_M^{(1)}}(x, y, \lambda)| &\leq |\sin \varphi|^{-4d-\frac{7}{2}n-6} \langle \lambda \rangle^{-2}, \\ |\mathcal{K}_{R_M^{(1)}PQ_\lambda}(x, y, \lambda)| &\leq |\sin \varphi|^{-4d-\frac{7}{2}n-7} \langle \lambda \rangle^{-2}, \\ |\mathcal{K}_{R_M^{(2)}PQ_\lambda}(x, y, \lambda)| &\leq |\sin \varphi|^{-\frac{3}{2}n-4} \langle \lambda \rangle^{-2}, \end{aligned} \quad (3.43)$$

*Proof.* For the use of Proposition 3.1, we note that when  $T$  is a  $\psi$ do of order  $\leq -n-1$ , then

$$\begin{aligned} \|T\|_{0,n+1} &\dot{\leq} \sum_{|\gamma| \leq n+1} \|D^\gamma T\|_{0,0}, \\ \|T^*\|_{0,n+1} &= \|T\|_{-n-1,0} \doteq \|T\langle D \rangle^{n+1}\|_{0,0}. \end{aligned}$$

Consider  $R_M^{(1)}$ . The  $N$  occurring in Proposition 3.11 can be written  $N = \frac{n}{2} + \delta$ ,  $\delta = \frac{1}{2}$  or 1. For  $|\alpha| \leq N$  and  $|\beta| \leq 1$ , the symbols  $D_x^\beta D_\xi^\alpha (\xi^\gamma \circ r_M^{(1)})$  are estimated by

$$|D_x^\beta D_\xi^\alpha (\xi^\gamma \circ r_M^{(1)})| \dot{\leq} |\sin \varphi|^{-2M-N-1-|\gamma|} \langle \xi \rangle^{2d-M+|\gamma|} \langle \lambda \rangle^{-2}.$$

To apply Proposition 3.1 with  $|\gamma|$  up to  $n+1$ , we must take the integer  $M$  such that  $2d - M + n + 1 \leq 0$ , so we let  $M = 2d + n + 1 + \delta'$  with  $\delta' \in [0, 1[$ . Then

$$\|D^\gamma R_M^{(1)}\|_{0,0} \dot{\leq} |\sin \varphi|^{-2M-1-N-|\gamma|} \langle \lambda \rangle^{-2},$$

and it follows that

$$\begin{aligned} \|R_M^{(1)}\|_{0,0} &\dot{\leq} |\sin \varphi|^{-2M-1-N} \langle \lambda \rangle^{-2} \\ \|R_M^{(1)}\|_{0,n+1} &\dot{\leq} \sum_{|\gamma| \leq n+1} \|D^\gamma R_M^{(1)}\|_{0,0} \dot{\leq} |\sin \varphi|^{-2M-N-n-2} \langle \lambda \rangle^{-2}. \end{aligned}$$

Moreover,

$$\|(R_M^{(1)})^*\|_{0,n+1} = \|R_M^{(1)}\langle D \rangle^{n+1}\|_{0,0} \dot{\leq} |\sin \varphi|^{-2M-1-N} \langle \lambda \rangle^{-2}.$$

Insertion in (3.1) with  $m = n+1$  gives that

$$\begin{aligned} |\mathcal{K}_{R_M^{(1)}}(x, y, \lambda)| &\dot{\leq} |\sin \varphi|^{(-2M-N-n-2)\frac{n}{n+1} + (-2M-N-1)(1-\frac{n}{n+1})} \langle \lambda \rangle^{-2} \\ &\dot{\leq} |\sin \varphi|^{-2M-N-n-1} \langle \lambda \rangle^{-2} = |\sin \varphi|^{-4d-\frac{7}{2}n-3-2\delta'-\delta} \langle \lambda \rangle^{-2} \\ &\leq |\sin \varphi|^{-4d-\frac{7}{2}n-6} \langle \lambda \rangle^{-2}. \end{aligned}$$

This shows the first estimate in (3.43).

For the second estimate, we reuse the operator norms established for  $R_M^{(1)}$ . They are now combined with some elementary norm estimates of  $PQ_\lambda$ , namely

$$\|PQ_\lambda\|_{0,0} = \|1 + \lambda Q_\lambda\|_{0,0} \dot{\leq} 1 + |\sin \varphi|^{-1}$$

holds in view of (3.18), and moreover, for any  $s \in \mathbb{R}$ ,

$$\|P Q_\lambda\|_{s,s} = \|P^{s/d} P Q_\lambda P^{-s/d}\|_{0,0} = \|P Q_\lambda\|_{0,0} \leq |\sin \varphi|^{-1}, \tag{3.44}$$

since the operators commute. The composition with  $P Q_\lambda$  thus results in an extra factor  $|\sin \varphi|^{-1}$  in the norm estimates, and hence likewise in the kernel estimate. This shows the second estimate in (3.43).

For the third estimate, we combine the elementary estimates

$$\|Q_\lambda\|_{s,s} \leq |\sin \varphi|^{-1} |\lambda|^{-1}, \tag{3.45}$$

shown earlier for  $s = 0$ , and extendible to all  $s$  by conjugation with  $P^{s/d}$ , with norm estimates of  $R_M^{(2)} P$ , derived similarly to above from the last two lines in (3.42). The latter give estimates in terms of  $|\sin \varphi|^{-1-N-1-n-1} \langle \lambda \rangle^{-1}$ . In the resulting combined estimate, we can replace  $|\lambda|^{-1}$  by  $\langle \lambda \rangle^{-1}$ , since we are working under the hypothesis that a possible nullspace of  $P$  has been removed. This shows the last line in (3.43).  $\square$

Then, we can show the estimate of the remainder kernel:

**THEOREM 3.13.** *Let  $P$  be selfadjoint strongly elliptic of order  $d > 0$  on  $M$ , with  $\gamma(P) \geq 0$ . The remainder kernel  $\mathcal{K}_{V'_M}$  satisfies for  $\arg t = \theta$ ,  $M = 2d + n + 1 + \delta'$  (with  $\delta' \in [0, 1[$ ):*

$$|\mathcal{K}_{V'_M}(x, y, t)| \leq (\cos \theta)^{-2d - \frac{7}{2}n - 7} e^{-c' \operatorname{Re} t |t|}, \tag{3.46}$$

where  $c' > 0$  if  $\gamma(P) > 0$ ,  $c' = 0$  if  $\gamma(P) = 0$ .

*Proof.* If  $\gamma(P) > 0$ , we use the preceding estimates directly to analyse

$$\begin{aligned} \partial_t \mathcal{K}_{V'_M} &= -\frac{i}{2\pi} \int_{\mathcal{C}} e^{-t\lambda} \mathcal{K}_{(Q_\lambda P)'_M} d\lambda, \\ (Q_\lambda P)'_M &= -R_M^{(1)} - R_M^{(2)} + R_M^{(1)} P Q_\lambda + R_M^{(2)} P Q_\lambda. \end{aligned}$$

The curve  $\mathcal{C}$  is chosen as in (3.3). The first, third, and fourth terms contribute with integrals of the form

$$\frac{i}{2\pi} \int_{\mathcal{C}} e^{-t\lambda} f(x, y, \lambda) d\lambda$$

where

$$|e^{-\lambda t} f(x, y, \lambda)| \leq e^{-c' \operatorname{Re} t} (\cos \theta)^{-4d - \frac{7}{2}n - 7} \langle \lambda \rangle^{-2}$$

on the curve by Theorem 3.12 (recall that  $\cos \theta \doteq \sin \varphi_0$ ). Since  $\langle \lambda \rangle^{-2}$  integrates to  $\infty$ , the resulting function is estimated by  $e^{-c' \operatorname{Re} t} (\cos \theta)^{-4d - \frac{7}{2}n - 7}$ .

To find the contribution from  $R_M^{(2)}$ , we first perform the integration on the symbol level:

$$\frac{i}{2\pi} \int_{\mathcal{C}} e^{-t\lambda} (p^0 - \lambda)^{-1} p'_M d\lambda = e^{-tp^0} p'_M.$$

Here, we can use an estimate from Lemma 3.5. By (3.8),

$$\begin{aligned} |D_x^\beta D_\xi^\alpha (e^{-tP^0} p'_M)| &\leq (\sin \varphi_0)^{-M-|\alpha|-|\beta|} \langle \xi \rangle^{-M-|\alpha|} e^{-c \operatorname{Re} t \langle \xi \rangle^d} \\ &\leq (\sin \varphi_0)^{-M-|\alpha|-|\beta|} \langle \xi \rangle^{-M-|\alpha|} e^{-c' \operatorname{Re} t}, \text{ hence} \\ |\mathcal{K}_{\operatorname{Op}(e^{-P^0} p'_M)}| &\leq (\sin \varphi_0)^{-M} e^{-c' \operatorname{Re} t} \text{ when } M \geq n + 1. \end{aligned}$$

Since the latter estimate is dominated by that from the other terms, we conclude that

$$|\partial_t \mathcal{K}_{V'_M}(x, y, t)| \leq e^{-c' \operatorname{Re} t} (\cos \theta)^{-4d - \frac{7}{2}n - 7}.$$

Then, an integration with respect to  $t$  using that  $\mathcal{K}_{V'_M}(x, y, 0) = 0$  shows (3.46).

In the case where  $\gamma(P) = 0$ , the above considerations will be valid for  $V^\varepsilon(t)$  as in (3.20). We then have to add  $(1 - e^{-\varepsilon t})\Pi_0$ , which has a smooth kernel bounded by  $\min\{|t|, 1\}$ , and we reach the conclusion in the theorem.  $\square$

We can then finally show the following:

**THEOREM 3.14.** *Let  $P$  be selfadjoint strongly elliptic of order  $d > 0$  on  $M$ , with  $\gamma(P) \geq 0$ . The heat kernel  $\mathcal{K}_V$  satisfies for all  $t \in \mathbb{C}_+$  (with  $\arg t = \theta \in ] -\frac{\pi}{2}, \frac{\pi}{2}[$ ) the Poisson estimate, where  $N = \max\{\frac{n}{d}, \frac{7n}{2} + 4d + 7\}$ :*

$$|\mathcal{K}_V(x, y, t)| \leq (\cos \theta)^{-N} e^{-\gamma(P) \operatorname{Re} t} \frac{|t|}{(d(x, y) + |t|^{1/d})^d} ((d(x, y) + |t|^{1/d})^{-n} + 1). \tag{3.47}$$

*Proof.* In local coordinates, the estimate follows from Theorems 3.7 and 3.13, by choosing  $M = n + 1 + 2d + \delta'$  in Theorem 3.13 and adding  $\mathcal{K}_{V_{-d-l}}$  for  $0 \leq l < M$ ; the most singular terms dominate. This leads to the global estimate (3.47) (the effect of the lower bound is handled as in Sect. 2).  $\square$

**REMARK 3.15.** Note that the order  $d$  and dimension  $n$  enter linearly in  $N' = \frac{7n}{2} + 4d + 7$ , and it is easy to see where the sizes come from:  $2n + 4d$  comes from the power  $-2M$  where  $M \sim 2d + n$ , one  $n$  comes from the requirement for Agmon’s estimate Proposition 3.1, and  $\frac{n}{2}$  comes from the requirement for Marschall’s estimate Proposition 3.11. The number 7 includes rounding up errors, and may be lowered. More substantial improvements would depend on choosing other general principles; e.g., the  $L_\infty$  kernel estimate in Beals [5, Lemma 2], which is slightly more efficient than Agmon’s estimate, might save  $\frac{n}{2}$  powers. Note that all orders  $d \in \mathbb{R}_+$  are allowed.

Our result applies in particular to the Dirichlet-to-Neumann operator  $P_{DN}$  of order  $d = 1$  associated with the Laplacian (and lower-order perturbations of it). For this operator, ter Elst and Ouhabaz [11] have estimates in terms of  $-N''$ th powers of  $\cos \theta$ , where the dimension  $n$  enters nonlinearly in  $N$ :

$$N'' = 2n(n + 1), \text{ compared to our } N' = \frac{7n}{2} + 11;$$

here  $N'' > N'$  for  $n \geq 6$ . They are proved by appealing to multiple commutator estimates for semigroups defined from iterates of  $P_{DN}$ , refined  $(L_p \rightarrow L_q)$ -estimates of Coifman-Meyer and others for pseudodifferential operators, Riesz potentials, interpolation, and other tools.

*REMARK 3.16.* Derivatives in  $x$  and  $y$  can also be estimated by these methods if needed. For example,  $D_{x_j} \mathcal{K}_V(x, y, t)$  is described by the above formulas composed to the left with  $D_{x_j}$ ; then, in the remainder terms,  $D_{x_j}$  is composed with the  $R_M^{(i)}$ , giving symbols described in Proposition 3.10. The remainder for  $D_{y_j} \mathcal{K}_V(x, y, t)$  is described by formulas, partly of the type where  $R_M^{(i)}$  is composed to the right with  $D_{x_j}$  which just gives a factor  $\xi_j$  on the symbol, partly of a type containing  $Q_\lambda D_{x_j}$ . In the latter cases, one can use, e.g., that

$$P Q_\lambda D_{x_j} = P D_{x_j} Q_\lambda + P [D_{x_j}, Q_\lambda] = D_{x_j} P Q_\lambda + [P, D_{x_j}] Q_\lambda + P Q_\lambda [D_{x_j}, P] Q_\lambda.$$

Here, the first term contributes a  $D_{x_j}$  that is absorbed in the  $\psi$ do's before it, and in the other terms, we note that  $[D_{x_j}, P]$  is of order  $d$  so that, by (3.44),

$$\begin{aligned} \|[P, D_{x_j}] Q_\lambda\|_{0,0} &\leq \|P Q_\lambda\|_{0,0} \leq |\sin \varphi|^{-1}, \\ \|P Q_\lambda [D_{x_j}, P] Q_\lambda\|_{0,0} &\leq \|P Q_\lambda\|_{0,0} \|[D_{x_j}, P] Q_\lambda\|_{0,0} \leq |\sin \varphi|^{-2}. \end{aligned}$$

#### 4. Kernels of heat semigroups for perturbations of fractional Laplacians and the Dirichlet-to-Neumann operator

This section complements the general upper bounds from Sect. 2 with lower estimates in the case of fractional powers of the Laplacian and the Dirichlet-to-Neumann operator and their perturbations.

Let  $\Delta$  be the (nonnegative) Laplace–Beltrami operator on the closed, compact Riemannian  $n$ -dimensional manifold  $M$ . The semigroups  $e^{-t\Delta}$  and  $V^d(t) = e^{-t\Delta^{d/2}}$  are related by subordination formulas, which lead to an alternative proof of the upper kernel estimate in this special case, as well as to lower bounds. For  $d = 1$ , they assume a simple form:

LEMMA 4.1. *Let  $\lambda \geq 0$ . One has for all  $t \geq 0$ :*

$$e^{-t\sqrt{\lambda}} = \frac{1}{2\sqrt{\pi}} \int_0^\infty e^{-s\lambda} t e^{-\frac{t^2}{4s}} s^{-\frac{3}{2}} ds. \tag{4.1}$$

*Proof.* Let  $\alpha = t\sqrt{\lambda}/2$  and let  $x = \frac{t}{2}s^{-\frac{1}{2}}$ ; then  $dx = -\frac{t}{4}s^{-\frac{3}{2}}ds$ , and Eq. (4.1) is turned into

$$\sqrt{\pi} e^{-2\alpha} = \int_0^\infty e^{-x^2 - \frac{\alpha^2}{x^2}} 2 dx. \tag{4.2}$$

To show this, note that the left-hand side  $I(\alpha)$  satisfies  $I(\alpha) \in C^1(\mathbb{R}_+)$ ,  $\lim_{\alpha \rightarrow 0^+} I(\alpha) = \sqrt{\pi}$ , and for  $\alpha > 0$  (with  $y = \alpha x^{-1}$ ,  $dy = -\alpha x^{-2} dx$ ):

$$\partial_\alpha I(\alpha) = \int_0^\infty e^{-x^2 - \frac{\alpha^2}{x^2}} (-4\alpha)x^{-2} dx = -2 \int_0^\infty e^{-\frac{\alpha^2}{y^2} - y^2} 2 dy = -2I(\alpha).$$

Thus,  $I(\alpha) = ce^{-2\alpha}$  with  $c = \sqrt{\pi}$ . □

By Zolotarev [27] (see also Grigor'yan [13]), there exists for any  $0 < d < 2$  a nonnegative function  $\eta_t^d(s)$  such that

$$e^{-t\lambda^{d/2}} = \int_0^\infty e^{-s\lambda} \eta_t^d(s) ds. \tag{4.3}$$

Here,  $\eta_t^d$  has the following properties

$$\eta_t^d(s) = t^{-2/d} \eta_1^d\left(\frac{s}{t^{2/d}}\right) \quad (s, t > 0), \tag{4.4}$$

$$\eta_t^d(s) \leq ts^{-1-\frac{d}{2}} \quad (s, t > 0), \tag{4.5}$$

$$\eta_t^d(s) \doteq ts^{-1-\frac{d}{2}} \quad (s \geq t^{2/d} > 0). \tag{4.6}$$

By an application of the spectral theorem, we obtain for all  $t > 0$ ,

$$V^d(t)f = e^{-t\Delta^{d/2}} f = \int_0^\infty e^{-\tau\Delta} f \eta_t^d(\tau) d\tau, \quad \text{for all } f \in H^s(M). \tag{4.7}$$

In view of (4.7), it holds that

$$\langle \delta_x, V^d(t)\delta_y \rangle = \left\langle \delta_x, \int_0^\infty e^{-\tau\Delta} \delta_y \eta_t^d(\tau) d\tau \right\rangle = \int_0^\infty \langle \delta_x, e^{-\tau\Delta} \delta_y \rangle \eta_t^d(\tau) d\tau,$$

resulting in an identity for the kernels: For all  $t > 0$ ,

$$\mathcal{K}_{V^d}(x, y, t) = \int_0^\infty \mathcal{K}_{e^{-\tau\Delta}}(x, y) \eta_t^d(\tau) d\tau, \quad \text{for } (x, y) \in M \times M. \tag{4.8}$$

Using this formula, we can deduce upper and lower estimates for  $\mathcal{K}_{V^d}$  from those known for  $\mathcal{K}_{e^{-\tau\Delta}}$ . The following upper and lower estimates are well known (see e.g., Saloff-Coste [22]):

$$\frac{c_1}{\mathcal{V}(x, \sqrt{\tau})} e^{-C_1 \frac{d(x,y)^2}{\tau}} \leq \mathcal{K}_{e^{-\tau\Delta}}(x, y) \leq \frac{c_2}{\mathcal{V}(x, \sqrt{\tau})} e^{-C_2 \frac{d(x,y)^2}{\tau}}. \tag{4.9}$$

Here,  $\mathcal{V}(x, r)$  denotes the volume of a ball of radius  $r$  around  $x$ . For a closed compact  $n$ -dimensional manifold  $M$ ,  $\mathcal{V}(x, r) \doteq r^n$  for small  $r$ , and  $\mathcal{V}(x, r)$  equals the volume of the connected component containing  $x$  when  $r \geq \text{diam } M$ . Hence

$$\mathcal{V}(x, \sqrt{\tau})^{-1} \doteq (\tau^{n/2})^{-1} + 1. \tag{4.10}$$

**THEOREM 4.2.** *Let  $0 < d < 2$ . The kernel of the semigroup  $V^d(t) = e^{-t\Delta^{d/2}}$  satisfies for all  $t \geq 0$ :*

$$\mathcal{K}_{e^{-t\Delta^{d/2}}}(x, y) \doteq \frac{t}{(d(x, y) + t^{1/d})^d} \left( (d(x, y) + t^{1/d})^{-n} + 1 \right). \tag{4.11}$$

*Proof.* The upper estimate follows already from Corollary 2.6. The following proof moreover extends to give the lower estimate. Inserting the heat kernel bounds (4.9), (4.10) into (4.8) and using (4.5), we find

$$\begin{aligned} \mathcal{K}_{V^d}(x, y, t) &\doteq \int_0^\infty (\tau^{-n/2} + 1) \eta_t^d(\tau) e^{-C\frac{d(x,y)^2}{\tau}} d\tau \\ &\doteq t \int_0^\infty \tau^{-n/2} \tau^{-1-\frac{d}{2}} e^{-C\frac{d(x,y)^2}{\tau}} d\tau + t \int_0^\infty \tau^{-1-\frac{d}{2}} e^{-C\frac{d(x,y)^2}{\tau}} d\tau. \end{aligned}$$

By a change of variables  $\tau \mapsto Cd(x, y)^2\tau$ , the first term equals

$$t(Cd(x, y)^2)^{-\frac{d+n}{2}} \int_0^\infty \tau^{-\frac{n+d}{2}-1} e^{-1/\tau} d\tau \doteq \frac{t}{d(x, y)^{n+d}}. \tag{4.12}$$

Similarly, the second term is

$$t(Cd(x, y)^2)^{-\frac{d}{2}} \int_0^\infty \tau^{-\frac{d}{2}-1} e^{-1/\tau} d\tau \doteq \frac{t}{d(x, y)^d},$$

and altogether,

$$\mathcal{K}_{V^d}(x, y, t) \doteq \frac{t}{d(x, y)^d} (d(x, y)^{-n} + 1).$$

On the other hand, using the uniform bound  $\mathcal{K}_{e^{-\tau\Delta}}(x, y) \doteq \tau^{-n/2} + 1$  and (4.4), we obtain

$$\begin{aligned} \mathcal{K}_{V^d}(x, y, t) &\doteq \int_0^\infty (\tau^{-n/2} + 1) \eta_t^d(\tau) d\tau = \int_0^\infty (\tau^{-n/2} + 1) \eta_1^d\left(\frac{\tau}{t^{2/d}}\right) t^{-2/d} d\tau \\ &= \int_0^\infty (t^{-n/d}\tau^{-n/2} + 1) \eta_1^d(\tau) d\tau \doteq t^{-n/d} + 1. \end{aligned}$$

Thus

$$\mathcal{K}_{V^d}(x, y, t) \doteq \min \left\{ t^{-n/d} + 1, \frac{t}{d(x, y)^d} (d(x, y)^{-n} + 1) \right\}.$$

If  $t^{1/d} \geq d(x, y)$ ,

$$t^{-n/d} \doteq t^{-n/d} \left( \frac{d(x, y)}{t^{1/d}} + 1 \right)^{-n-d} = t(d(x, y) + t^{1/d})^{-n-d}$$

and

$$1 \doteq \left( \frac{d(x, y)}{t^{1/d}} + 1 \right)^{-d} = t(d(x, y) + t^{1/d})^{-d}.$$

On the other hand, for  $t^{1/d} \leq d(x, y)$  we have  $d(x, y) \doteq d(x, y) + t^{1/d}$  and hence

$$\frac{t}{d(x, y)^d} (d(x, y)^{-n} + 1) \leq \frac{t}{(d(x, y) + t^{1/d})^d} \left( (d(x, y) + t^{1/d})^{-n} + 1 \right).$$

This shows “ $\leq$ ” in (4.11).

To show the opposite inequality in (4.11), note that the integrand in (4.8) is non-negative, and (4.9), (4.10) imply

$$\mathcal{K}_{V^d}(x, y, t) = \int_0^\infty \mathcal{K}_{e^{-\tau\Delta}}(x, y) \eta_t^d(\tau) \, d\tau \geq \int_\alpha^\infty (\tau^{-n/2} + 1) \eta_t^d(\tau) e^{-C\frac{d(x,y)^2}{\tau}} \, d\tau$$

for  $\alpha = \max\{t^{2/d}, d(x, y)^2\}$ . Now, for  $\tau \geq d(x, y)^2$ ,  $e^{-C\frac{d(x,y)^2}{\tau}} \geq e^{-C}$ . Then by (4.6),

$$\begin{aligned} \mathcal{K}_{V^d}(x, y, t) &\geq \int_\alpha^\infty (\tau^{-n/2} + 1) t\tau^{1-\frac{1}{2}} \, d\tau \doteq t(\alpha^{-\frac{n+d}{2}} + \alpha^{-\frac{d}{2}}) \\ &= \min\{t^{-n/d}, td(x, y)^{-n-d}\} + \min\{1, td(x, y)^{-d}\} \\ &\geq t(d(x, y) + t^{1/d})^{-n-d} + t(d(x, y) + t^{1/d})^{-d}. \end{aligned}$$

□

For  $d = 1$ , this complies well with the explicit kernel formula (2.3) for the Poisson operator solving the Dirichlet problem for the Laplacian on  $\mathbb{R}_+^{n+1}$ .

We also consider the case where  $M$  is the boundary of a compact  $(n + 1)$ -dimensional Riemannian manifold  $\tilde{M}$  with boundary. With  $\Delta$  denoting the nonnegative Laplace–Beltrami operator on  $M$ , we shall compare  $\mathcal{K}_{e^{-t\sqrt{\Delta}}}$  with the kernel of the semigroup generated by the (nonnegative) Dirichlet-to-Neumann operator  $P_{DN}$  on  $M$ .  $P_{DN}$  is the operator mapping  $u$  to the normal derivative  $\partial_\nu \tilde{u}$ , where  $\tilde{u}$  is the harmonic function on  $\tilde{M}$  with boundary value  $u$ . It is known (cf. [15]) that  $P_{DN}$  is an elliptic pseudodifferential operator of order 1 on  $M$  with the same principal symbol as  $\sqrt{\Delta}$ .

Since  $\Delta^{d/2}$  is a classical strongly elliptic  $\psi$ do of order  $d$ , Theorem 2.5 applies to all operators of the form  $P = \Delta^{d/2} + P'$  with  $P'$  classical of order  $d - 1$ , giving upper estimates of the absolute value of the kernels; note that no selfadjointness is required. For such operators, we can also show lower estimates.

**THEOREM 4.3.** *Let  $d \in ]0, 2[$  and let  $P$  be a classical  $\psi$ do of order  $d$  with the same principal symbol as  $\Delta^{d/2}$ . Then the kernel of  $V(t) = e^{-tP}$  satisfies for all  $t \geq 0$ :*

$$\begin{aligned} |\mathcal{K}_V(x, y, t)| &\leq \frac{t}{(d(x, y) + t^{1/d})^d} \left( \frac{1}{(d(x, y) + t^{1/d})^{-n}} + 1 \right) \\ &\quad + e^{-c_1 t} \frac{t}{(d(x, y) + t^{1/d})^{d+n-1}}, \end{aligned} \tag{4.13}$$

for any  $c_1 < \gamma(P)$  ( $c_1 = \gamma(P)$  if Corollary 2.6 applies). Moreover, there is an  $r > 0$  such that

$$|\mathcal{K}_V(x, y, t)| \geq t(d(x, y) + t^{1/d})^{-d-n}, \quad \text{for } d(x, y) + t^{1/d} \leq r. \tag{4.14}$$



*Proof.* As  $P$  and  $\Delta^{d/2}$  have the same principal symbol,

$$V(t) = V^d(t) + V',$$

where  $V'$  is of lower order; more precisely  $V'$  is the difference between the first remainders for  $V(t) = e^{-tP}$  and  $V^d(t) = e^{-t\Delta^{d/2}}$ , as in the second line of (2.25). Hence,

$$|\mathcal{K}_{V'}(x, y, t)| \leq e^{-c_1 t} t (d(x, y) + t^{1/d})^{1-n-d}. \tag{4.15}$$

Now, (4.11) and (4.15) together imply (4.13).

To obtain the lower estimate (4.14), we note that

$$c s^{-n-d} - c' s^{1-n-d} = c s^{-n-d} (1 - c' c^{-1} s) \geq 2^{-1} c s^{-n-d}, \text{ when } s \leq c/(2c'), \tag{4.16}$$

so for all  $t$  in a bounded set where  $e^{-c_1 t} \leq c'$ , the lower estimate in (4.11) implies that (4.14) holds for all small  $d(x, y) + t^{1/d}$ .  $\square$

We can also obtain upper and lower estimates for the Dirichlet-to-Neumann operator.

**THEOREM 4.4.** *The kernel of  $e^{-tP_{DN}}$  satisfies for all  $t \geq 0$ :*

$$\mathcal{K}_{e^{-tP_{DN}}}(x, y, t) \leq \frac{t}{d(x, y) + t} ((d(x, y) + t)^{-n} + 1), \tag{4.17}$$

and there is an  $r > 0$  such that it satisfies

$$\mathcal{K}_{e^{-tP_{DN}}}(x, y, t) \geq t (d(x, y) + t)^{-1-n}, \text{ for } d(x, y) + t \leq r. \tag{4.18}$$

*Proof.* Here,  $P_{DN}$  is known to be selfadjoint nonnegative, and the semigroup has real, nonnegative kernel [3,4], so that we may omit absolute values. The upper estimate (4.17) follows from Corollary 2.6. The lower estimate (4.18) follows from Theorem 4.3 since  $P_{DN}$  differs from  $\Delta^{1/2}$  by a classical  $\psi$ do of order 0.  $\square$

**REMARK 4.5.** This work was inspired from a conversation of the second author with W. Arendt and A. ter Elst in August 2012 on the need for kernel estimates for the Dirichlet-to-Neumann semigroup, where we suggested the applicability of pseudo-differential methods as in [16]. When our first version of this paper was posted in arXiv:1302.6529, we learned of the efforts of ter Elst and Ouhabaz [11], giving an analysis of the Dirichlet-to-Neumann semigroup kernel by somewhat different methods, and obtaining some of the same results as those presented here.

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