

# Distributional asymptotic expansions of spectral functions and of the associated Green kernels \*

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## Abstract

Asymptotic expansions of Green functions and spectral densities associated with partial differential operators are widely applied in quantum field theory and elsewhere. The mathematical properties of these expansions can be clarified and more precisely determined by means of tools from distribution theory and summability theory. (These are the same, insofar as recently the classic Cesàro–Riesz theory of summability of series and integrals has been given a distributional interpretation.) When applied to the spectral analysis of Green functions (which are then to be expanded as series in a parameter, usually the time), these methods show: (1) The “local” or “global” dependence of the expansion coefficients on the background geometry, etc., is determined by the regularity of the asymptotic expansion of the integrand at the origin (in “frequency space”); this marks the difference between a heat kernel and a Wightman two-point function, for instance. (2) The behavior of the integrand at infinity determines whether the expansion of the Green function is genuinely asymptotic in the literal, pointwise sense, or is merely valid in a distributional (Cesàro-averaged) sense; this is the difference between the heat kernel and the Schrödinger kernel. (3) The high-frequency expansion of the spectral density itself is local in a distributional sense (but not pointwise). These observations make rigorous sense out of calculations in the physics literature that are sometimes dismissed as merely formal.

## 1 Introduction

The aim of this article is to study several issues related to the small- $t$  behavior of various Green functions  $G(t, x, y)$  associated to an elliptic differential operator  $H$ . These are the integral kernels of operator-valued functions of  $H$ , such as the heat operator  $e^{-tH}$ , the Schrödinger propagator  $e^{-itH}$ , various wave-equation operators such as  $\cos(t\sqrt{H})$ , the operator  $e^{-t\sqrt{H}}$  that solves a certain elliptic boundary-value problem involving  $H$ , etc. All these kernels are expressed

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(possibly after some redefinitions of variables) in the form

$$G(t, x, y) = \int_0^\infty g(t\lambda) dE_\lambda(x, y), \quad (1)$$

where  $E_\lambda$  is the spectral decomposition of  $H$ , and  $g$  is a smooth function on  $(0, \infty)$ .

Each such Green function raises a set of interrelated questions, which are illumined by a set of familiar examples. (To avoid cluttering this introduction with the details of these examples, we have put the formulas in an appendix, which the reader may wish to read at this point.)

(i) *Does  $G(t, x, y)$  have an asymptotic expansion as  $t \downarrow 0$ ?* For the heat problem, (A1), it is well known [34, 22] that

$$K(t, x, x) \sim (4\pi t)^{-d/2} \sum_{n=0}^{\infty} a_n(x, x) t^{n/2}, \quad (2a)$$

where  $d$  is the dimension of the manifold  $\mathcal{M}$  and  $a_0(x, x) = 1$ . Similar formulas hold off-diagonal; for example, if  $\mathcal{M} \subseteq \mathbb{R}^d$  and the leading term in  $H$  is the Laplacian, then

$$K(t, x, y) \sim (4\pi t)^{-d/2} e^{-|x-y|^2/4t} \sum_{n=0}^{\infty} a_n(x, y) t^{n/2}. \quad (2b)$$

In the case (A7b), the elementary heat kernel on  $\mathbb{R}^1$ , all  $a_n = 0$  except the first. In fact, this is true also of (A11b), the elementary Dirichlet heat kernel on  $(0, \pi)$ , because as  $t$  goes to 0 the ratio of any other term to the largest term ( $e^{-(x-y)^2/4t}$ ) vanishes faster than any power of  $t$ . In particular, therefore, the expansion (2) for fixed  $(x, y) \in (0, \pi) \times (0, \pi)$  does not distinguish between the finite region  $(0, \pi)$  and the infinite region  $\mathbb{R}$ . (However, the smallness of the two nearest image terms in (A11b) is not uniform near the boundary, and hence  $\int_0^\pi K(t, x, x)$  has an asymptotic expansion  $(4\pi t)^{-1/2} \sum_{n=0}^{\infty} A_n$  with nontrivial higher-order terms  $A_n$ .) This “locality” property will concern us again in questions (iv) and (v).

The Schrödinger problem, (A2), gives rise to an expansion (4) that is formally identical to (2) (more precisely, obtained from it by the obvious analytic continuation) [37, 6]. However, it is obvious from (A12b) that this expansion (which again reduces to a single term in the examples (A8) and (A12) is *not literally valid*, because each image term in (A12b) is exactly as large in modulus as the “main” term!

(ii) *In what sense does such an expansion correspond to an asymptotic expansion for  $E_\lambda(x, y)$  as  $\lambda \rightarrow +\infty$ ?* Formulas (2) would follow immediately from (1) if

$$E_\lambda(x, y) \sim \lambda^{d/2} \sum_{n=0}^{\infty} \alpha_n \lambda^{-n/2} \quad (3)$$

with  $\alpha_n$  an appropriate multiple of  $a_n$ . The converse implication from (2) to (3), however, is generally not valid beyond the first (“Weyl”) term. (For example,

in (A11a) or any other discrete eigenvector expansion the  $E_\lambda$  is a step function; its growth is described by  $\alpha_0$  but there is an immediate contradiction with the form of the higher terms in (3).) It has been known at least since the work of Brownell [1, 2] that (3) is, nevertheless, correct if somehow “averaged” over sufficiently large intervals of the variable  $\lambda$ . That is, it is valid in a certain *distributional* sense. Hörmander [27, 28] reformulated this principle in terms of literal asymptotic expansions up to some nontrivial finite order for each of the *Riesz means* of  $E_\lambda$ . Riesz means generalize to (Stieltjes) integrals the *Cesàro sums* used to create or accelerate convergence for infinite sequences and series (see Section 2).

(iii) *If an ordinary asymptotic expansion for  $G$  does not exist, does an expansion exist in some “averaged” sense?* We noted above that the Schwinger–DeWitt expansion

$$U(t, x, y) \sim (4\pi it)^{-d/2} e^{i|x-y|^2/4t} \sum_{n=0}^{\infty} a_n(x, y) (it)^{n/2} \quad (4)$$

is not a true asymptotic expansion under the most general conditions. Nevertheless, this expansion gives correct information for the purposes for which it is used by (competent) physicists. Clearly, the proper response in such a situation is not to reject the expansion as false or nonrigorous, but to define a sense (or more than one) in which it is true. At this point we cannot go into the uses made of the Schwinger–DeWitt expansion in renormalization in quantum field theory (where, actually,  $H$  is a hyperbolic operator instead of elliptic). We can note, however, that if  $U$  is to satisfy the initial condition in (A2), then as  $t \downarrow 0$  the main term in (A12b), which coincides with the whole of (A8b), must “approach a delta function”, while the remaining terms of (A12b) must effectively vanish in the context of the integral  $\lim_{t \downarrow 0} \int_0^\pi U(t, x, y) f(y) dy$ . These things happen by virtue of the increasingly rapid oscillations of the terms, integrated against the fixed test function  $f(y)$ . That is, this instance of (4) is literally true when interpreted as a relation among distributions (in the variable  $y$ ). All this is, of course, well known, but our purpose here is to examine it in a more general context. We shall show that the situation for expansions like (4) is much like that for (3): They can be rigorously established in a Riesz–Cesàro sense, or, equivalently, in the sense of distributions in the variable  $t$ . This leaves open the next question.

(iv) *If an asymptotic expansion does not exist pointwise, does it exist distributionally in  $x$  and/or  $y$ ; and does the spectral expansion converge in this distributional sense when it does not converge classically? What is the connection between this distributional behavior and that in  $t$ ?* Such formulas as (A8a), (A10), (A12a), (A14a) are not convergent, but only summable or, at most, conditionally convergent. The Riesz–Cesàro theory handles the summability issue, and, as remarked, can be rephrased in terms of distributional behavior in  $t$ . However, one suspects that such integrals or sums should be literally convergent in the topology of distributions on  $\mathcal{M}$  or  $\mathcal{M} \times \mathcal{M}$ .

This interpretation is especially appealing in the case of the Wightman func-

tion (see (A4)–(A5), (A10), (A14)). To calculate observable quantities such as energy density in quantum field theory, one expects to subtract from  $W(t, x, y)$  the leading, singular terms in the limit  $y \rightarrow x$ ; those terms are “local” or “universal”, like the  $a_n$  in the heat kernel. The remainder will be nonlocal but finite; it contains the information about physical effects caused by boundary and initial conditions on the field. (See, for instance, [16], Chapters 5 and 9.) The fact that this renormalized  $W(t, x, x)$  is finite does not guarantee that a spectral integral or sum for it will be absolutely convergent. Technically, this problem may be handled by Riesz means or some other definition of summability; but in view of the formulation of quantum field theory in terms of operator-valued distributions, one expects that such summability should be equivalent to distributional convergence on  $\mathcal{M}$ . It was, in fact, this problem that originally motivated the present work and a companion paper [17].

A fully satisfactory treatment of these issues cannot be limited to the interior of  $\mathcal{M}$ ; it should take into account the special phenomena that occur at the boundary. These questions are related to the “heat content asymptotics” recently studied by Gilkey et al. [39, 5] and McAvity [32, 33]. (A longer reference list, especially of earlier work by Van den Berg, is given by Gilkey in [21].)

(v) *Is the expansion “local” or “global” in its dependence on  $H$ ?* We have already encountered this issue in connection with the Wightman function, but it is more easily demonstrated by what we call the “cylinder kernel”  $T(t, x, y)$ , defined by (A3). Examination of (A9b) and (A13b-c) shows that  $T$  has a non-trivial power-series expansion in  $t$ , which is different for the two cases ( $\mathcal{M} = \mathbb{R}$  and  $(0, \pi)$ ). (See [17] for more detailed discussion.) More generally speaking,  $T(t, x, x)$  differs in an essential way from  $K(t, x, x)$  in that its asymptotic expansion as  $t \downarrow 0$  is not uniquely determined by the coefficient functions (symbol) of  $H$ , evaluated at  $x$ .  $T(t, x, x)$  can depend upon boundary conditions, existence of closed classical paths (geodesics or bicharacteristics), and other global structure of the problem. In terms of an inverse spectral problem, the asymptotic expansion of  $T$  gives more information about the spectrum of  $H$  and about  $E_\lambda(x, y)$  than that of  $K$  does. (Of course, the *exact* heat kernel contains, in principle, all the information, as it is the Laplace transform of  $E_\lambda$ .) We shall investigate the issue of locality for a general Green function (1).

In summary, the four basic examples introduced in the Appendix demonstrate all possible combinations of pointwise or distributional asymptotic expansions with local or global dependence on the symbol of the operator:

	Pointwise	Distributional
Local	Heat	Schrödinger
Global	Cylinder	Wightman

(5)

In this paper we show that the answers to questions (i) and (iii), and the distinction between the columns of the table above, are determined by the behavior of  $g$  at infinity: If

$$g^{(n)}(t) = O(t^{\gamma-n}) \quad \text{as } t \rightarrow +\infty \quad \text{for some } \gamma \in \mathbb{R} \quad (6)$$

(i.e.,  $g$  has at infinity the behavior characterizing the test-function space  $\mathcal{K}$  — see Sec. 2), then the answer to (i) is *Yes*. On the other hand, when  $g$  is of slow growth at infinity but does not necessarily belong to  $\mathcal{K}$ , then the expansion holds in the distributional sense mentioned in (iii).

The answer to (v), and the distinction between the rows of the table, depend on the behavior of  $g$  at the origin. If  $g(t)$  has an expansion of the form  $\sum_{n=0}^{\infty} a_n t^n$  as  $t \downarrow 0$  (even in the distributional sense) then the expansion of  $G(t, x, y)$  is local. However, if the expansion of  $g(t)$  contains fractional powers, logarithms, or any other term, then the locality property is lost. This subject is treated from a different point of view in [17].

We hope to return to question (iv) in later work.

Our basic tool is the study of the *distributional* behavior of the spectral density  $e_\lambda = dE_\lambda/d\lambda$  of the operator  $H$  as  $\lambda \rightarrow \infty$ . We are able to obtain a quite general expansion of  $e_\lambda$  when  $H$  is self-adjoint. Using the results of a previous paper [9], one knows that distributional expansions are equivalent to expansions of Cesàro–Riesz means. Thus our results become an extension of those of Hörmander [27, 28]. They sharpen and complement previous publications by one of us [13, 15, 17].

The other major tool we use is an extension of the “moment asymptotic expansion” to distributions, as explained in Section 5.

The plan of the paper is as follows. In Section 2 we give some results from [9] that play a major role in our analysis. In particular we introduce the space of test functions  $\mathcal{K}$  and its dual  $\mathcal{K}'$ , the space of distributionally small generalized functions.

In the third section we consider the distributional asymptotic expansion of spectral decompositions and of spectral densities. Many of our results hold for general self-adjoint operators on a Hilbert space, and we give them in that context. We then specialize to the case of a pseudodifferential operator acting on a manifold and by exploiting the pseudolocality of such operators we are able to show that the asymptotic behavior of the spectral density of a pseudodifferential operator has a local character *in the Cesàro sense*. That such spectral densities have a local character in “some sense” has been known for years [18, 13, 14, 15]; here we provide a precise meaning to this locality property.

In the next section we consider two model examples for the asymptotic expansion of spectral densities. Because of the local behavior, they are more than examples, since they give the asymptotic development of any operator locally equal to one of them.

In Section 5 we show that the moment asymptotic expansion, which is the basic building block in the asymptotic expansion of series and integrals [12], can be generalized to distributions, giving expansions that hold in an “averaged” or distributional sense explaining, for instance, the small- $t$  behavior of the Schrödinger propagator.

In the last two sections we apply our machinery to the study of the asymptotic expansion of general Green kernels. In Section 6 we show that the small- $t$  expansion of a propagator  $g(tH)$  that corresponds to a function  $g$  that has a Taylor-type expansion at the origin is local and that it is an ordinary or an

averaged expansion depending on the behavior of  $g$  at infinity: If  $g \in \mathcal{K}$  then the regular moment asymptotic expansion applies, while if  $g \notin \mathcal{K}$  then the “averaged” results of Section 5 apply. In the last section we consider the case when  $g$  does not have a Taylor expansion at the origin and show that in that case  $g(tH)$  has a global expansion, which depends on such information as boundary conditions.

Some applications of both of the main themes of this paper have been made elsewhere [10], most notably a mathematical sharpening of the work of Chamseddine and Connes [3] on a “universal bosonic functional”.

We do not claim that the machinery of distribution theory is indispensable in obtaining the results of this paper. Undoubtedly, most of them could be, and some of them have been, obtained by more classical methods, in the same sense that the quantum mechanics of atoms could be developed without using the terminology of group theory. We believe that our work extends and fills in previous results, and, perhaps more importantly, provides a framework in which they are better understood and appreciated.

## 2 Preliminaries

The principal tool for our study of the behavior of spectral functions and of the associated Green kernels is the distributional theory of asymptotic expansions, as developed by several authors [40, 35, 11, 12]. The main idea is that one may obtain the “average” behavior of a function, in the Riesz or Cesàro sense, by studying its parametric or distributional behavior [9].

In this section we give a summary of these results. We also set the notation for the spaces of distributions and test functions used.

If  $\mathcal{M}$  is a smooth manifold, then  $\mathcal{D}(\mathcal{M})$  is the space of compactly supported smooth functions on  $\mathcal{M}$ , equipped with the standard Schwartz topology [12, 36, 29]. Its dual,  $\mathcal{D}'(\mathcal{M})$ , is the space of standard distributions on  $\mathcal{M}$ . The space  $\mathcal{E}(\mathcal{M})$  is the space of all smooth functions on  $\mathcal{M}$ , endowed with the topology of uniform convergence of all derivatives on compacts. Its dual,  $\mathcal{E}'(\mathcal{M})$ , can be identified with the subspace of  $\mathcal{D}'(\mathcal{M})$  formed by the compactly supported distributions. Naturally the two constructions coincide if  $\mathcal{M}$  is compact.

The space  $\mathcal{S}'(\mathbb{R}^n)$  consists of the tempered distributions on  $\mathbb{R}^n$ . It is the dual of the space of rapidly decreasing smooth functions  $\mathcal{S}(\mathbb{R}^n)$ ; a smooth function  $\phi$  belongs to  $\mathcal{S}(\mathbb{R}^n)$  if  $D^\alpha \phi(x) = o(|x|^{-\infty})$  as  $|x| \rightarrow \infty$ , for each  $\alpha \in \mathbb{R}^n$ . Here we use the usual notation,  $D^\alpha = \partial^{|\alpha|} / \partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_n}$ ,  $|\alpha| = \alpha_1 + \cdots + \alpha_n$ ;  $o(x^{-\infty})$  means a quantity that is  $o(x^{-\beta})$  for all  $\beta \in \mathbb{R}$ .

A not so well known pair of spaces that plays a fundamental role in our analysis is  $\mathcal{K}(\mathbb{R}^n)$  and  $\mathcal{K}'(\mathbb{R}^n)$ . The space  $\mathcal{K}$  was introduced in [23]. A smooth function  $\phi$  belongs to  $\mathcal{K}_q$  if  $D^\alpha \phi(x) = O(|x|^{q-|\alpha|})$  as  $|x| \rightarrow \infty$  for each  $\alpha \in \mathbb{R}^n$ . The space  $\mathcal{K}$  is the inductive limit of the spaces  $\mathcal{K}_q$  as  $q \rightarrow \infty$ .

Any distribution  $f \in \mathcal{K}'(\mathbb{R})$  satisfies the *moment asymptotic expansion*,

$$f(\lambda x) \sim \sum_{j=0}^{\infty} \frac{(-1)^j \mu_j \delta^{(j)}(x)}{j! \lambda^{j+1}} \quad \text{as } \lambda \rightarrow \infty, \quad (7)$$

where  $\mu_j = \langle f(x), x^j \rangle$  are the moments of  $f$ . The interpretation of (7) is in the topology of the space  $\mathcal{K}'$ ; observe, however, that there is an equivalence between weak and strong convergence of one-parameter limits in spaces of distributions, such as  $\mathcal{K}'$ .

The moment asymptotic expansion does not hold for general distributions of the spaces  $\mathcal{D}'$  or  $\mathcal{S}'$ . Actually, it was shown recently [9] that any distribution  $f \in \mathcal{D}'$  that satisfies the moment expansion (7) for some sequence of constants  $\{\mu_j\}$  must belong to  $\mathcal{K}'$  (and then the  $\mu_j$  are the moments).

There is still another characterization of the elements of  $\mathcal{K}'$ . They are precisely the distributions of rapid decay at infinity *in the Cesàro sense*. That is why the elements of  $\mathcal{K}'$  are referred to as *distributionally small*.

The notions of Cesàro summability of series and integrals are well known [25]. In [9] this theory is generalized to general distributions. The generalization includes the classical notions as particular cases, since the behavior of a sequence  $\{a_n\}$  as  $n \rightarrow \infty$  can be studied by studying the generalized function  $\sum_{n=0}^{\infty} a_n \delta(x-n)$ . The basic concept is that of the order symbols in the Cesàro sense: Let  $f \in \mathcal{D}'(\mathbb{R})$  and let  $\beta \in \mathbb{R} \setminus \{-1, -2, -3, \dots\}$ ; we say that

$$f(x) = O(x^\beta) \quad (C) \quad \text{as } x \rightarrow \infty, \quad (8)$$

if there exists  $N \in \mathbb{R}$ , a function  $F$  whose  $N$ th derivative is  $f$ , and a polynomial  $p$  of degree  $N-1$  such that  $F$  is locally integrable for  $x$  large and the ordinary relation

$$F(x) = p(x) + O(x^{\beta+N}) \quad \text{as } x \rightarrow \infty \quad (9)$$

holds. The relation  $f(x) = o(x^\beta) \quad (C)$  is defined similarly by replacing the big  $O$  by the little  $o$  in (9).

Limits and evaluations can be handled by using the order relations. In particular,  $\lim_{x \rightarrow \infty} f(x) = L \quad (C)$  means that  $f(x) = L + o(1) \quad (C)$  as  $x \rightarrow \infty$ . If  $f \in \mathcal{D}'$  has support bounded on the left and  $\phi \in \mathcal{E}$ , then in general the evaluation  $\langle f(x), \phi(x) \rangle$  does not exist, but we say that it has the value  $S$  in the Cesàro sense if  $\lim_{x \rightarrow \infty} G(x) = S \quad (C)$ , where  $G$  is the primitive of  $f\phi$  with support bounded on the left. The Cesàro interpretation of evaluations  $\langle f(x), \phi(x) \rangle$  with  $\text{supp } f$  bounded on the right is similar, while the general case can be considered by writing  $f = f_1 + f_2$ , with  $\text{supp } f_1$  bounded on the left and  $\text{supp } f_2$  bounded on the right.

The main result that allows one to obtain the Cesàro behavior from the parametric behavior is the following.

**Theorem 2.1.** *Let  $f$  be in  $\mathcal{D}'$  with support bounded on the left. If  $\alpha > -1$ , then*

$$f(x) = O(x^\alpha) \quad (C) \quad \text{as } x \rightarrow \infty \quad (10)$$

if and only if

$$f(\lambda x) = O(\lambda^\alpha) \quad \text{as } \lambda \rightarrow \infty \quad (11)$$

distributionally.

When  $-(k+1) > \alpha > -(k+2)$  for some  $k \in \mathbb{R}$ , (10) holds if and only if there are constants  $\mu_0, \dots, \mu_k$  such that

$$f(\lambda x) = \sum_{j=0}^k \frac{(-1)^j \mu_j \delta^{(j)}(x)}{j! \lambda^{j+1}} + O(\lambda^\alpha) \quad (12)$$

distributionally as  $\lambda \rightarrow \infty$ .

*Proof:* See [9].  $\diamond$

The fact that the distributions that satisfy the moment asymptotic expansion are exactly those that satisfy  $f(x) = O(x^{-\infty})$  (C) follows from the theorem by letting  $\alpha \rightarrow -\infty$ . Thus the elements of  $\mathcal{K}'$  are the distributions of rapid distributional decay at infinity in the Cesàro sense. Hence the space  $\mathcal{K}'$  is a distributional analogue of  $\mathcal{S}$ . We apply this idea in Section 5, where we build a duality between  $\mathcal{S}'$  and  $\mathcal{K}'$ .

Another important corollary of the theorem is the fact that one can relate the (C) expansion of a generalized function and its parametric expansion in a simple fashion. Namely, if  $\{\alpha_j\}$  is a sequence with  $\Re \alpha_j \searrow -\infty$ , then

$$f(x) \sim \sum_{j=0}^{\infty} a_j x^{\alpha_j} \quad (C) \quad \text{as } x \rightarrow \infty \quad (13)$$

if and only if

$$f(\lambda x) \sim \sum_{j=0}^{\infty} a_j g_{\alpha_j}(\lambda x) + \sum_{j=0}^{\infty} \frac{(-1)^j \mu_j \delta^{(j)}(x)}{j! \lambda^{j+1}} \quad (14)$$

as  $\lambda \rightarrow \infty$ , where the  $\mu_j$  are the (generalized) moments of  $f$  and where

$$g_\alpha(x) = x_+^\alpha \quad \text{if } \alpha \neq -1, -2, -3, \dots, \quad (15)$$

while in the exceptional cases  $g_\alpha$  is a finite-part distribution [12]:

$$g_{-k}(x) = \mathcal{P}.f. (\chi(x)x^{-k}) \quad \text{if } k = 1, 2, 3, \dots, \quad (16)$$

$\chi$  being the Heaviside function, the characteristic function of the interval  $(0, \infty)$ . Notice that

$$g_\alpha(\lambda x) = \lambda^\alpha g_\alpha(x), \quad \alpha \neq -1, -2, -3, \dots, \quad (17)$$

$$g_{-k}(\lambda x) = \frac{g_{-k}(x)}{\lambda^k} + \frac{(-1)^{k-1} \ln \lambda \delta^{(k-1)}(x)}{(k-1)! \lambda^k}, \quad k = 1, 2, 3, \dots \quad (18)$$



### 3 The asymptotic expansion of spectral decompositions

Let  $\mathcal{H}$  be a Hilbert space and let  $H$  be a self-adjoint operator on  $\mathcal{H}$ , with domain  $\mathcal{X}$ . Then  $H$  admits a spectral decomposition  $\{E_\lambda\}_{\lambda=-\infty}^{\infty}$ . The  $\{E_\lambda\}$  is an increasing family of projectors that satisfy

$$I = \int_{-\infty}^{\infty} dE_\lambda, \quad (19)$$

where  $I$  is the identity operator, and

$$H = \int_{-\infty}^{\infty} \lambda dE_\lambda \quad (20)$$

in the weak sense, that is,

$$(Hx|y) = \int_{-\infty}^{\infty} \lambda d(E_\lambda x|y), \quad (21)$$

for  $x \in \mathcal{X}$  and  $y \in \mathcal{H}$ , where  $(x|y)$  is the inner product in  $\mathcal{H}$ .

Perhaps more natural than the spectral function  $E_\lambda$  is the spectral density  $e_\lambda = dE_\lambda/d\lambda$ . This spectral density does not have a pointwise value for all  $\lambda$ . Rather, it should be understood as an operator-valued distribution, an element of the space  $\mathcal{D}'(\mathbb{R}, L(\mathcal{X}, \mathcal{H}))$ . Thus (19)–(20) become

$$I = \langle e_\lambda, 1 \rangle \quad (22)$$

$$H = \langle e_\lambda, \lambda \rangle, \quad (23)$$

where  $\langle f(\lambda), \phi(\lambda) \rangle$  is the evaluation of a distribution  $f(\lambda)$  on a test function  $\phi(\lambda)$ .

The spectral density  $e_\lambda$  can be used to build a functional calculus for the operator  $H$ . Indeed, if  $g$  is continuous and with compact support in  $\mathbb{R}$  then we can define the operator  $g(H) \in L(\mathcal{X}, \mathcal{H})$  (extendible to  $L(\mathcal{H}, \mathcal{H})$ ) by

$$g(H) = \langle e_\lambda, g(\lambda) \rangle. \quad (24)$$

One does not need to assume  $g$  of compact support in (24), but in a contrary case the domain of  $g(H)$  is not  $\mathcal{X}$  but the subspace  $\mathcal{N}_g$  consisting of the  $x \in \mathcal{H}$  for which the improper integral  $\langle (e_\lambda x|y), g(\lambda) \rangle$  converges for all  $y \in \mathcal{H}$ .

One can even define  $f(H)$  when  $f$  is a distribution such that the evaluation  $\langle e_\lambda, f(\lambda) \rangle$  is defined. For instance, if  $E_\lambda$  is continuous at  $\lambda = \lambda_0$  then  $E_{\lambda_0} = \chi(\lambda_0 - H)$  where  $\chi$  is again the Heaviside function. Differentiation yields the useful symbolic formula

$$e_\lambda = \delta(\lambda - H). \quad (25)$$

Let  $\mathcal{X}_n$  be the domain of  $H^n$  and let  $\mathcal{X}_\infty = \bigcap_{n=1}^{\infty} \mathcal{X}_n$ . Then

$$\langle e_\lambda, \lambda^n \rangle = H^n \quad (26)$$

in the space  $L(\mathcal{X}_\infty, \mathcal{H})$ . But, as shown recently [9], a distribution  $f \in \mathcal{D}'(\mathbb{R})$  whose moments  $\langle f(x), x^n \rangle$ ,  $n \in \mathbb{R}$ , all exist belongs to  $\mathcal{K}'(\mathbb{R})$  — that is, it is distributionally small. Hence,  $e_\lambda$ , as a function of  $\lambda$ , belongs to the space  $\mathcal{K}'(\mathbb{R}, L(\mathcal{X}_\infty, \mathcal{H}))$ . Therefore, the asymptotic behavior of  $e_{\lambda\sigma}$ , as  $\sigma \rightarrow \infty$ , can be obtained by using the moment asymptotic expansion:

$$e_{\lambda\sigma} \sim \sum_{n=0}^{\infty} \frac{(-1)^n H^n \delta^{(n)}(\lambda\sigma)}{n!} \quad \text{as } \sigma \rightarrow \infty, \quad (27)$$

while  $e_\lambda$  vanishes to infinite order at infinity in the Cesàro sense:

$$e_\lambda = o(|\lambda|^{-\infty}) \quad (C) \quad \text{as } |\lambda| \rightarrow \infty. \quad (28)$$

The asymptotic behavior of the spectral function  $E_\lambda$  is obtained by integration of (27) and by recalling that  $\lim_{\lambda \rightarrow -\infty} E_\lambda = 0$ ,  $\lim_{\lambda \rightarrow \infty} E_\lambda = I$ . We obtain

$$E_\lambda \sim \chi(\lambda\sigma)I + \sum_{n=0}^{\infty} \frac{(-1)^{n+1} H^{n+1} \delta^{(n)}(\lambda\sigma)}{(n+1)!} \quad \text{as } \sigma \rightarrow \infty. \quad (29)$$

Similarly, the Cesàro behavior is given by

$$E_\lambda = I + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty, \quad (30)$$

$$E_\lambda = o(|\lambda|^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow -\infty. \quad (31)$$

These formulas are most useful when  $H$  is an unbounded operator. Indeed, if  $H$  is bounded, with domain  $\mathcal{X} = \mathcal{H}$ , then  $e_\lambda = 0$  for  $\lambda > \|H\|$  and  $E_\lambda = 0$  for  $\lambda < -\|H\|$ ,  $E_\lambda = I$  for  $\lambda > \|H\|$ , so (28), (30), and (31) are trivial in that case.

In the present study we are mostly interested in the case when  $H$  is an elliptic differential operator with smooth coefficients defined on a smooth manifold  $\mathcal{M}$ . Usually  $\mathcal{H} = L^2(\mathcal{M})$  and  $\mathcal{X}$  is the domain corresponding to the introduction of suitable boundary conditions. Usually the operator  $H$  will be positive, but at present we shall just assume  $H$  to be self-adjoint.

In this case the space  $\mathcal{D}(\mathcal{M})$  of test functions on  $\mathcal{M}$  is a subspace of  $\mathcal{X}_\infty$ . Observe also that the operators  $K$  acting on  $\mathcal{D}(\mathcal{M})$  can be realized as distributional kernels  $k(x, y)$  of  $\mathcal{D}'(\mathcal{M} \times \mathcal{M})$  by

$$(K\phi)(x) = \langle k(x, y), \phi(y) \rangle_y. \quad (32)$$

In particular,  $\delta(x - y)$  is the kernel corresponding to the identity  $I$ , and  $H\delta(x - y)$  is the kernel of  $H$ . The spectral density  $e_\lambda$  also has an associated kernel  $e(x, y; \lambda)$ , an element of  $\mathcal{D}'(\mathbb{R}, \mathcal{D}'(\mathcal{M} \times \mathcal{M}))$ . Since  $H$  is elliptic it follows that  $e(x, y; \lambda)$  is smooth in  $(x, y)$ . *Warning:* Much of the literature uses “ $e(x, y; \lambda)$ ” for what we call “ $E(x, y; \lambda)$ ”.

The expansions (27)–(31) will hold in  $\mathcal{X}_\infty$  and thus, a fortiori, in  $\mathcal{D}(\mathcal{M})$ . Hence

$$e(x, y; \lambda\sigma) \sim \sum_{n=0}^{\infty} \frac{(-1)^n H^n \delta(x - y) \delta^{(n)}(\lambda\sigma)}{n!} \quad \text{as } \sigma \rightarrow \infty, \quad (33)$$

$$E(x, y; \lambda\sigma) \sim \chi(\lambda\sigma)\delta(x-y) + \sum_{n=0}^{\infty} \frac{(-1)^{n+1} H^{n+1} \delta(x-y) \delta^{(n)}(\lambda\sigma)}{(n+1)!} \quad \text{as } \sigma \rightarrow \infty, \quad (34)$$

in the space  $\mathcal{D}'_{\lambda}(\mathbb{R}, \mathcal{D}'_{xy}(\mathcal{M} \times \mathcal{M}))$ . Furthermore,

$$e(x, y; \lambda) = o(|\lambda|^{-\infty}) \quad (C) \quad \text{as } |\lambda| \rightarrow \infty, \quad (35)$$

$$E(x, y; \lambda) = \delta(x-y) + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty, \quad (36a)$$

$$E(x, y; \lambda) = o(|\lambda|^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow -\infty, \quad (36b)$$

in the space  $\mathcal{D}'(\mathcal{M} \times \mathcal{M})$ .

Actually, an easy argument shows that the expansions also hold distributionally in one variable and pointwise in the other. (For instance, (35) says that if  $y$  is fixed and  $\phi \in \mathcal{D}(\mathcal{M})$  then  $\langle e(x, y; \lambda), \phi(x) \rangle = o(|\lambda|^{-\infty}) \quad (C) \quad \text{as } |\lambda| \rightarrow \infty$ .)

That the expansions cannot hold pointwise in both variables  $x$  and  $y$  should be clear since we cannot set  $x = y$  in the distribution  $\delta(x-y)$ . And indeed,  $e(x, x; \lambda)$  is *not* distributionally small. However, as we now show, the expansions are valid pointwise outside of the diagonal of  $\mathcal{M} \times \mathcal{M}$ .

Indeed, let  $U, V$  be open sets with  $U \cap V = \emptyset$ . If  $f \in \mathcal{D}'(\mathcal{M})$  and  $\phi \in \mathcal{D}(\mathbb{R})$ , then  $\phi(H)$  is a smoothing pseudodifferential operator, so  $\phi(H)f$  is smooth in  $\mathcal{M}$ . Thus,  $\langle e(x, y; \lambda), f(x)g(y)\phi(\lambda) \rangle = \langle \phi(H)f(x), g(x) \rangle$  is well-defined if  $f \in \mathcal{D}'(\mathcal{M}), \text{supp } f \subseteq U, g \in \mathcal{D}'(\mathcal{M}), \text{supp } g \subseteq V$ . Therefore  $e(x, y; \lambda)$  belongs to  $\mathcal{D}'(\mathbb{R}, \mathcal{E}(U \times V))$ . But

$$\langle e(x, y; \lambda), f(x)g(y)\lambda^n \rangle = \langle H^n f(x), g(x) \rangle = 0, \quad (37)$$

thus  $e(x, y; \lambda)$  actually belongs to  $\mathcal{K}'(\mathbb{R}, \mathcal{E}(U \times V))$ ; that is, it is a distributionally small distribution in that space whose moments vanish. Therefore

$$e(x, y; \lambda\sigma) = o(\sigma^{-\infty}) \quad \text{as } \sigma \rightarrow \infty, \quad (38)$$

$$E(x, y; \lambda\sigma) = \chi(\lambda\sigma)\delta(x-y) + o(\sigma^{-\infty}) \quad \text{as } \sigma \rightarrow \infty, \quad (39)$$

in the space  $\mathcal{K}'(\mathbb{R}, \mathcal{E}(U \times V))$ . Similarly, (35)–(36) also hold in  $\mathcal{E}(U \times V)$ . Convergence in  $\mathcal{E}(U \times V)$  implies pointwise convergence on  $U \times V$ , but it gives more; namely, it gives uniform convergence of all derivatives on compacts. Thus (35), (36), (38), and (39) hold uniformly on compacts of  $U \times V$  and the expansion can be differentiated as many times as we please with respect to  $x$  or  $y$ .

**Example.** Let  $Hy = -y''$  considered on the domain  $\mathcal{X} = \{y \in C^2[0, \pi] : y(0) = y(\pi) = 0\}$  in  $L^2[0, \pi]$ . The eigenvalues are  $\lambda_n = n^2$ ,  $n = 1, 2, 3, \dots$ , with normalized eigenfunctions  $\phi_n(x) = \sqrt{\frac{2}{\pi}} \sin nx$ . Therefore,

$$e(x, y; \lambda) = \frac{2}{\pi} \sum_{n=1}^{\infty} \sin nx \sin ny \delta(\lambda - n^2), \quad (40)$$

where  $0 < x < \pi$ ,  $0 < y < \pi$ . Then

$$\frac{2}{\pi} \sum_{n=1}^{\infty} \sin nx \sin ny \delta(\lambda\sigma - n^2) \sim \sum_{j=0}^{\infty} \frac{\delta^{(2j)}(x-y)\delta^{(j)}(\lambda)}{j! \sigma^{j+1}} \quad \text{as } \sigma \rightarrow \infty \quad (41)$$

in  $\mathcal{D}'(\mathbb{R}, \mathcal{D}'((0, \pi) \times (0, \pi)))$ , while

$$\frac{2}{\pi} \sum_{n=1}^{\infty} \sin nx \sin ny \delta(\lambda\sigma - n^2) = o(\sigma^{-\infty}) \quad \text{as } \sigma \rightarrow \infty \quad (42)$$

if  $x$  and  $y$  are fixed,  $x \neq y$ . On the other hand,

$$e(x, x; \lambda) = \frac{2}{\pi} \sum_{n=1}^{\infty} \sin^2 nx \delta(\lambda - n^2), \quad (43)$$

thus if  $0 < x < \pi$ ,

$$\begin{aligned} e(x, x; \lambda\sigma) &= \frac{1}{\pi} \sum_{n=1}^{\infty} (1 - \cos 2nx) \delta(\lambda\sigma - n^2) \\ &= \frac{1}{\pi} \sum_{n=1}^{\infty} \delta(\lambda\sigma - n^2) + \frac{1}{2\pi\sigma} \delta(\lambda) + o(\sigma^{-\infty}) \quad \text{as } \sigma \rightarrow \infty, \end{aligned}$$

because the generalized function  $\sum_{n=1}^{\infty} \cos 2nx \delta(\lambda - n^2)$  is distributionally small if  $0 < x < \pi$ , with moments  $\mu_0 = -1/2$  and  $\mu_k = 0$  for  $k \geq 1$ , since [8]

$$\begin{aligned} \sum_{n=1}^{\infty} \cos 2nx &= -\frac{1}{2} \quad (C), \\ \sum_{n=1}^{\infty} n^{2k} \cos 2nx &= 0 \quad (C), \quad k = 1, 2, 3, \dots \end{aligned}$$

But ([12], Chapter 5)

$$\sum_{n=1}^{\infty} \phi(\varepsilon n^2) = \frac{1}{2\varepsilon^{1/2}} \int_0^{\infty} u^{-1/2} \phi(u) du - \frac{1}{2} \phi(0) + o(\varepsilon^{\infty}) \quad (44)$$

as  $\varepsilon \rightarrow 0^+$  if  $\phi \in \mathcal{S}$ , thus

$$e(x, x; \lambda\sigma) = \frac{1}{2\pi\sigma^{1/2}} \lambda_+^{-1/2} + o(\sigma^{-\infty}) \quad \text{as } \sigma \rightarrow \infty. \quad (45)$$

It is then clear that  $e(x, x; \lambda)$  is not distributionally small; rather,

$$e(x, x; \lambda) = \frac{1}{2\pi\lambda^{1/2}} + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty, \quad (46)$$

that is,  $e(x, x; \lambda) \sim (1/2\pi)\lambda^{-1/2}$ , as  $\lambda \rightarrow \infty$ , in the Cesàro sense.  $\diamond$

Neither is the spectral density  $e(x, y; \lambda)$  distributionally small at the boundaries, as follows from the heat content asymptotics of Refs. [39, 5]. That there is a sharp change of behavior at the boundary can be seen from the behavior of the spectral density  $e(x, x; \lambda)$  given by (43). Indeed, if  $0 < x < \pi$  then  $e(x, x; \lambda) = (1/2\pi)\lambda^{-1/2} + o(\lambda^{-\infty})$  (C), but when  $x = 0$  or  $x = \pi$  then  $e(0, 0; \lambda) = e(\pi, \pi; \lambda) = 0$ .

It is important to observe that in the Cesàro or distributional sense, the behavior at infinity of the spectral density  $e(x, y; \lambda)$  depends only on the local behavior of the coefficients of  $H$ . That is, if  $H_1$  and  $H_2$  are two operators that coincide on the open subset  $U$  of  $\mathcal{M}$  and if  $e_1(x, y; \lambda)$  and  $e_2(x, y; \lambda)$  are the corresponding spectral densities, then

$$e_1(x, y; \sigma\lambda) = e_2(x, y; \sigma\lambda) + o(\sigma^{-\infty}) \quad \text{as } \sigma \rightarrow \infty \tag{47}$$

in  $\mathcal{D}'(U \times U)$ . This follows immediately from (33). In fact, it follows from Theorem 7.2 that

$$e_1(x, y; \lambda) = e_2(x, y; \lambda) + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty, \tag{48}$$

pointwise on  $(x, y) \in U \times U$  (even on the diagonal!). More than that, (48) holds in the space  $\mathcal{E}(U \times U)$ , so that it is uniform on compacts of  $U$ . These results are useful in connection with the suggestion [18, 13, 14, 15] to replace a general second-order operator  $H$  by another,  $H_0$ , that agrees locally with  $H$  and for which the spectral density can be calculated. In the next section we treat two special classes of operators where this idea has been implemented.

**Example.** The spectral density for the operator  $-y''$  on the whole real line is

$$e_1(x, y; \lambda) = \frac{\chi(\lambda) \cos \lambda^{1/2}(x - y)}{2\pi\lambda^{1/2}}, \tag{49}$$

as can be seen from (A7a) and (A8a). Therefore, comparison with (40) yields

$$\frac{2}{\pi} \sum_{n=1}^{\infty} \sin nx \sin ny \delta(\lambda - n^2) = \frac{\cos \lambda^{1/2}(x - y)}{2\pi\lambda^{1/2}} + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty. \tag{50}$$

In particular, if we set  $x = y$  we recover (46).

Formula (50) is uniform in compacts of  $(0, \pi) \times (0, \pi)$  but ceases to hold as  $x$  or  $y$  approaches 0 or  $\pi$ . For instance, if  $y = 0$ , the left side vanishes while [cf. (33)]

$$\frac{\chi(\sigma\lambda) \cos(\sigma\lambda)^{1/2}x}{2\pi(\sigma\lambda)^{1/2}} \sim \frac{\delta(x)\delta(\lambda)}{\sigma} + \frac{\delta''(x)\delta'(\lambda)}{\sigma^2} + \dots$$

as  $\sigma \rightarrow \infty$ .  $\diamond$

## 4 Special cases

In this section we give two model cases for the asymptotic expansion of spectral densities. They are not just examples, since according to the results of the

previous section, the spectral density of any operator locally equal to such a model case will have the same behavior at infinity in the Cesàro sense.

Let us start with a constant-coefficient elliptic operator  $H$  defined on the whole space  $\mathbb{R}^n$ . Then  $H$  admits a unique self-adjoint extension (which we also denote as  $H$ ), given as follows. Let  $p = \sigma(H)$  be the symbol of  $H$  (i.e.,  $H = p(-i\partial)$ ). Then the spectral function is given by

$$E(x, y; \lambda) = \frac{1}{(2\pi)^n} \int_{p(\xi) < \lambda} e^{i(x-y)\cdot\xi} d\xi, \quad (51)$$

so that the spectral density can be written as

$$e(x, y; \lambda) = \frac{1}{(2\pi)^n} \left\langle e^{i(x-y)\cdot\xi}, \delta(p(\xi) - \lambda) \right\rangle. \quad (52)$$

For the definition of  $\delta(f(x))$  see [20, 4].

To obtain the behavior of  $e(x, y; \lambda)$  as  $\lambda \rightarrow \infty$  in the Cesàro or in the distributional sense, we should consider the parametric behavior of  $e(x, y; \sigma\lambda)$  as  $\sigma \rightarrow \infty$ . Setting  $\varepsilon = 1/\sigma$  and evaluating at a test function  $\phi(\lambda)$ , one is led to the function

$$\Phi(\varepsilon) = \langle e(x, y; \lambda), \phi(\varepsilon\lambda) \rangle_\lambda. \quad (53)$$

But in view of (52) we obtain

$$\Phi(\varepsilon) = \frac{1}{(2\pi)^n} \left\langle e^{i(x-y)\cdot\xi}, \phi(\varepsilon p(\xi)) \right\rangle_\xi. \quad (54)$$

When  $x \neq y$  are fixed,  $e^{i(x-y)\cdot\xi}$  is distributionally small as a function of  $\xi$ . This also holds distributionally in  $(x, y)$ . Thus the expansion of (54) follows from the following lemma.

**Lemma 4.1.** *Let  $f \in \mathcal{K}'(\mathbb{R}^n)$ , so that it satisfies the moment asymptotic expansion*

$$f(\lambda x) \sim \sum_{k \in \mathbb{R}^n} \frac{(-1)^{|k|} \mu_k D^k \delta(x)}{k! \lambda^{|k|+n}} \quad \text{as } \lambda \rightarrow \infty, \quad (55)$$

where  $\mu_k = \langle f(x), x^k \rangle$ ,  $k \in \mathbb{R}^n$ , are the moments. Then if  $p$  is an elliptic polynomial and  $\phi \in \mathcal{K}$ ,

$$\langle f(x), \phi(\varepsilon p(x)) \rangle \sim \sum_{m=0}^{\infty} \frac{\langle f(x), p(x)^m \rangle \phi^{(m)}(0) \varepsilon^m}{m!} \quad \text{as } \varepsilon \rightarrow 0. \quad (56)$$

*Proof:* The proof consists in showing that the Taylor expansion in  $\varepsilon$ ,

$$\phi(\varepsilon p(x)) = \sum_{m=0}^N \frac{\phi^{(m)}(0) p(x)^m \varepsilon^m}{m!} + O(\varepsilon^{N+1}), \quad (57)$$

not only holds pointwise but actually holds in the topology of  $\mathcal{K}(\mathbb{R}^n)$ . But the remainder in this Taylor approximation is

$$R_N(x, \varepsilon) = \frac{\phi^{(N+1)}(\theta p(x)) p(x)^{N+1} \varepsilon^{N+1}}{(N+1)!}, \quad (58)$$

for some  $\theta \in (0, \varepsilon)$ . Since  $\phi \in \mathcal{K}$ , there exists  $q \in \mathbb{R}$  such that  $\phi^{(j)}(x) = O(|x|^{q-j})$  as  $x \rightarrow \infty$ . If  $p$  has degree  $m$  it follows that

$$|R_N(x, \varepsilon)| \leq \frac{M \max\{1, |x|^{mq}\} \varepsilon^{N+1}}{(N+1)!} \quad (59)$$

for some constant  $M$ , and the convergence of the Taylor expansion in the topology of the space  $\mathcal{K}$  follows.  $\diamond$

Thus, applying (56) with  $f(x) = e^{i(x-y)\cdot\xi}$  for  $x \neq y$  or distributionally in  $(x, y)$ , we obtain

$$\Phi(\varepsilon) \sim \frac{1}{(2\pi)^n} \sum_{k=0}^{\infty} \frac{\langle e^{i(x-y)\cdot\xi}, p(\xi)^k \rangle \phi^{(k)}(0) \varepsilon^k}{k!},$$

or

$$\Phi(\varepsilon) \sim \sum_{k=0}^{\infty} \frac{H^k \delta(x-y) \phi^{(k)}(0) \varepsilon^k}{k!}. \quad (60)$$

Therefore,

$$e(x, y; \lambda \sigma) \sim \sum_{k=0}^{\infty} \frac{(-1)^k H^k \delta(x-y) \delta^{(k)}(\lambda)}{k! \sigma^{k+1}} \quad \text{as } \sigma \rightarrow \infty, \quad (61)$$

in accordance with the general result.

Observe also that if  $H_1$  is any operator corresponding to the same differential expression, considered in some open set  $\mathcal{M}$  with some boundary conditions, then its spectral density  $e_1(x, y; \lambda)$  satisfies

$$e_1(x, y; \lambda) = \frac{1}{(2\pi)^n} \langle e^{i(x-y)\cdot\xi}, \delta(p(\xi) - \lambda) \rangle + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty. \quad (62)$$

**Example.** Let  $\mathcal{M}$  be a region in  $\mathbb{R}^n$  and let  $H$  be any self-adjoint extension of the negative Laplacian  $-\Delta$  obtained by imposing suitable boundary conditions on  $\mathcal{M}$ . Let  $e_{\mathcal{M}}(x, y; \lambda)$  be the spectral density. Then

$$e_{\mathcal{M}}(x, y; \lambda) = \frac{1}{(2\pi)^n} \langle \delta(|\xi|^2 - \lambda), e^{i(x-y)\cdot\xi} \rangle + o(\lambda^{-\infty}) \quad (C). \quad (63)$$

We now use the one-variable formula

$$\delta(f(x)) = \frac{\delta(x - x_0)}{|f'(x_0)|},$$

valid if  $f$  has a single zero at  $x_0$ , and pass to polar coordinates  $\xi = r\omega$ , where  $r = |\xi|$ ,  $\omega = (\omega_1, \dots, \omega_n)$  satisfies  $|\omega| = 1$ , and  $d\xi = r^{n-1} dr d\sigma(\omega)$ , to obtain

$$\begin{aligned} & \frac{1}{(2\pi)^n} \langle \delta(|\xi|^2 - \lambda), e^{i(x-y)\cdot\xi} \rangle \\ &= \frac{1}{(2\pi)^n} \int_{|\omega|=1} \int_0^\infty \langle \delta(r^2 - \lambda), e^{ir(x-y)\cdot\omega} \rangle r^{n-1} dr d\sigma(\omega) \\ &= \frac{\lambda^{n/2-1}}{2(2\pi)^n} \int_{|\omega|=1} e^{i\lambda^{1/2}(x-y)\cdot\omega} d\sigma(\omega) \\ &= \frac{\lambda^{n/2-1}}{2(2\pi)^n} \int_{|\omega|=1} e^{i\lambda^{1/2}\omega_1|x-y|} d\sigma(\omega) \\ &= \frac{\lambda^{n/2-1}}{2(2\pi)^n} \frac{2\pi^{(n-1)/2}}{\Gamma(\frac{n-1}{2})} \int_{-1}^1 e^{i\lambda^{1/2}u|x-y|} (1-u^2)^{\frac{n-3}{2}} du \\ &= \frac{\lambda^{n/4-1/2} J_{n/2-1}(\lambda^{1/2}|x-y|)}{2^{n/2+1}\pi^{n/2}|x-y|^{n/2-1}}, \end{aligned}$$

where  $J_p(x)$  is the Bessel function of order  $p$ . Therefore

$$e_{\mathcal{M}}(x, y; \lambda) = \frac{\lambda^{n/4-1/2} J_{n/2-1}(\lambda^{1/2}|x-y|)}{2^{n/2+1}\pi^{n/2}|x-y|^{n/2-1}} + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty, \quad (64)$$

uniformly over compacts of  $\mathcal{M} \times \mathcal{M}$ .  $\diamond$

Our second model is an ordinary differential operator  $H$  with variable coefficients, as treated in [13, 14, 15]. There are two major simplifications in this one-dimensional case. First, the Weyl–Titchmarsh–Kodaira theory [38, 30] expresses the spectral density as

$$e(x, y; \lambda) d\lambda = \sum_{j,k=0}^1 \psi_{\lambda_j}(x) d\mu^{jk}(\lambda) \overline{\psi_{\lambda_k}(y)}, \quad (65)$$

where  $d\mu^{jk}$  are certain Stieltjes measures supported on the spectrum of  $H$ , and  $\psi_{\lambda_j}$  are the classical solutions of  $H\psi - \lambda\psi$  with the basic data

$$\begin{aligned} \psi_{\lambda_0}(x_0) &= 1, & \psi'_{\lambda_0}(x_0) &= 0, \\ \psi_{\lambda_1}(x_0) &= 0, & \psi'_{\lambda_1}(x_0) &= 1, \end{aligned} \quad (66)$$

at some  $x_0 \in \mathcal{M}$ . Thus

$$\begin{aligned} \mu^{00}(\lambda) &= E(x_0, x_0; \lambda), & \mu^{01}(\lambda) &= \frac{\partial E}{\partial y}(x_0, x_0; \lambda), \\ \mu^{10}(\lambda) &= \frac{\partial E}{\partial x}(x_0, x_0; \lambda), & \mu^{11}(\lambda) &= \frac{\partial^2 E}{\partial x \partial y}(x_0, x_0; \lambda). \end{aligned} \quad (67)$$

Second, the eigenfunctions  $\psi_{\lambda_j}$  can be approximated for large  $\lambda$  quite explicitly by the phase-integral (WKB) method. (Thirdly, but less essentially, there is no



loss of generality in considering

$$H = -\frac{d^2}{dx^2} + V(x), \quad (68)$$

since the general second-order operator can be reduced to this form by change of variables.)

In [13] the phase-integral representation of the eigenfunctions was used to obtain in a direct and elementary way the expansion

$$d\mu^{jk}(\lambda) \sim \frac{1}{\pi} \sum_{n=0}^{\infty} \rho_n^{jk}(x_0) \omega^{2\delta_{j1}\delta_{k1}-2n} d\omega, \quad (69)$$

where  $\lambda = \omega^2$  and

$$\begin{aligned} \rho_0^{00} &= 1, & \rho_1^{00} &= \frac{1}{2}V, & \rho_2^{00} &= \frac{1}{8}(-V'' + 3V^2), & \dots, \\ \rho_0^{11} &= 1, & \rho_1^{11} &= -\frac{1}{2}V, & \rho_2^{11} &= \frac{1}{8}(V'' - 3V^2), & \dots, \end{aligned} \quad (70)$$

$$\rho_n^{10} = \rho_n^{01} = \frac{1}{2} \frac{d}{dx_0}(\rho_n^{00}).$$

Formula (69) is a rigorous asymptotic expansion when  $\mathcal{M} = \mathbb{R}$  and  $V$  is a  $C^\infty$  function of compact support. The relevance of (69) in more general cases, where it is certainly not a literal pointwise asymptotic expansion, was discussed at length in [13]; the results of the present paper simplify and sharpen that discussion by showing that *the error in (69) is  $O(\lambda^{-\infty})$  in the  $(C)$  sense for any operator locally equivalent to one for which (69) holds pointwise.*

## 5 Pointwise and average expansions

Let  $f \in \mathcal{K}'(\mathbb{R})$ . Since the elements of  $\mathcal{K}'(\mathbb{R})$  are precisely the distributionally small generalized functions, it follows that  $f$  satisfies the moment asymptotic expansion; that is,

$$f(\lambda x) \sim \sum_{j=0}^{\infty} \frac{(-1)^j \mu_j \delta^{(j)}(x)}{j! \lambda^{j+1}} \quad \text{as } \lambda \rightarrow \infty, \quad (71)$$

where

$$\mu_j = \langle f(x), x^j \rangle, \quad j \in \mathbb{R}, \quad (72)$$

are the moments.

The moment asymptotic expansion allows us to obtain the small- $t$  behavior of functions  $G(t)$  that can be written as

$$G(t) = \langle f(x), g(tx) \rangle, \quad (73)$$

as long as  $g \in \mathcal{K}$ . Indeed, (71) gives

$$G(t) = \sum_{j=0}^{\infty} \frac{\mu_j g^{(j)}(0) t^j}{j!} \quad \text{as } t \rightarrow 0. \quad (74)$$

Naturally, this would be valuable if  $f(\lambda) = e(x, y; \lambda)$  is the spectral density of the elliptic differential operator  $H$  and  $G(t, x, y) = \langle e(x, y; \lambda), g(\lambda t) \rangle$  is an associated Green kernel.

However, we emphasize that the derivation of (74) holds only when  $g \in \mathcal{K}$ . What if  $g \notin \mathcal{K}$ ? A particularly interesting example is the kernel  $U(t, x, y) = \langle e(x, y; \lambda), e^{-i\lambda t} \rangle$  that solves the Schrödinger equation

$$i \frac{\partial U}{\partial t} = HU, \quad t > 0 \quad (75a)$$

with initial condition

$$U(0^+, x, y) = \delta(x - y). \quad (75b)$$

In this case  $g(x) = e^{-ix}$  is smooth, but because of its behavior at infinity, it does not belong to  $\mathcal{K}$ . We pointed out in the introduction, however, that (74) is still valid in some “averaged” sense.

Indeed, we shall now show that formula (73) permits one to define  $G(t)$  as a distribution when instead of asking  $g \in \mathcal{K}$  we assume  $g$  to be a tempered distribution of the space  $\mathcal{S}'$  which has a distributional expansion at the origin. We then show that (74) holds in an averaged or distributional sense. The fact that the space of smooth functions  $\mathcal{K}$  is replaced by the space of tempered distributions is not casual: the distributions of  $\mathcal{S}'$  are exactly those that have the behavior at  $\infty$  of the elements of  $\mathcal{K}$  in the Cesàro or distributional sense. Indeed, we have

**Lemma 5.1** *Let  $g \in \mathcal{S}'(\mathbb{R})$ . Then there exists  $\alpha \in \mathbb{R}$  such that*

$$g^{(n)}(\lambda x) = O(\lambda^{\alpha-n}) \quad \text{as } \lambda \rightarrow \infty, \quad (76)$$

*distributionally.*

*Proof:* See [9], where it is shown that (76) is actually a characterization of the tempered distributions.  $\diamond$

Let  $g \in \mathcal{S}'(\mathbb{R})$  and let  $\alpha$  be as in (76). If  $\phi \in \mathcal{S}(\mathbb{R})$  then the function  $\Phi$  defined by

$$\Phi(x) = \langle g(tx), \phi(t) \rangle \quad (77)$$

is smooth in the open set  $(-\infty, 0) \cup (0, \infty)$  and, because of (76), satisfies

$$\Phi^{(n)}(x) = O(|x|^{\alpha-n}) \quad \text{as } |x| \rightarrow \infty. \quad (78)$$

It follows that we can define  $G(t) = \langle f(x), g(tx) \rangle$  as an element of  $\mathcal{S}'(\mathbb{R})$  by

$$\langle G(t), \phi(t) \rangle = \langle f(x), \Phi(x) \rangle, \quad (79)$$

whenever  $f \in \mathcal{K}'$  and  $0 \notin \text{supp } f$ .

When  $0 \in \text{supp } f$  then (79) cannot be used unless  $\Phi$  is smooth at the origin. And in order to have  $\Phi$  smooth we need to ask the existence of the *distributional* values  $g^{(n)}(0)$ ,  $n = 0, 1, 2, \dots$

Recall that following Lojasiewicz [31], one says that a distribution  $h \in \mathcal{D}'$  has the value  $\gamma$  at the point  $x = x_0$ , written as

$$h(x_0) = \gamma \quad \text{in } \mathcal{D}', \tag{80}$$

if

$$\lim_{\varepsilon \rightarrow 0} h(x_0 + \varepsilon x) = \gamma \tag{81}$$

distributionally; that is, if for each  $\phi \in \mathcal{D}$

$$\lim_{\varepsilon \rightarrow 0} \langle h(x_0 + \varepsilon x), \phi(x) \rangle = \gamma \int_{-\infty}^{\infty} \phi(x) dx. \tag{82}$$

It can be shown that  $h(x_0) = \gamma$  in  $\mathcal{D}'$  if and only if there exists a primitive  $h_n$  of some order  $n$ ,  $h_n^{(n)} = h$ , which is continuous in a neighborhood of  $x = x_0$  and satisfies

$$h_n(x) = \frac{\gamma(x - x_0)^n}{n!} + o(|x - x_0|^n), \quad \text{as } x \rightarrow x_0. \tag{83}$$

In our present case, we need to ask the existence of the distributional values  $g^{(n)}(0) = a_n$  for  $n \in \mathbb{R}$ . We can then say that  $g(x)$  has the small- $x$  ‘‘averaged’’ or distributional expansion

$$g(x) \sim \sum_{n=0}^{\infty} \frac{a_n x^n}{n!}, \quad \text{as } x \rightarrow 0, \quad \text{in } \mathcal{D}', \tag{84}$$

in the sense that the parametric expansion

$$g(\varepsilon x) \sim \sum_{n=0}^{\infty} \frac{a_n \varepsilon^n x^n}{n!}, \quad \text{as } \varepsilon \rightarrow 0, \tag{85}$$

holds, or, equivalently, that

$$\langle g(\varepsilon x), \phi(x) \rangle \sim \sum_{n=0}^{\infty} \frac{a_n}{n!} \left( \int_{-\infty}^{\infty} x^n \phi(x) dx \right) \varepsilon^n, \tag{86}$$

for each  $\phi \in \mathcal{D}$ .

**Lemma 5.2.** *Let  $g \in \mathcal{S}'$  be such that the distributional values  $g^{(n)}(0) = a_n$ , in  $\mathcal{D}'$ , exist for  $n \in \mathbb{R}$ . Let  $\phi \in \mathcal{S}$  and put  $\Phi(x) = \langle g(tx), \phi(t) \rangle$ . Then  $\Phi \in \mathcal{K}$ .*

*Proof:* Indeed,  $\Phi$  is smooth for  $x \neq 0$ , but since the distributional values  $g^{(n)}(0) = a_n$  exist, it follows that  $\Phi(x) \sim \sum_{n=0}^{\infty} b_n x^n$  as  $x \rightarrow 0$ , where  $b_n = (a_n/n!) \int_{-\infty}^{\infty} x^n \phi(x) dx$ . Thus  $\Phi$  is also smooth at  $x = 0$ . Finally, let  $\alpha$  be as in (76); then  $\Phi^{(n)}(x) = O(|x|^{\alpha-n})$  as  $|x| \rightarrow \infty$ . Hence  $\Phi \in \mathcal{K}$ .  $\diamond$

Using this lemma we can give the following

**Definition.** Let  $f \in \mathcal{K}'$ . Let  $g \in \mathcal{S}'$  have distributional values  $g^{(n)}(0)$ ,  $n \in \mathbb{R}$ . Then we can define the tempered distribution

$$G(t) = \langle f(x), g(tx) \rangle \quad (87)$$

by

$$\langle G(t), \phi(t) \rangle = \langle f(x), \Phi(x) \rangle, \quad (88)$$

where

$$\Phi(x) = \langle g(tx), \phi(t) \rangle, \quad (89)$$

if  $\phi \in \mathcal{S}$ .

In general the distribution  $G(t)$  is not smooth near the origin, but its distributional behavior can be obtained from the moment asymptotic expansion.

**Theorem 5.1.** Let  $f \in \mathcal{K}'$  with moments  $\mu_n = \langle f(x), x^n \rangle$ . Let  $g \in \mathcal{S}'$  have distributional values  $g^{(n)}(0)$  for  $n \in \mathbb{R}$ . Then the tempered distribution  $G(t) = \langle f(x), g(tx) \rangle$  has distributional values  $G^{(n)}(0)$ ,  $n \in \mathbb{R}$ , which are given by  $G^{(n)}(0) = \mu_n g^{(n)}(0)$ , and  $G$  has the distributional expansion

$$G(t) \sim \sum_{n=0}^{\infty} \frac{\mu_n g^{(n)}(0) t^n}{n!}, \quad \text{in } \mathcal{D}', \quad \text{as } t \rightarrow 0. \quad (90)$$

*Proof:* Let  $\phi \in \mathcal{S}$  and let  $\Phi(x) = \langle g(tx), \phi(t) \rangle$ . Then

$$\langle G(\varepsilon t), \phi(t) \rangle = \langle f(x), \Phi(\varepsilon x) \rangle, \quad (91)$$

and since  $\Phi^{(n)}(0) = g^{(n)}(0) \int_{-\infty}^{\infty} t^n \phi(t) dt$ , the moment asymptotic expansion yields

$$\langle G(\varepsilon t), \phi(t) \rangle \sim \sum_{n=0}^{\infty} \frac{\mu_n g^{(n)}(0)}{n!} \left( \int_{-\infty}^{\infty} t^n \phi(t) dt \right) \varepsilon^n \quad \text{as } \varepsilon \rightarrow 0, \quad (92)$$

and (90) follows.  $\diamond$

Before we continue, it is worthwhile to give some examples.

**Example.** Let  $g \in \mathcal{S}'$  be such that the distributional values  $g^{(n)}(0)$  exist for  $n \in \mathbb{R}$ . Since the Fourier transform  $\hat{g}(\lambda)$  can be written as  $\hat{g}(\lambda) = \lambda^{-1} \langle e^{ix}, g(\lambda^{-1}x) \rangle$ , and since all the moments  $\mu_n = \langle e^{ix}, x^n \rangle$  vanish, it follows that  $\hat{g}(\varepsilon^{-1}) = O(\varepsilon^\infty)$  distributionally as  $\varepsilon \rightarrow 0$  and thus  $\hat{g}(\lambda) = O(|\lambda|^{-\infty})$  ( $C$ ) as  $|\lambda| \rightarrow \infty$ . Therefore  $\hat{g} \in \mathcal{K}'$ .

Conversely, if  $f \in \mathcal{K}'$ , then its Fourier transform  $\hat{f}(t)$  is equal to  $F(t) = \langle f(x), e^{itx} \rangle$  for  $t \neq 0$ . Thus  $\hat{f}(t) = F(t) + \sum_{j=0}^n a_j \delta^{(j)}(t)$  for some constants  $a_0, \dots, a_n$ . But the distributional values  $F^{(n)}(0)$  exist for  $n \in \mathbb{R}$  and are given by  $F^{(n)}(0) = i^n \langle f(x), x^n \rangle$ , and hence  $\hat{F} \in \mathcal{K}'$ , and it follows that  $a_0 = \dots = a_n = 0$ . In summary,  $\hat{f}^{(n)}(0)$  exists in  $\mathcal{D}'$  for each  $n \in \mathbb{R}$ .

Therefore, a distribution  $g \in \mathcal{S}'$  is smooth at the origin in the distributional sense (that is, the distributional values  $g^{(n)}(0)$  exist for  $n \in \mathbb{R}$ ) if and only if its Fourier transform  $\hat{g}$  is distributionally small (i.e.,  $\hat{g} \in \mathcal{K}'$ ).  $\diamond$

**Example.** Let  $\xi \in \mathbb{C}$  with  $|\xi| = 1$ ,  $\xi \neq 1$ . Then the distribution  $f(x) = \sum_{n=-\infty}^{\infty} \xi^n \delta(x-n)$  belongs to  $\mathcal{K}'$ . All its moments vanish:  $\mu_k = \sum_{n=-\infty}^{\infty} \xi^n n^k = 0$  ( $C$ ) for  $k = 0, 1, 2, \dots$ . It follows that if  $g \in \mathcal{S}'$  is distributionally smooth at the origin, then

$$\sum_{n=-\infty}^{\infty} \xi^n g(nx) = o(x^\infty) \quad \text{in } \mathcal{D}' \quad \text{as } x \rightarrow 0. \tag{93}$$

When  $\xi = 1$ ,  $\sum_{n=-\infty}^{\infty} \delta(x-n)$  does not belong to  $\mathcal{K}'$  but  $\sum_{n=-\infty}^{\infty} \delta(x-n) - 1$  does. Thus, if  $g \in \mathcal{S}'$  is distributionally smooth at the origin and  $\int_{-\infty}^{\infty} g(u) du$  is defined, then

$$\sum_{n=-\infty}^{\infty} g(nx) = \left( \int_{-\infty}^{\infty} g(u) du \right) x^{-1} + o(x^\infty) \quad \text{in } \mathcal{D}' \quad \text{as } x \rightarrow 0. \tag{94}$$

Actually, many number-theoretical expansions considered in [7] and Chapter 5 of [12] will hold in the averaged or distributional sense when applied to distributions.  $\diamond$

Many times,  $\text{supp } f \subseteq [0, \infty)$  and one is interested in  $G(t) = \langle f(x), g(tx) \rangle$  for  $t > 0$  only. In those cases the values of  $g(x)$  for  $x < 0$  are irrelevant and one may assume that  $\text{supp } g \subseteq [0, \infty)$ . Since we need to consider  $\Phi(x) = \langle g(tx), \phi(t) \rangle$  for  $x > 0$  only, we do not require the existence of the distributional values  $g^{(n)}(0)$ ; instead, we assume the existence of the one-sided distributional values  $g^{(n)}(0^+) = a_n$  for  $n \in \mathbb{R}$ . This is equivalent to asking  $g(\varepsilon x)$  to have the asymptotic development

$$g(\varepsilon x) \sim \sum_{n=0}^{\infty} \frac{a_n \varepsilon^n x_+^n}{n!} \quad \text{as } \varepsilon \rightarrow 0^+; \tag{95}$$

that is,

$$\langle g(\varepsilon x), \phi(x) \rangle \sim \sum_{n=0}^{\infty} \frac{a_n}{n!} \left( \int_0^\infty x^n \phi(x) dx \right) \varepsilon^n \quad \text{as } \varepsilon \rightarrow 0^+ \tag{96}$$

for  $\phi \in \mathcal{S}$ . We shall use the notation

$$g(x) \sim \sum_{n=0}^{\infty} \frac{a_n x^n}{n!} \quad \text{in } \mathcal{D}' \quad \text{as } x \rightarrow 0^+ \tag{97}$$

in such a case.

**Lemma 5.3.** *Let  $g \in \mathcal{S}'$  with  $\text{supp } g \subseteq [0, \infty)$  and let  $g^{(n)}(0^+) = a_n$  exist in  $\mathcal{D}'$  for  $n \in \mathbb{R}$ . Let  $\phi \in \mathcal{S}$  and put  $\Phi(x) = \langle g(tx), \phi(t) \rangle$  for  $x > 0$ . Then  $\Phi$  admits extensions  $\tilde{\Phi}$  to  $\mathbb{R}$  with  $\tilde{\Phi} \in \mathcal{K}(\mathbb{R})$ .*

*Proof:* It suffices to show that  $\Phi$  is smooth up to the origin from the right and that it satisfies estimates of the form  $\Phi^{(j)}(x) = O(|x|^{\alpha-n})$  as  $|x| \rightarrow \infty$ . But the first statement follows because  $g^{(n)}(0^+)$  exists for all  $n \in \mathbb{R}$ , while the latter is true because of (76).  $\diamond$

From this lemma it follows that when  $f \in \mathcal{K}'$ ,  $\text{supp } f \subseteq [0, \infty)$ ,  $\text{supp } g \subseteq [0, \infty)$ , and the distributional values  $g^{(n)}(0^+)$  exist for  $n \in \mathbb{R}$ , then  $G(t) = \langle f(x), g(tx) \rangle$  can be defined as a tempered distribution with support contained in  $[0, \infty)$  by

$$\langle G(t), \phi(t) \rangle = \langle f(x), \tilde{\Phi}(x) \rangle, \quad (98)$$

where  $\tilde{\Phi}$  is any extension of  $\Phi(x) = \langle g(tx), \phi(t) \rangle$ ,  $x > 0$ , such that  $\tilde{\Phi} \in \mathcal{K}$ .

**Theorem 5.2.** *Let  $f \in \mathcal{K}'$  with  $\text{supp } f \subseteq [0, \infty)$  and moments  $\mu_n = \langle f(x), x^n \rangle$ . Let  $g \in \mathcal{S}'$  with  $\text{supp } g \subseteq [0, \infty)$  have distributional one-sided values  $g^{(n)}(0^+)$  for  $n \in \mathbb{R}$ . Then the tempered distribution  $G(t) = \langle f(t), g(tx) \rangle$  defined by (98) has distributional one-sided values  $G^{(n)}(0^+)$ ,  $n \in \mathbb{R}$ , which are given by  $G^{(n)}(0^+) = \mu_n g^{(n)}(0^+)$ , and  $G$  has the distributional expansion*

$$G(t) \sim \sum_{n=0}^{\infty} \frac{\mu_n g^{(n)}(0^+) t^n}{n!} \quad \text{in } \mathcal{D}' \quad \text{as } t \rightarrow 0^+. \quad (99)$$

*Proof:* Quite similar to the proof of Theorem 5.1.  $\diamond$

## 6 Expansion of Green kernels I: Local expansions

In this section we shall consider the small- $t$  behavior of Green kernels of the type  $G(t; x, y) = \langle e(x, y; \lambda), g(\lambda t) \rangle$  for some  $g \in \mathcal{S}'$ . Here  $e(x, y; \lambda)$  is the spectral density kernel corresponding to a positive elliptic operator  $H$  that acts on the smooth manifold  $\mathcal{M}$ .

Our results can be formulated in a general framework. So, let  $H$  be a positive self-adjoint operator on the domain  $\mathcal{X}$  of the Hilbert space  $\mathcal{H}$ . Let  $\mathcal{X}_\infty$  be the common domain of  $H^n$ ,  $n \in \mathbb{R}$ , and let  $e_\lambda$  be the associated spectral density. Let  $g \in \mathcal{S}'$  with  $\text{supp } g \subseteq [0, \infty)$  such that the one-sided distributional values  $a_n = g^{(n)}(0^+)$  exist for  $n \in \mathbb{R}$ . Then we can define

$$G(t) = g(tH), \quad t > 0, \quad (100)$$

that is,

$$G(t) = \langle e_\lambda, g(t\lambda) \rangle, \quad t > 0. \quad (101)$$

Hence,  $G$  can be considered as an operator-valued distribution in the space  $\mathcal{S}'(\mathbb{R}, L(\mathcal{X}_\infty, \mathcal{H}))$ . The behavior of  $G(t)$  as  $t \rightarrow 0^+$  can be obtained from the moment asymptotic expansion (27) for  $e_\lambda$ . The expansion of  $G(t)$  as  $t \rightarrow 0^+$  will be a distributional or ‘‘averaged’’ expansion, in general, but when  $g$  has the behavior of the elements of  $\mathcal{K}$  at  $\infty$  it becomes a pointwise expansion. In

particular, if  $g$  is smooth in  $[0, \infty)$ , the expansion is pointwise or not depending on the behavior of  $g$  at infinity.

**Theorem 6.1.** *Let  $H$  be a positive self-adjoint operator on the domain  $\mathcal{X}$  of the Hilbert space  $\mathcal{H}$ . Let  $\mathcal{X}_\infty$  be the intersection of the domains of  $H^n$  for  $n \in \mathbb{R}$ . Let  $g \in \mathcal{S}'$  with  $\text{supp } g \subseteq [0, \infty)$  be such that the distributional one-sided values*

$$g^{(n)}(0^+) = a_n \quad \text{in } \mathcal{D}' \quad (102)$$

*exist for  $n \in \mathbb{R}$ . Let  $G(t) = g(tH)$ , an element of  $\mathcal{S}'(\mathbb{R}, L(\mathcal{X}_\infty, \mathcal{H}))$  with support contained in  $[0, \infty)$ . Then  $G(t)$  admits the distributional expansion in  $L(\mathcal{X}_\infty, \mathcal{H})$ ,*

$$G(t) \sim \sum_{n=0}^{\infty} \frac{a_n H^n t^n}{n!}, \quad \text{as } t \rightarrow 0^+, \quad \text{in } \mathcal{D}', \quad (103)$$

*so that the distributional one-sided values  $G^{(n)}(0^+)$  exist and are given by*

$$G^{(n)}(0^+) = a_n H^n \quad \text{in } \mathcal{D}'. \quad (104)$$

*When  $g$  admits an extension that belongs to  $\mathcal{K}$ , (103) is an ordinary pointwise expansion while the  $G^{(n)}(0^+)$  exist as ordinary one-sided values.*

*Proof:* Follows immediately from Theorem 5.2.  $\diamond$

When  $H$  is a positive elliptic differential operator acting on the manifold  $\mathcal{M}$ , then Theorem 6.1 gives the small- $t$  expansion of Green kernels. Let  $e(x, y; \lambda)$  be the spectral density kernel and let

$$G(t, x, y) = \langle e(x, y; \lambda), g(t\lambda) \rangle, \quad t > 0, \quad (105)$$

be the Green function kernel corresponding to the operator  $G(t) = g(tH)$ . Then  $G$  belongs to  $\mathcal{S}'(\mathbb{R}) \hat{\otimes} \mathcal{D}'(\mathcal{M} \times \mathcal{M})$ , has spectrum in  $[0, \infty)$ , and as  $t \rightarrow 0^+$  admits the distributional expansion

$$G(t, x, y) \sim \sum_{n=0}^{\infty} \frac{a_n H^n \delta(x-y) t^n}{n!}, \quad \text{as } t \rightarrow 0^+, \quad \text{in } \mathcal{D}'; \quad (106)$$

that is,

$$G(\varepsilon t, x, y) \sim \sum_{n=0}^{\infty} \frac{a_n H^n \delta(x-y) \varepsilon^n t_+^n}{n!} \quad \text{as } \varepsilon \rightarrow 0^+, \quad (107)$$

in  $\mathcal{D}'(\mathcal{M} \times \mathcal{M})$ . Also, the distributional one-sided values  $\frac{\partial^n}{\partial t^n} G(0^+, x, y)$  exist for  $n \in \mathbb{R}$  and are given by

$$\frac{\partial^n}{\partial t^n} G(0^+, x, y) = a_n H^n \delta(x-y) \quad \text{in } \mathcal{D}'. \quad (108)$$

If  $g$  admits extension to  $\mathcal{K}$ , then (106) and (108) are valid in the ordinary pointwise sense with respect to  $t$  (and distributionally in  $(x, y)$ ).

Pointwise expansions in  $(x, y)$  follow when  $x \neq y$ . Indeed, if  $U$  and  $V$  are open subsets of  $\mathcal{M}$  with  $U \cap V = \emptyset$ , then  $G$  belongs to  $\mathcal{S}'(\mathbb{R}) \hat{\otimes} \mathcal{E}(U \times V)$  and as  $t \rightarrow 0^+$  we have the distributional expansion

$$G(t, x, y) = o(t^\infty), \quad \text{in } \mathcal{D}', \quad \text{as } t \rightarrow 0^+, \quad (109)$$

in  $\mathcal{E}(U \times V)$ , and in particular pointwise on  $x \in U$  and  $y \in V$ . The expansion becomes pointwise in  $t$  when  $g$  admits an extension to  $\mathcal{K}$ .

These expansions depend only on the local behavior of the differential operator. Let  $H_1$  and  $H_2$  be two differential operators that coincide on the open subset  $U$  of  $\mathcal{M}$ . Let  $e_1(x, y, \lambda)$ ,  $e_2(x, y, \lambda)$  be the corresponding spectral densities and  $G_1(t, x, y)$  and  $G_2(t, x, y)$  the corresponding kernels for the operators  $g(tH_1)$  and  $g(tH_2)$ , respectively. Then

$$G_1(t, x, y) = G_2(t, x, y) + o(t^\infty), \quad \text{in } \mathcal{D}', \quad \text{as } t \rightarrow 0^+, \quad (110)$$

in  $\mathcal{E}(U \times U)$ ; and when  $g$  admits an extension that belongs to  $\mathcal{K}$  this also holds pointwise in  $t$ .

Let us consider some illustrations.

**Example.** Let  $K(t, x, y) = \langle e(x, y; \lambda), e^{-\lambda t} \rangle$  be the heat kernel, corresponding to the operator  $K(t) = e^{-tH}$ , so that

$$\frac{\partial K}{\partial t} = -HK, \quad t > 0, \quad (111)$$

and

$$K(0^+, x, y) = \delta(x - y). \quad (112)$$

In this case  $g(t) = \chi(t)e^{-t}$  admits extensions in  $\mathcal{K}$ . Thus the expansions

$$K(t, x, y) \sim \sum_{n=0}^{\infty} \frac{(-1)^n H^n \delta(x - y) t^n}{n!} \quad \text{as } t \rightarrow 0^+ \quad (113)$$

in the space  $\mathcal{D}'(\mathcal{M} \times \mathcal{M})$ , and

$$K(t, x, y) = o(t^\infty) \quad \text{as } t \rightarrow 0^+, \quad \text{with } x \neq y, \quad (114)$$

hold *pointwise* in  $t$ .  $\diamond$

**Example.** Let  $U(t, x, y) = \langle e(x, y; \lambda), e^{-i\lambda t} \rangle$  be the Schrödinger kernel, corresponding to  $U(t) = e^{-itH}$ , so that

$$i \frac{\partial U}{\partial t} = HU, \quad t > 0 \quad (115)$$

and

$$U(0^+, x, y) = \delta(x - y). \quad (116)$$

Here the function  $e^{-it}$  belongs to  $\mathcal{S}'$  but not to  $\mathcal{K}$ . Therefore, the expansions

$$U(t, x, y) \sim \sum_{n=0}^{\infty} \frac{(-i)^n H^n \delta(x - y) t^n}{n!}, \quad \text{as } t \rightarrow 0^+, \quad \text{in } \mathcal{D}', \quad (117)$$



and

$$U(t, x, y) = o(t^\infty), \quad \text{in } \mathcal{D}', \quad \text{as } t \rightarrow 0^+ \quad \text{with } x \neq y, \quad (118)$$

are distributional or “averaged” in  $t$ .

Consider, for instance,  $U(t, x, y) = (4\pi t)^{-n/2} e^{i|x-y|^2/4t}$ , corresponding to the case when  $H$  is the negative Laplacian,  $-\Delta$ , acting on  $\mathcal{M} = \mathbb{R}^n$ . If  $x \neq y$  are fixed,  $U(t, x, y)$  oscillates as  $t \rightarrow 0^+$ , but (118) holds in the distributional sense. (This also follows from the results of [9], because  $\lim_{s \rightarrow \infty} e^{ias} = 0$  ( $C$ ) if  $a \neq 0$ .)

Notice that it also follows that if  $U_1$  is the Schrödinger kernel associated to  $-\Delta$  in any open subset  $\mathcal{M}$  of  $\mathbb{R}^n$  with boundary conditions that make the operator positive and self-adjoint, then

$$U_1(t, x, y) = (4\pi t)^{-n/2} e^{i|x-y|^2/4t} + o(t^\infty), \quad \text{in } \mathcal{D}', \quad \text{as } t \rightarrow 0^+, \quad (119)$$

uniformly and strongly on compacts of  $\mathcal{M}$ . In particular,

$$U_1(t, x, x) = (4\pi t)^{-n/2} + o(t^\infty), \quad \text{in } \mathcal{D}', \quad \text{as } t \rightarrow 0^+, \quad (120)$$

uniformly and strongly on compacts of  $\mathcal{M}$ . (We reiterate that this holds in the interior of  $\mathcal{M}$  only.)  $\diamond$

Apart from (120) we have had little to say in this section about the much-studied *diagonal* expansions of the heat and Schrödinger kernels. See, however, [10], where the methods of this paper are applied in that arena.

## 7 Expansion of Green kernels II: Global expansions

When considering a second-order differential operator on a one-dimensional manifold, the variable  $\lambda$  of the spectral density  $e(x, y; \lambda)$  is often replaced by the variable  $\omega$  defined by  $\omega^2 = \lambda$ . For instance, the asymptotic behavior of  $\omega_n = \lambda_n^{1/2}$ , the square root of the  $n$ th eigenvalue, has a more convenient form than that for  $\lambda_n$  in the case of regular Sturm–Liouville equations. But, does this change of variable have any effect on the expansion of the associated Green kernels?

Consider, for instance, the behavior of the kernel

$$e(x, y; \lambda) = \frac{2}{\pi} \sum_{n=1}^{\infty} \sin nx \sin ny \delta(\lambda - n^2), \quad (121)$$

which we studied before. Let  $\omega^2 = \lambda$ , and consider the kernel  $\tilde{e}(x, y; \omega)$  given by

$$\tilde{e}(x, y; \omega) = 2\omega e(x, y; \omega^2) = \frac{2}{\pi} \sum_{n=1}^{\infty} \sin nx \sin ny \delta(\omega - n). \quad (122)$$

The behavior of  $\tilde{e}(x, y; \omega)$  at infinity can be obtained by studying the parametric behavior, i.e.,  $\tilde{e}(x, y; \sigma\omega)$  as  $\sigma \rightarrow \infty$ . Letting  $\varepsilon = 1/\sigma$ , we are led to consider the development of

$$\frac{2}{\pi} \sum_{n=1}^{\infty} \sin nx \sin ny \phi(\varepsilon n) = \langle \tilde{e}(x, y; \omega), \phi(\varepsilon\omega) \rangle_{\omega} \quad (123)$$

as  $\varepsilon \rightarrow 0^+$ . The even moments of  $\tilde{e}$  coincide with those of  $e$  of half the order; i.e.,

$$\langle \tilde{e}(x, y; \omega), \omega^{2k} \rangle = \delta^{(2k)}(x - y). \quad (124)$$

But we also have to consider odd-order moments, such as

$$J(x, y) = \langle \tilde{e}(x, y; \omega), \omega \rangle = \frac{2}{\pi} \sum_{n=1}^{\infty} n \sin nx \sin ny. \quad (125)$$

The operator corresponding to  $J$  is not the derivative  $d/dx$ , but rather  $(d/dx)Q$ , where  $Q$  is a Hilbert transform. Thus,  $J$  is not a local operator: in general  $\text{supp } J(\phi)$  is not contained in  $\text{supp } \phi$ . Thus, the expansion

$$\tilde{e}(x, y; \sigma\omega) \sim \frac{\delta(x - y)\delta(\omega)}{\sigma} - \frac{J(x, y)\delta'(\omega)}{\sigma^2} + \frac{\delta''(x - y)\delta''(\omega)}{2\sigma^3} - \dots \quad (126)$$

has a nonlocal character: The expansion of  $\langle \tilde{e}(x, y; \sigma\omega), f(y) \rangle$  as  $\sigma \rightarrow \infty$  may have nonzero contributions outside of  $\text{supp } f$ .

The change of variable  $\omega^2 = \lambda$ , which seems so innocent, has introduced a new phenomenon into the expansion of the spectral density: the appearance of nonlocal terms. This will also apply to the expansion of the corresponding Green kernels. Consider the expansion of the cylinder kernel (A9b)

$$T(t, x, y) = \frac{t}{\pi((x - y)^2 + t^2)}. \quad (127)$$

We have

$$\frac{t}{\pi((x - y)^2 + t^2)} \sim \delta(x - y) + \frac{t}{\pi(x - y)^2} - \frac{\delta''(x - y)t^2}{2} + \frac{t^3}{\pi(x - y)^3} + \dots \quad (128)$$

as  $t \rightarrow 0^+$ , which is a nonlocal expansion because the odd-order terms are nonlocal. In particular, the expansion does not vanish when  $x \neq y$ .

Why? Why do the results of the previous section fail? The operator corresponding to (127) is  $e^{-tH^{1/2}}$ , where  $H = -d^2/dx^2$  on  $\mathbb{R}$ . Thus, we arrive at the same question: How does the change  $\lambda \mapsto \lambda^{1/2} = \omega$  affect our results? However, the answer is now clearer:  $H^{1/2}$  is a *nonlocal* pseudodifferential operator, and  $J(x, y)$  is simply its kernel. The nonlocality of the odd-order moments just reflects the fact that the basic operator  $H^{1/2}$  is not local.

The behavior of summability after changes of variables was already studied at the beginning of the century by Hardy [24, 26] and is the central theme in [17].

When using the distributional approach, we can see that the change  $\omega = \lambda^{1/2}$ , and similar ones, do not introduce problems at infinity. Rather, the point is that the change introduces a new structure at the origin.

Let  $f \in \mathcal{D}'$  have  $\text{supp } f \subseteq (0, \infty)$ . Then  $f(\omega^2)$  is a well-defined distribution, given by

$$\langle f(\omega^2), \phi(\omega) \rangle = \frac{1}{2} \langle f(\lambda), \lambda^{-1/2} \phi(\lambda^{1/2}) \rangle. \quad (129)$$

When  $0 \in \text{supp } f$ , however, there is no canonical way to define  $f(\omega^2)$ . That there are no problems at infinity follows from the results of [9].

**Lemma 7.1.** *Let  $f$  be in  $\mathcal{D}'(\mathbb{R})$  with  $\text{supp } f \subseteq (0, \infty)$ . Then  $f$  is distributionally small at infinity if and only if  $f(\omega^2)$  is.*

*Proof:* The generalized function  $f$  is distributionally small at infinity if and only if it belongs to  $\mathcal{K}'$ . Thus it suffices to see that  $f(\lambda)$  belongs to  $\mathcal{K}'$  if and only if  $f(\omega^2)$  does, and, by duality, it suffices to see that if  $\text{supp } \phi \subseteq (0, \infty)$  then  $\phi(\omega)$  belongs to  $\mathcal{K}$  if and only if  $\lambda^{-1/2} \phi(\lambda^{1/2})$  does.  $\diamond$

Therefore, if  $e(x, y; \lambda)$  is the spectral density kernel corresponding to a positive self-adjoint operator  $H$ , then  $e(x, y; \omega^2)$  is also distributionally small as a function of  $\omega$ , both distributionally and pointwise on  $x \neq y$ . However, as we have seen, the corresponding moment expansion for  $e(x, y; \omega^2)$  will contain extra terms. These arise as a special case of a general theorem that extends the conclusions of Sections 5 and 6 to the situation where the function or distribution  $g$  does not have a Taylor expansion at the origin.

The spaces  $\mathcal{A}\{\phi_n\}$  associated to an asymptotic sequence are discussed in Refs. [11, 12]. In particular, if  $\alpha_n$  is a sequence with  $\Re \alpha_n \nearrow \infty$ , then the space  $\mathcal{K}\{x^{\alpha_n}\}$  consists of those smooth functions  $\phi$  defined on  $(0, \infty)$  that have the behavior of the space  $\mathcal{K}$  at infinity but at the origin can be developed in a strong expansion

$$\phi(x) \sim a_1 x^{\alpha_1} + a_2 x^{\alpha_2} + a_3 x^{\alpha_3} + \cdots \quad \text{as } x \rightarrow 0^+. \quad (130)$$

The point is that the  $\alpha_n$  need not be nonnegative integers.

The functionals  $\delta_j \in \mathcal{K}'\{x^{\alpha_n}\}$  given by

$$\langle \delta_j(x), \phi(x) \rangle = a_j \quad (131)$$

play the role of the traditional delta functions. Each  $f \in \mathcal{K}'\{x^{\alpha_n}\}$  admits a generalized moment asymptotic expansion,

$$f(\lambda x) \sim \sum_{j=1}^{\infty} \frac{\mu(\alpha_j) \delta_j(x)}{\lambda^{\alpha_j+1}} \quad \text{as } \lambda \rightarrow \infty, \quad (132)$$

where  $\mu(\alpha_j) = \langle f(x), x^{\alpha_j} \rangle$  are the moments. Therefore, if  $g \in \mathcal{K}\{x^{\alpha_n}\}$  then the expansion of  $G(t) = \langle f(x), g(tx) \rangle$  can be obtained from (132) as

$$G(t) \sim \sum_{j=1}^{\infty} \mu(\alpha_j) a_j t^{\alpha_j} \quad \text{as } t \rightarrow 0^+, \quad (133)$$

where  $a_j = \langle \delta_j(x), g(x) \rangle$ . But following the ideas of Section 5 we can define  $G(t) = \langle f(x), g(tx) \rangle$  when  $g$  is a distribution of  $\mathcal{S}'$  with  $\text{supp } g \subseteq [0, \infty)$ , whose behavior at the origin is of the form

$$g(\varepsilon x) \sim \sum_{j=1}^{\infty} a_j \varepsilon^{\alpha_j} x_+^{\alpha_j} \quad \text{as } \varepsilon \rightarrow 0^+, \quad (134a)$$

a fact that we express by saying that

$$g(x) \sim \sum_{j=1}^{\infty} a_j x^{\alpha_j}, \quad \text{distributionally, as } x \rightarrow 0^+. \quad (134b)$$

Then  $G(t)$  will have the same expansion (133), but in the average or distributional sense. A corresponding result for operators also holds.

**Theorem 7.1.** *Let  $H$  be a positive self-adjoint operator on the domain  $\mathcal{X}$  of the Hilbert space  $\mathcal{H}$ . Let  $\mathcal{X}_\infty$  be the intersection of the domains of  $H^n$  for  $n \in \mathbb{R}$ . Let  $g \in \mathcal{S}'$  with  $\text{supp } g \subseteq [0, \infty)$  have a distributional expansion of the type  $g(x) \sim \sum_{j=1}^{\infty} a_j x^{\alpha_j}$  as  $x \rightarrow 0^+$ , where  $\Re \alpha_n \nearrow \infty$ . Then  $G(t) = g(tH)$  can be defined as an element of  $\mathcal{S}'(\mathbb{R}, L(\mathcal{X}_\infty, \mathcal{H}))$  with support contained in  $[0, \infty)$ , and  $G(t)$  admits the distributional expansion*

$$G(t) \sim \sum_{j=1}^{\infty} a_j H^{\alpha_j} t^{\alpha_j}, \quad \text{as } t \rightarrow 0^+, \quad \text{in } \mathcal{D}'. \quad (135)$$

When  $g$  belongs to  $\mathcal{K}\{x^{\alpha_n}\}$ , (135) becomes a pointwise expansion.  $\diamond$

Therefore, we may generalize our previous discussion as follows: *If  $H$  is a differential operator, then the expansion of the Green function of  $g(tH)$  is local or global depending on whether the expansion (134) of  $g$  at the origin is of the Taylor-series type or not.*

**Example.** The small- $t$  expansion of the cylinder function  $T(t, x, y)$  described in (A3) is given by

$$T(t, x, y) \sim \sum_{n=0}^{\infty} \frac{(-1)^n H_x^{n/2} (\delta(x-y)) t^n}{n!} \quad \text{as } t \rightarrow 0^+. \quad (136)$$

The expansion is pointwise in  $t$  and distributional in  $(x, y)$ . The expansion is also pointwise in  $t$  for  $x \neq y$ , but we do not get  $T(t, x, y) = o(t^\infty)$  because the odd terms in the expansion do not vanish for  $x \neq y$ . This type of behavior is typical of harmonic functions near boundaries.  $\diamond$

We may look at the locality problem from a different perspective. Suppose  $H_1$  and  $H_2$  are two different self-adjoint extensions of the same differential operator on a subset  $U$  of  $\mathcal{M}$ . Then the two cylinder kernels  $T_1(t, x, y)$  and  $T_2(t, x, y)$  have different expansions as  $t \rightarrow 0^+$  even if  $(x, y) \in U \times U$ . The same is true of the associated Wightman functions. In both cases the small- $t$

expansion of the Green kernel reflects some global properties of the operators  $H_1$  and  $H_2$ . Since the cylinder and Wightman functions are constructed from the operators  $H_1^{1/2}$  and  $H_2^{1/2}$ , one may ask if this nonlocal character can already be observed in the spectral densities  $e_{H_j^{1/2}}(x, y; \lambda)$ ,  $j = 1, 2$ . Interestingly, the nonlocal character cannot be seen in the Cesàro behavior, since according to Theorem 7.2 below we have

$$e_{H_1^{1/2}}(x, y; \lambda) = e_{H_2^{1/2}}(x, y; \lambda) + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty, \quad (137)$$

for  $(x, y) \in U \times U$ . Instead, the nonlocal character of the small- $t$  expansion of the Green kernels is explained by the difference in the moments. (Recall Theorem 2.1 and the formula (14).)

We finish by giving a result that justifies (137) and also has an interest of its own.

**Theorem 7.2.** *Let  $H_1$  and  $H_2$  be two pseudodifferential operators acting on the manifold  $\mathcal{M}$ , with spectral densities  $e_j(x, y; \lambda)$  for  $j = 1, 2$ . Let  $U$  be an open set of  $\mathcal{M}$  and suppose that  $H_1 - H_2$  is a smoothing operator in  $U$ . Then*

$$e_1(x, y; \lambda) = e_2(x, y; \lambda) + o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty, \quad (138)$$

in the topology of the space  $\mathcal{E}(U \times U)$  and, in particular, pointwise on  $(x, y) \in U \times U$ .

*Proof:* If  $\phi \in \mathcal{D}(\mathbb{R})$ , then  $\phi(H_1) - \phi(H_2)$  is a smoothing operator, thus  $\langle e_1(x, y; \lambda) - e_2(x, y; \lambda), f(x)g(y) \rangle$  is a well-defined element of  $\mathcal{D}'(\mathbb{R})$  given by

$$\langle \langle e_1(x, y; \lambda) - e_2(x, y; \lambda), f(x)g(y) \rangle, \phi(\lambda) \rangle = \langle (\phi(H_1) - \phi(H_2))f, g \rangle. \quad (139)$$

In general this generalized function is not a distributionally small function of  $\lambda$ , but if  $\text{supp } f \subset U$  and  $\text{supp } g \subset U$  then all the moments

$$\langle \langle e_1(x, y; \lambda) - e_2(x, y; \lambda), f(x)g(y) \rangle, \lambda^n \rangle = \langle (H_1^n - H_2^n)f, g \rangle \quad (140)$$

exist because  $H_1 - H_2$  is smoothing in  $U$ . Therefore,

$$\langle e_1(x, y; \lambda) - e_2(x, y; \lambda), f(x)g(y) \rangle$$

belongs to  $\mathcal{K}'(\mathbb{R})$ ; that is, it is a distributionally small function. Hence,

$$\langle e_1(x, y; \lambda) - e_2(x, y; \lambda), f(x)g(y) \rangle = o(\lambda^{-\infty}) \quad (C) \quad \text{as } \lambda \rightarrow \infty \quad (141)$$

for each  $f, g \in \mathcal{E}'(U)$ , and (138) follows by duality.  $\diamond$

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## Appendix: The simplest one-dimensional examples

Let  $H$  be a positive, self-adjoint, second-order linear differential operator on scalar functions, on a manifold or region  $\mathcal{M}$ . We are concerned with distributions of the type  $G(t, x, y)$  ( $t \in \mathbb{R}$ ,  $x \in \mathcal{M}$ ,  $y \in \mathcal{M}$ ) that are integral kernels of parametrized operator-valued functions of  $H$ . In particular:

(1) The *heat kernel*,  $K(t, x, y)$ , represents the operator  $e^{-tH}$ , which solves the heat equation

$$-\frac{\partial \Psi}{\partial t} = H\Psi, \quad \lim_{t \downarrow 0} \Psi(t, x) = f(x), \quad (\text{A1})$$

for  $(t, x) \in (0, \infty) \times \mathcal{M}$ , by  $\Psi(t, x) = e^{-tH}f(x)$ .

(2) The *Schrödinger propagator*,  $U(t, x, y)$ , is the kernel of  $e^{-itH}$ , which solves the Schrödinger equation

$$i\frac{\partial \Psi}{\partial t} = H\Psi, \quad \lim_{t \rightarrow 0} \Psi(t, x) = f(x), \quad (\text{A2})$$

for  $(t, x) \in \mathbb{R} \times \mathcal{M}$ , by  $\Psi(t, x) = e^{-itH}f(x)$ .

(3) Let  $T(t, x, y)$  be the integral kernel of the operator  $e^{-t\sqrt{H}}$ , which solves the elliptic equation

$$-\frac{\partial^2 \Psi}{\partial t^2} + H\Psi = 0, \quad \lim_{t \downarrow 0} \Psi(t, x) = f(x), \quad \lim_{t \rightarrow +\infty} \Psi(t, x) = 0, \quad (\text{A3})$$

in the infinite half-cylinder  $(0, \infty) \times \mathcal{M}$ , by  $\Psi(t, x) = e^{-t\sqrt{H}}f(x)$ . We shall call this the *cylinder kernel* of  $H$ . It may also be regarded as the heat kernel of the first-order pseudodifferential operator  $\sqrt{H}$ .

(4) The *Wightman function*,  $W(t, x, y)$ , is the kernel of  $(2\sqrt{H})^{-1}e^{-it\sqrt{H}}$ . This operator solves the wave equation

$$-\frac{\partial^2 \Psi}{\partial t^2} = H\Psi \quad (\text{A4})$$

with the nonlocal initial data

$$\lim_{t \downarrow 0} \Psi(t, x) = (2\sqrt{H})^{-1}f(x), \quad \lim_{t \downarrow 0} \frac{\partial \Psi}{\partial t}(t, x) = -\frac{i}{2}f(x). \quad (\text{A5})$$

The significance of  $W$  is that it is the two-point vacuum expectation value of a quantized scalar field satisfying the time-independent, linear field equation (A4):

$$W(t, x, y) = \langle 0 | \phi(t, x) \phi(0, y) | 0 \rangle$$

(e.g., [16], Chapters 3–5).

These four kernels are rather diverse in their asymptotic behavior as  $t$  approaches 0 and also in the convergence properties of their spectral expansions.

Most of the relevant mathematical phenomena that distinguish them can be demonstrated already in the simplest case,

$$H = -\frac{\partial^2}{\partial x^2} \quad (\text{A6})$$

with  $\mathcal{M}$  either  $\mathbb{R}$  or a bounded interval  $(0, \pi)$ . (For other one-dimensional  $\mathcal{M}$  see [17].) We record here the spectral expansion (Fourier transform or series) of each kernel and also its actual functional value (closed form or image sum).

### Case $\mathcal{M} = \mathbb{R}$

*Heat kernel:*

$$K(t, x, y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-y)} e^{-k^2 t} dk. \quad (\text{A7a})$$

$$K(t, x, y) = (4\pi t)^{-1/2} e^{-(x-y)^2/4t}. \quad (\text{A7b})$$

*Schrödinger propagator:*

$$U(t, x, y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-y)} e^{-ik^2 t} dk. \quad (\text{A8a})$$

$$U(t, x, y) = e^{-i(\text{sgn } t)\pi/4} (4\pi t)^{-1/2} e^{i(x-y)^2/4t}. \quad (\text{A8b})$$

*Cylinder kernel:*

$$T(t, x, y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-y)} e^{-|k|t} dk. \quad (\text{A9a})$$

$$T(t, x, y) = \frac{t}{\pi} \frac{1}{(x-y)^2 + t^2}. \quad (\text{A9b})$$

*Wightman function:*

$$W(t, x, y) = \frac{1}{4\pi} \int_{-\infty}^{\infty} e^{ik(x-y)} \frac{e^{-i|k|t}}{|k|} dk. \quad (\text{A10})$$

This integral is divergent at  $k = 0$  and does not make sense even as a distribution except on a restricted class of test functions. This “infrared” problem, which is irrelevant to the main issues of the present paper, disappears when one (1) goes to higher dimension, (2) adds a positive constant (“mass”) to  $H$ , or (3) takes one or more derivatives of  $W$  with respect to any of its variables. Therefore, we do not list an integrated form of (A10). (If we gave one, it would be nonunique and would grow logarithmically in  $(x-y)^2$ , thus being useless for forming an image sum for (A14).) For more information about infrared complications in simple model quantum field theories, see [19] and references therein.

Case  $\mathcal{M} = (0, \pi)$

Heat kernel:

$$K(t, x, y) = \frac{2}{\pi} \sum_{k=1}^{\infty} \sin(kx) \sin(ky) e^{-k^2 t}. \quad (\text{A11a})$$

$$K(t, x, y) = (4\pi t)^{-1/2} \sum_{N=-\infty}^{\infty} \left[ e^{-(x-y-2N\pi)^2/4t} - e^{-(x+y-2N\pi)^2/4t} \right]. \quad (\text{A11b})$$

Schrödinger propagator:

$$U(t, x, y) = \frac{2}{\pi} \sum_{k=1}^{\infty} \sin(kx) \sin(ky) e^{-ik^2 t}. \quad (\text{A12a})$$

$$U(t, x, y) = e^{-i(\operatorname{sgn} t)\pi/4} (4\pi t)^{-1/2} \sum_{N=-\infty}^{\infty} \left[ e^{i(x-y-2N\pi)^2/4t} - e^{i(x+y-2N\pi)^2/4t} \right]. \quad (\text{A12b})$$

Cylinder kernel:

$$T(t, x, y) = \frac{2}{\pi} \sum_{k=1}^{\infty} \sin(kx) \sin(ky) e^{-kt}. \quad (\text{A13a})$$

$$T(t, x, y) = \frac{t}{\pi} \sum_{N=-\infty}^{\infty} \left[ \frac{1}{(x-y-2N\pi)^2 + t^2} - \frac{1}{(x+y-2N\pi)^2 + t^2} \right]. \quad (\text{A13b})$$

In this case a closed form is obtainable:

$$T(t, x, y) = \frac{1}{2\pi} \left[ \frac{\sinh t}{\cosh t - \cos(x-y)} - \frac{\sinh t}{\cosh t - \cos(x+y)} \right]. \quad (\text{A13c})$$

Wightman function:

$$W(t, x, y) = -\frac{1}{\pi} \sum_{k=1}^{\infty} \sin(kx) \sin(ky) \frac{e^{-ikt}}{k}. \quad (\text{A14a})$$

This is expressible in the closed form

$$W(t, x, y) = \frac{1}{4\pi} \ln \left| \frac{\cos t - \cos(x+y)}{\cos t - \cos(x-y)} \right| + \frac{i}{4} P(t, x, y), \quad (\text{A14b})$$

where

$$P(t, x, y) = \begin{cases} -1 & \text{for } 2k\pi - f(x+y) < t < 2k\pi - |x-y|, \\ 0 & \text{for } 2k\pi - |x-y| < t < 2k\pi + |x-y|, \\ 1 & \text{for } 2k\pi + |x-y| < t < 2k\pi + f(x+y), \\ 0 & \text{for } 2k\pi + f(x+y) < t < 2(k+1)\pi - f(x+y), \end{cases} \quad (\text{A15})$$



for  $k \in \mathbb{Z}$ , with

$$f(z) = \begin{cases} z & \text{if } 0 \leq z \leq \pi, \\ 2\pi - z & \text{if } \pi \leq z \leq 2\pi. \end{cases} \quad (\text{A16})$$

( $P$  is essentially the standard Green function for the Dirichlet problem for the wave equation — the d'Alembert solution modified by reflections.)

*Proof of (A13c):* Write (A13a) as

$$-\frac{1}{2\pi} \sum_{k=1}^{\infty} \left[ e^{ik(x+y)-kt} + e^{-ik(x+y)-kt} - e^{ik(x-y)-kt} - e^{-ik(x-y)-kt} \right].$$

Evaluate each sum by the geometric series

$$\sum_{k=1}^{\infty} e^{kz} = \frac{e^z}{1 - e^z}. \quad (\text{A17})$$

Some algebraic reduction yields (A13c).  $\diamond$

*Proof of (A14b):* Start with the well-known dispersion relation

$$\frac{1}{x \pm i0} = \mathcal{P} \frac{1}{x} \mp \pi i \delta(x), \quad (\text{A18})$$

where  $\mathcal{P} \frac{1}{x}$  is a principal-value distribution, whose antiderivative is  $\ln|x| + \text{constant}$ . This generalizes easily to:

**Lemma A.1.** *Let  $F$  be analytic in a region  $\Omega \setminus \{x_1, \dots, x_n\}$ ,  $x_j \in \mathbb{R}$ , where  $\Omega$  intersects  $\mathbb{R}$  on  $(a, b)$  and each  $x_j$  is a simple pole of  $F$  with residue  $\alpha_j$ . Then*

$$F(x - i0) = \mathcal{P}F(x) + \pi i \sum_{j=1}^n \alpha_j \delta(x - x_j). \quad (\text{A19})$$

$\diamond$

To apply this to (A14b), replace  $t$  by  $ib$  in (A13a) and (A13c):

$$\sum_{k=1}^{\infty} \sin(kx) \sin(ky) e^{-ikb} = \frac{i}{4} \left( \frac{\sin b}{\cos b - \cos(x-y)} - \frac{\sin b}{\cos b - \cos(x+y)} \right),$$

for  $\text{Im } b < 0$ . There are poles at  $b = 2k\pi \pm (x-y)$  with residue  $i/4$  and at  $b = 2k\pi \pm (x+y)$  with residue  $-i/4$ . Thus for  $b \in \mathbb{R}$ ,

$$\begin{aligned} & \sum_{k=1}^{\infty} \sin kx \sin ky e^{-ikb} \\ &= \frac{i}{4} \left[ \mathcal{P} \left( \frac{\sin b}{\cos b - \cos(x-y)} - \frac{\sin b}{\cos b - \cos(x+y)} \right) \right. \\ & \quad \left. + \pi i \sum_{k=-\infty}^{\infty} \left( \delta(b - 2k\pi - x + y) + \delta(b - 2k\pi + x - y) \right. \right. \\ & \quad \left. \left. - \delta(b - 2k\pi - x - y) - \delta(b - 2k\pi + x + y) \right) \right]. \end{aligned} \quad (\text{A20})$$

Also, integrating (A13a) and (A13c) and letting  $t \rightarrow 0^+$ , one gets

$$\sum_{k=1}^{\infty} \frac{\sin kx \sin ky}{k} = \frac{1}{4} \ln \left( \frac{1 - \cos(x+y)}{1 - \cos(x-y)} \right). \quad (\text{A21})$$

Therefore, integrating (A20) yields

$$\begin{aligned} & \sum_{k=1}^{\infty} \frac{\sin kx \sin ky e^{-ikt}}{k} \\ &= -i \int_0^t \sum_{k=1}^{\infty} \sin kx \sin ky e^{-ikb} db + \sum_{k=1}^{\infty} \frac{\sin kx \sin ky}{k} \\ &= \frac{1}{4} \int_0^t \mathcal{P} \left( \frac{\sin b}{\cos b - \cos(x-y)} - \frac{\sin b}{\cos b - \cos(x+y)} \right) db \\ & \quad + \frac{1}{4} \ln \left( \frac{1 - \cos(x+y)}{1 - \cos(x-y)} \right) \\ & \quad + \frac{\pi i}{4} \int_0^t \sum_{k=-\infty}^{\infty} \left( \delta(b - 2k\pi - x + y) + \delta(b - 2k\pi + x - y) \right. \\ & \quad \left. - \delta(b - 2k\pi - x - y) - \delta(b - 2k\pi + x + y) \right) db \\ &= \frac{1}{4} \ln \left| \frac{\cos t - \cos(x+y)}{\cos t - \cos(x-y)} \right| + \frac{\pi i}{4} P(t, x, y), \end{aligned}$$

which is (A14b).  $\diamond$

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### Addendum: July 22, 2005.

The two formulas given for the (well known) Green kernel of the time-dependent free Schrödinger equation do not agree with each other nor with the truth.

In equations (119) and (120) and the text paragraph above them, the factor  $(4\pi t)^{-n/2}$  should be  $(4\pi it)^{-n/2}$  with the branch cut for  $(it)^{1/2}$  understood to be the negative real axis.

In equations (A8b) and (A12b) the factor  $(4\pi t)^{-1/2}$  should be  $(4\pi|t|)^{-1/2}$ .  
These transcription errors in no way affect the conclusions of the paper.