HEAT KERNEL-ZETA FUNCTION RELATIONSHIP COMING FROM THE CLASSICAL MOMENT PROBLEM.

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Abstract

By using ideas and strong results borrowed from the classical moment problem, we show how —under very general conditions— a discrete number of values of the spectral zeta function (associated generically with a non-decreasing sequence of numbers, and not necessarily with an operator) yields all the moments corresponding to the density of states, as well as those of the partition function of the sequence (the two basic quantities that are always considered in a quantum mechanical context). This goes beyond the well known expression of the small−t asymptotic expansion of the heat kernel of an operator in terms of zeta function values. The precise result for a given situation depends dramatically on the singularity structure of the zeta function. The different specific situations that can appear are discussed in detail, using seminal results from the zeta function literature. Attention is paid to formulations involving zeta functions with a non-standard pole structure (as those arising in noncommutative theories and others). Finally, some misuses of the classical moment problem are pointed out.
1 Introduction

There are two well known spectral functions associated with a sequence of numbers \( \{e_n\} \) (ordered, non-negative), which in a physical context may correspond to some realistic quantum sequence. By realistic we mean that the energy levels of a quantum system usually have some constraints in its growth, given by Schrödinger’s equation. These two functions are the following.

The trace of the heat kernel, or partition function:

\[
K(t) = \sum_{n=0}^{\infty} e^{-te_n},
\]

and the spectral zeta function

\[
\zeta(s) = \sum_{n=0}^{\infty} e^{-sne_n}.
\]

By simple contour integration it is immediate to show that these two spectral functions are related by a Mellin transformation (up to a gamma function). The relation is:

\[
\zeta(s) = \frac{1}{\Gamma(s)} \int_{0}^{\infty} t^{s-1} K(t) dt = \frac{1}{\Gamma(s)} M[K(t); s]
\]

It follows from its definition that the Mellin transformed, \( M[k(t); s] \), gives all the moments of the function \( K(t) \). In probabilistic terms, it provides all the moments of a random variable whose probability density function is proportional to \( K(t) \). As we will see below, provided some conditions are satisfied, the proportionality constant that normalizes \( K(t) \) (as a probability measure) is given by \( \zeta(1)^{-1} \). The extreme importance of the possibility of normalization of the probability measure will become clear below.

Let us also recall that, in the theory of pseudodifferential operators (ΨDO) the relation between heat kernel and zeta functions is much more profound. Let \( A \) a ΨDO, fulfilling the conditions of existence of a heat kernel and a zeta function (see, e.g., [1]). Its corresponding heat kernel is given by (see, for instance,[2] and references therein)

\[
K_A(t) = \text{Tr} e^{-tA} = \sum_{\lambda \in \text{Spec } A} e^{-t\lambda},
\]

which converges for \( t > 0 \), and where the prime means that the kernel of the operator has been projected out before computing the trace, and the corresponding zeta function (as a Mellin transform)

\[
\zeta_A(s) = \frac{1}{\Gamma(s)} \text{Tr} \int_{0}^{\infty} t^{s-1} e^{-tA} dt.
\]
For \( t \downarrow 0 \), we have the following asymptotic expansion:

\[
K_A(t) \sim \alpha_n(A) + \sum_{n \neq j \geq 0} \alpha_j(A) t^{-s_j} + \sum_{k \geq 1} \beta_k(A) t^k \ln t, \quad t \downarrow 0, \tag{6}
\]

being

\[
\alpha_n(A) = \zeta_A(0), \quad \alpha_j(A) = \Gamma(s_j)\text{Res}_{s=s_j} \zeta_A(s), \quad \text{if } s_j \notin \mathbb{Z} \text{ or } s_j > 0,
\]

\[
\alpha_j(A) = \frac{(-1)^k}{k!} \left[ \text{PP} \zeta_A(-k) + \left(1 + \frac{1}{2} + \cdots + \frac{1}{k} - \gamma\right) \text{Res}_{s=-k} \zeta_A(s) \right],
\]

\[
\beta_k(A) = \frac{(-1)^{k+1}}{k!} \text{Res}_{s=-k} \zeta_A(s),
\]

where PP means the principal part:

\[
\text{PP } \varphi = \lim_{s \to p} \left[ \varphi(s) - \frac{\text{Res}_{s=p} \varphi(s)}{s-p} \right], \tag{7}
\]

a finite number. It turns out that all \( \beta_k = 0 \) if \( A \) is a differential operator. Note that, in the case of a generic \( \Psi \)DO fulfilling the conditions of existence of the zeta function, this one provides the asymptotic expansion \( (t \downarrow 0) \) of the heat kernel of the operator.

The main result we are going to obtain here can be viewed as a sort of complement or completion of the above expansion. Rather than dealing with the asymptotics of the heat kernel we will make use of results known for the classical moment problem in order to gain knowledge of the heat kernel itself, from the behavior of the zeta function. And this, moreover, will not be restricted to a family of differentiable or \( \Psi \)DOs, but will hold in a quite general setting.

Now we comment briefly on some basic issues of the moment problem (for a recent review and further details see [3]). The two fundamental moment problems are the following.

**Problem 1. The Hamburger moment problem.**

Given a sequence of reals \( E_0, E_1, \ldots \), does it exist a measure, \( d\rho \), on \((-\infty, \infty)\), so that:

\[
E_n = \int_{-\infty}^{\infty} x^n d\rho(x)
\]

and, if such a measure exists, is it unique?

**Problem 2. The Stieltjes moment problem.**

Given a sequence of reals \( E_0, E_1, \ldots \), does it exist a measure, \( d\rho \), on \((0, \infty)\), so that:

\[
E_n = \int_{0}^{\infty} x^n d\rho(x)
\]
and, if such a measure exists, is it unique?

There is an extensive theory behind these so simply stated problems. In our case, we will be interested in just a couple of results, that we quote explicitly here because of their simplicity, and also in order to keep this paper self-contained. In this context, the following proposition is useful.

**Proposition 1** Suppose that \( \{E_n\}_{n=0}^\infty \) is a set of Hamburger moments and that for some \( C, R > 0 \),

\[
|E_n| \leq CR^n n!,
\]

Then the Hamburger problem is determinate. If \( \{E_n\}_{n=0}^\infty \) is a set of Stieltjes moments and

\[
|E_n| \leq CR^n (2n)!.
\]

Then the Stieltjes moment problem is determinate.

2. **Encoding of the heat kernel in terms of zeta values**

The preceding proposition is quite interesting, since it provides a sufficient condition for the existence and uniqueness of the solution to the problems. Also, it follows from equation 3 that \( \zeta(s) = E_{s-1}/\Gamma(s) \), for integer \( s \), and the (non-normalized) measure is given by \( d\rho(t) = K(t)dt \).

That is, we have that the moments, relative to our measure, are given by:

\[
E_n = \zeta(n+1)\Gamma(n+1) = \zeta(n+1) n!.
\] (8)

As we can see, this is a remarkable relationship, because the connection between the two spectral functions—heat kernel and zeta function—stems not only from the fact that the second is the Mellin transformed of the first, and that then it encodes all the moments of the first, but especially that it is the Mellin transform up to a gamma function, so it is, in some sense, even more tied to the problem of moments since it introduces the factorial. And this implies that it is not only a Stieltjes determined problem but also that we can construct an associated Hamburger problem that is also determinate, since it saturates the bound. On the other hand, the analytical continuations of the zeta and gamma functions on the variable \( n \) to the whole of the complex plane, provides also a natural extension of the corresponding moments to complex values of the argument.

We can now state our main result.

**Theorem 2** The trace of the heat kernel \( K(t) \) is a function exactly reproducible by its moments only if its associated zeta function \( \zeta(s) \) does not have any pole at any integer value of \( s \).
**Proof.** From equation 8 we see that the moments of the heat kernel satisfy the bound stated in the proposition, as long as \( \zeta(n + 1) \leq CR^n \), which is certainly the case if there is no singularity in the zeta function for any positive integer \( n \).

**Example 3** From the well known pole at \( s = 1 \), that we can interpret as lack of normalization of the associated heat kernel, we should immediately exclude from the list of the functions that satisfy the theorem the following important cases.

1. The Riemann zeta function: \( \zeta(s) = \sum_{n=1}^{\infty} n^{-s} \).
2. The Hurwitz zeta function: \( \zeta(s,a) = \sum_{n=0}^{\infty} (n + a)^{-s} \).
3. The Epstein zeta function in dimension two:

\[
E(s;a,b,c) = \sum_{n,m} (an^2 + bmn + cn^2)^{-s}.
\]

All of them having its rightmost pole at \( s = 1 \). Trivially, all these zeta functions give rise to indeterminate problems, in spite of the fact that all of their moments, except the zeroth one, are perfectly well behaved. Their associated heat kernels are not normalizable. One example of well-behaved (in our context) zeta function is:

\[
G(s;a,c;q) = \left[a(n+c)^2 + q\right]^{-s}.
\]

It is often called Epstein-Hurwitz in the physics literature \([1,4]\); and it has its rightmost pole at \( s = \frac{1}{2} \).

Let us now quote another Proposition from \([3]\) that will help us to check some of the statements mentioned above, and to get some identities.

**Proposition 4** (Krein \([3]\)) Suppose that \( d\rho(t) = K(t)dt \), where \( 0 \leq K(t) \leq 1 \) and either

(i) \( sup p(K) = (-\infty, \infty) \) and

\[
\int_{-\infty}^{\infty} \frac{\ln K(t) dt}{1 + t^2} < \infty,
\]

(ii) \( sup p(K) = (0, \infty) \) and

\[
\int_{0}^{\infty} \frac{\ln K(t) dt}{1 + t} \frac{1}{\sqrt{t}} < \infty,
\]

Suppose also that, for all \( n \):

\[
\int_{-\infty}^{\infty} |t|^n K(t) < \infty,
\]
Then the moment problem, with moments:

\[ E_n = \frac{\int t^n K(t)dt}{K(t)dt}, \]

is indeterminate.

**Remark 5** By the same method, Krein proved a stronger result: \( K(t) \) need not be bounded and the measure defining the moments can have an arbitrary singular part. It is also important to comment that Krein’s conditions are close to optimal. That is, for example, if the moments under consideration saturate the conditions stated in our first proposition, then the integrals in Krein’s proposition are barely divergent. Thus, taking into account our theorem and the last proposition we have the following one.

**Proposition 6** For the kind of heat kernels that belong to the category stated in the theorem, we have that the following integral:

\[ \int_0^\infty \ln K(t)dt \]

is divergent.

### 3. The example of the theta function.

**Example 7** Let us consider the family of functions \( K(t) = \sum_{n=1}^{\infty} e^{-n^\alpha t}, \) with \( \alpha \) a real parameter with \( \alpha \neq \frac{1}{n} \) with \( n \) any integer (thought it is maybe necessary to distinguish between \( \alpha > 1 \) and \( \alpha < 1 \)). Its associated zeta function has the rightmost pole moved from \( s = 1 \) in the Riemann case (\( \alpha = 1 \)) to \( s = \frac{1}{\alpha} \). Thus, in principle this is an example of the kind of function that satisfies our theorem and also the last proposition.

Let us apply what we have learned up to now to a very basic situation. From what we have said, it is clear that we cannot work out the Riemann case, since it has a pole at \( s = 1 \). But it turns out that we can in fact consider the following heat kernel:

\[ K(t) = \sum_{n=1}^{\infty} e^{-n^\alpha t}, \quad (9) \]

which is a particular case of the elliptic theta function:

\[ \theta_3(z, \tau) = \sum_{n=-\infty}^{\infty} e^{-\pi n^2 \tau + 2\pi nz} \quad (10) \]

with \( z \in C, \tau \in R^+. \) More precisely: \( K(t) = \frac{1}{2} [\theta_3(0, t/\pi) - 1] \)
Thus, we are dealing with a particular case of a theta function. Its zeta function counterpart is:

\[ \tilde{\zeta}(s) = \sum_{n=1}^\infty n^{-2s} = \zeta_R(2s), \]

where the last one is the Riemann zeta function.

It is well known that with theta functions one is usually able to obtain remarkable identities, some of them coming basically from the Jacobi identity (or the “equivalent” summation formulas), but not so often completely closed, evaluable expressions. In the light of the theory of moments and from what has been stated above, we now have all the information about the theta function encoded in the integer values of \( \zeta_R(2s) \). But the theory of moments does not say anything about how to do the reconstruction. We can try, for example, the well known “probabilistic approach”, that consists in the construction of the characteristic or generating function. In general, the characteristic (or generating) function is given by:

\[ \phi(k) = \sum_{n=0}^\infty \frac{<X^n>}{n!}k^n = \sum_{n=1}^\infty \frac{\zeta(n)\Gamma(n)}{(n-1)!}k^{n-1} = \sum_{n=1}^\infty \zeta(n)k^{n-1}. \]  

(11)

And, in the particular case we are studying,

\[ \phi(k) = \sum_{s=1}^\infty \zeta_R(2s)(-k)^s = -1 + \frac{\pi \sqrt{k} \coth(\pi \sqrt{k})}{2k}. \]

(12)

In principle, this expression should be equal to the Laplace transform of our theta function, and this would imply a confirmation of our theorem in this particular case. Let us show that this is indeed the case. Consider

\[ \int_0^\infty e^{-sx} \sum_{n=1}^\infty e^{-n^2s} \, dx = \sum_{n=1}^\infty \frac{1}{n^2 + s}, \]

(13)

and using the well known series expansion of the cotangent, we get that the Laplace transform is just our \( \phi(k) \). Thus, such very simple case provides a practical confirmation of our theorem. Now we have two possible different ways to arrive to the same result. The direct one, of computing the Laplace (or Fourier) transform of the theta function, and the other—a consequence of our theorem—by a direct construction using the associated zeta function. It would be interesting to investigate which kind of information can be obtained from the comparison of the two methods in more complicated or practical cases than the one considered here. On the other side, we see that the Laplace transform of our theta function presents periodic singularities at \( k = n^2 \), with \( n = 1, 2, 3... \). It would be interesting to know whether this can be related with to fact that our theta function, for example, has some kind of special features like the lack of an analytical continuation around the origin. Or, more probably, to the presence of the pole at \( s = \frac{1}{2} \) of the associated zeta function, to which the theory of moments is blind (and that always implies the divergence of a certain integral associated to the heat kernel). In this particular case, the divergent integral is \( \int_0^\infty K(t)/\sqrt{t} \).
4. Inversion problems and possible encoding of the heat kernel in terms of negative zeta values

The classical moment problem, as can be readily appreciated from [3], has to do essentially with the uniqueness issue. In this spirit, we have seen that, under the restriction on the position of the poles, we can guarantee determinacy: the positive integer values of the zeta function determine in a unique way the partition function of the system. This is equivalent to saying that there is only one partition function with the same given moments: if there is another with the same integer values of the associated zeta function it should necessarily be the same partition function. This is an important formal statement, since it implies that only with a very restricted part of the information included in the spectral zeta function (the set of positive integer values against the whole complex plane), we have completely determined and fixed the partition function. Nevertheless, it is not guaranteed that the inversion, from the practical point of view, can always be performed in a straightforward way, as explained in the previous section. More precisely, the construction of the characteristic function used above is based on the following series and integral commutation:

\[
\int_0^\infty e^{-\beta t} K(t) dt = \int_0^\infty \sum_{k=0}^\infty \frac{(-\beta)^k}{k!} K(t) dt = \sum_{k=0}^\infty \left( \int_0^\infty t^k K(t) dt \right) \frac{(-\beta)^k}{k!} = \sum_{k=0}^\infty \frac{\zeta(k+1)}{\beta^k}.
\]

Of course, this is cannot be always carried out in such a simple way (see [9], and [7] for a discussion in a QFT context). In our case, our main concern will be precisely the situation when regularized values appear (see [1]). As we will see later, it is of course also possible to do this in such cases, since we deal with a function \(K(t)\) of the type \(K(t) = \sum_ne^{-e_n t}\). Then we can proceed as

\[
\int_0^\infty e^{-\beta t} K(t) dt = \int_0^\infty e^{-\beta x} \sum_{n=1}^\infty e^{-\epsilon_n x} dx = \sum_{n=1}^\infty \frac{1}{e_n + \beta} = \sum_{n=1}^\infty \sum_{k=0}^\infty \frac{(-\beta)^k}{\epsilon_{n+k+1}}.
\]

Clearly, the two expression are only equal under the validity of the commutation of the two series in the last expression:

\[
\sum_{n=1}^\infty \sum_{k=0}^\infty \frac{(-\beta)^k}{\epsilon_{n+k+1}} = \sum_{k=0}^\infty \sum_{n=1}^\infty \frac{(-\beta)^k}{\epsilon_{n+k+1}} = \sum_{k=0}^\infty \zeta(k+1)(-\beta)^k.
\]

This is exactly the case of the example considered, as checked above, and it is to be expected in general whenever the rightmost pole is at \(s < 1\) and, in addition, it has been shown that the moments, as in our case, directly satisfy the bound that guarantees that the Taylor expansion can be done. Nevertheless, the case
with \( s > 1 \) should be considered with more care since regularized values for the
moments appear and it is in general known that commutation of series cannot
be performed in a direct way, as we will see. To begin with, a representation
of the Laplace transform by \( \sum_{n=1}^{\infty} \frac{1}{\Gamma_n + \beta} \) is clearly a regularized series if the
rightmost pole is at the right of \( s = 1 \).

We now consider the possibility that the zeta function encodes, in the posi-
tive integer values of its argument, all the information that describes the heat
kernel (and not only that of its asymptotic expansion). Again, from the very
simple expansion of the exponential: \( e^{-e_n t} = \sum_{j=0}^{\infty} \frac{(-e_n t)^j}{j!} \), we can wonder
whether

\[
K(t) = \sum_{n=1}^{\infty} \sum_{j=0}^{\infty} \frac{-(e_n t)^j}{j!}
\]

has something to do with the following quantity:

\[
\tilde{K}(t) = \sum_{j=0}^{\infty} \sum_{n=1}^{\infty} \frac{(e_n)^j t^j}{j!} = \sum_{j=0}^{\infty} \frac{\zeta(-j)(-t)^j}{j!}.
\]

The first thing one can wonder about is, whether these two expressions
are equal, that is, if we can proceed with the commutation of the series. The validity
of the commutation of the two series would imply the use of the regularized
sums \( \sum_n e_n^j \) (essentially this is a divergent series and we use its regularized
value, expressed by the zeta function). So, this makes unlikely that this is the
case, and actually, it has been shown in the theory of spectral zeta functions
that commutations of series cannot be done, in general, without the additional
contributions \[1\]. This implies, in principle, that we cannot reproduce the heat-
kernel from the values of the associated zeta function at negative integer values
of \( s \), at least not in such a naive way. Nevertheless, we can use the functional
equation satisfied by the zeta function.

In the particular example considered, it is the well known functional equation
for the Riemann zeta function \[12\]:

\[
\pi^{-s/2} \Gamma(s/2) \zeta_R(s) = \pi^{-(1-s)/2} \Gamma(\frac{1-s}{2}) \zeta_R(1-s)
\]

It provides the analytic continuation of the Riemann zeta function to the whole
complex plane (with the pole at \( s = 1 \)), so it allows to express the negative
integer values of the zeta function in terms of the positive ones. Then, we arrive
at the formal result that the existence of a functional equation implies that our
statement also holds for the negative integer values of the zeta function (but
then we probably have to include gamma functions and other factors in order to
reproduce the numerical value of the zeta function in the positive integer value,
which actually is the fundamental quantity in our study).
5. The role of the non-integer poles and the regularized values of the moments

A natural question that arises is: What is the role played by the pole or poles at the non-integer positions in the determinate case? To answer this we consider the Laplace transform of a generic heat kernel:

\[ \int_0^\infty e^{-\beta x} \sum_{n=1}^\infty e^{-e_n x} dx = \sum_{n=1}^\infty \frac{1}{e_n + \beta} \quad (20) \]

We see that the Laplace transform is related to the associated spectral zeta function in the following simple way. Being the associated spectral zeta function \( \zeta(s) = \sum e^{-e_n s} \), we associate to this last one, a shifted spectral zeta function: \( \zeta(s, \beta) = \sum (e_n + \beta)^{-s} \) (in particular, this leads from the Riemann zeta function to the Hurwitz zeta function). We see clearly, that the Laplace transform of the heat kernel is the shifted zeta function evaluated at \( s = 1 \) and with the parameter \( \beta \) being the variable of the function. Since the addition of the shift does not change the rightmost pole, we see that the divergence at \( s = 1 \) is the most problematic one, since our expression for the Laplace transform is expressed then as a genuine divergent series. This is in some sense, to be expected, since the pole at \( s = 1 \) implies lack of normalization of the heat kernel. For the case when we have the rightmost pole at \( s > 1 \), the expression is a regularized series, while for \( s < 1 \) it is a convergent series.

Let us now study the case where \( e_n = n^\alpha \). Then, the associated zeta function has its rightmost pole at \( s = \frac{1}{\alpha} \). Thus, for \( \alpha \) running from 1 to \( \infty \), the rightmost pole moves from \( s = 1 \) to \( s = 0 \). And we see that the pattern of singularities in the Laplace transform of the heat kernel goes like \( n^\alpha \), so we have less and less singular behavior corresponding to the pole tending towards the origin.

With this simple example we observe that, in spite of the fact that, regarding uniqueness and inversion questions, only the positive integer moments play a role (and this is due to the fact that the distribution and its moments are related by a Taylor series expansion of a certain function of the distribution), we see how the non-integer poles do also play a role, not in the fact that the problem is determinate or not, but in the actual form and behavior of the characteristic function (the integral transform of the distribution). This was to be expected.

Now, consider that the parameter \( \alpha \) ranges between \( (0, 1) \). Then we move the rightmost pole to the right of \( s = 1 \) (of course, avoiding values of the parameter such that we get a pole in another integer position). We see, directly from the Laplace transform, that the more the pole goes to the right, the more divergences are to be accounted for. It is worth to remark that in this case, all the zeta function values that are on the left of the pole (that defines the abscissa of convergence) correspond to regularized values, and this implies that in our series expansion we have a finite number of moments whose expression is a regularized one. This is in contrast with the case discussed above, and we can in fact relate it with the commutation of series above mentioned.
6. The density of states in terms of the zeta function

Let us now consider the density of states of the system:

$$\rho(E) = \sum_n \delta(E - e_n).$$  \hfill (21)

Its relation with the zeta function can be simply written as:

$$\zeta(s) = \sum_n e^{-s e_n} = \int_{-\infty}^{\infty} \delta(E - e_n) E^{-s} = \int_{-\infty}^{\infty} \rho(E) E^{-s} dE$$ \hfill (22)

That is, the zeta function at its negative integer values gives all the (regularized) moments of the density of states. As long as there are no poles, this implies that the negative integer values of the zeta function determine in a unique way the density of states, thanks to the functional equation, that gives us the analytical prolongation to the whole complex plane and implies, together with the considerations for the partition function case, that the bound for the moments is equally satisfied.

As before, some difficulties can appear at the practical level, especially when one is dealing with a certain number of moments (a finite number in the previous example, with $(0, 1)$, and an infinite number in this case) that come from a regularized divergent series. But, at least in this last case, taking into account that the Laplace transform of the density of states is the own heat kernel, and that the result on commutation on series (or zeta function regularization theorem) tells us that:

$$K(t) = \sum_n e^{-t e_n} = \sum_n \sum_j \frac{(-t)^j e_n}{j!} \neq \sum_j \sum_n \frac{(-t)^j e_n}{j!} = \sum_j \frac{(-\beta)^j}{j!} \zeta(-j).$$ \hfill (23)

The crucial point is to understand that the classical moment problem give us several conditions that lead us know whether the measure is unique or not. There is a very simple and enlightening example, due to Stieltjes, and included in, e.g. \cite{3}. It is based on the following observation.

For any $\theta \in [-1, 1]$, we have that

$$\int_0^{\infty} u^k u^{-\ln u} [1 + \theta \sin(2\pi \ln u)] = \sqrt{\pi} e^{\frac{\theta}{2}(k+1)^2},$$ \hfill (24)

and we thus arrive to a one-parameter family of different functions all of them having the same sequence of moments. Clearly, $\gamma_k = e^{\frac{\theta}{2}(k+1)^2}$ is an indeterminate set of Stieltjes moments. It is not necessary that the relationship with the moments should be given as the usual series expansion in straightforward probability theory for example. It is valid for the simple example of the theta
function, shown above. In fact there are papers in the physical literature dealing with the classical moment problem for the case of the moments of a random quantity, but they fail to appreciate altogether, that the condition on the bound we have used to show determinacy in our context, is just a sufficient condition, that came from analyticity of the Fourier transform of the measure. In fact, as clearly stated in [3], there can be sets of moments of an arbitrary high growth which constitute nevertheless a determinate moment problem. One should be careful since, on the other hand, there are sets of moments that are only slightly bigger than the ones in our proposition (1) and that constitute an indeterminate moment problem. Let us go further into the results of the commutation of series in order to see what happens with a practical implementation of the relationship between the density of states and the trace of the heat kernel by the moments of the last one. In [1], it is shown that:

\[ K_{\alpha}(t = 1) = \sum_{n=1}^{\infty} e^{-n^\alpha} = \sum_{a=1}^{\infty} \frac{(-1)^a}{a!} \zeta(-a\alpha) + \frac{1}{\alpha} \Gamma(\alpha) - \Delta_\alpha, \]  

(25)

being \( \Delta_\alpha \) an additional contribution coming from series commutation. The particular case of the zeta function regularization says that: 1. For \(-\infty < \alpha < 2\), the contribution of the additional term is \( \Delta_\alpha = 0 \). 2. For \( \alpha = 2 \), the contribution of the additional term is \( \Delta_\alpha = -\sqrt{\pi} K_2(\pi^2) \). 3. For \( \alpha > 2 \), the contribution is increasingly bigger. Following our line of reasoning, we identify each situation with the position of the rightmost (and in this case only) pole, the correspondence being 1. The pole of the zeta function lies in \((-\infty, 0) \cup \left( \frac{1}{2}, \infty \right)\). 2. The pole of the zeta function is at \( s = \frac{1}{2} \). 3. The pole lies in \((0, \frac{1}{2})\). No conclusion seems to be implied by this observation. Notice, nevertheless, that we are in the particular case \( t = 1 \). For the general case, the expression:

\[ K_{\alpha}(t) = \sum_{n=1}^{\infty} e^{-n^\alpha t} = \sum_{a=1}^{\infty} \frac{(-t)^a}{a!} \zeta(-a\alpha) + \frac{1}{\alpha} \Gamma(\alpha) - \Delta_\alpha \]  

(26)

is only valid for \( \alpha \in (0, 1] \) and for \( \alpha \in 2N \). These last value of the parameter are the ones that make the associated operator a differential operator.

We have restricted our discussion up to now to zeta functions that only posses one pole. It is worth to complete our characterization comparing with cases where more poles appear. In particular, when we have an infinite sequence of poles in the left half-plane. These appear in a natural way, when we introduce a constant shift in the spectrum. In this case, we go, for example, from the Hurwitz zeta function to the Epstein-Hurwitz zeta function mentioned above:

\[ G(s; a, c; q) = \sum_{n=-\infty}^{\infty} [a(n + c)^2 + q]^{-s}. \]

(27)

This has, like the Hurwitz or the Riemann with \( \alpha = 2 \), its rightmost pole at \( s = \frac{1}{2} \), but exhibits, in addition, an infinite number of poles at \( s = -\frac{1}{2}, -\frac{3}{2}, ... \).
produced by the $q$ term. The Laplace transform of the heat kernel is:

$$\mathcal{L}\{K(t)\} = \int_0^\infty e^{-\beta x} \sum_{n=1}^\infty e^{-[a(n+c)^2+q]x} \, dx = \sum_{n=1}^\infty \frac{1}{[a(n+c)^2+q]+\beta}$$  \hspace{1cm} (28)

We see that the introduction of the parameter $q$, the responsible for the new poles, only shifts by a constant value the pattern of divergences of this function.

It should be clear that we can apply our results as soon as we know the structure of the zeta function. This allows us to consider, for example, cases as general as:

$$\sum_{n_1,\ldots,n_N} [a_1(n_1+c)^{\alpha_1} + \ldots + a_N(n_N+c)^{\alpha_N} + q]^{-s},$$  \hspace{1cm} (29)

with its rightmost pole at $s_0 = \max (\alpha_1, \ldots, \alpha_N)$. Notice that this example (considered in detail in the seminal paper [4]) does not correspond generically to a ΨDO. As we pointed out before, our approach is not necessarily limited to ΨDOs. But, even in the family of ΨDOs, very general pole structures for the zeta function can show up (in particular, in the case of noncommutative spaces, see e.g. [10, 11, 13]).

7. The problem in the framework of noncommutative geometry

It is clear that we can state the condition of absence of a pole at a certain position in more mathematical terms as a zero value for the residue of the zeta function at the point. This allows a more direct comparison with usual heat kernel asymptotic expansion since, as we have seen, the coefficients are given essentially by the residues of the zeta function at certain points. To begin with, we have seen that, if the operator is a differential operator then all $\beta_k = 0$ and, since $\beta_k(A) = \frac{(-1)^{k+1}}{k!} \text{Res}_{s=-k} \zeta_A(s)$, then we have automatically implemented the condition $\text{Res}_{s=-k} \zeta_A(s) = 0$, that is, absence of pole at the negative integer values. Then we can clearly state that for a differential operator the density of states is uniquely determined by all its moments, that is, by the values of the associated zeta function at its negative integer values. Of course, the condition $\beta_k = 0$ does not imply that the operator is differential, and we have seen an example in the case of the spectrum $\{e_n\} = n\alpha$. For, then we have always $\beta_k = 0$, but it corresponds to a differential operator only when $\alpha \in 2\mathbb{N}$. Also, for example, we see that determinacy for the density of states not only implies $\beta_k = 0$, but also that $\alpha_j(A) = \frac{(-1)^k}{k!} \zeta (-k)$ (for the case $s = -k$).

We can now put our problem into the context of noncommutative geometry, given that the tool used to compute the zeta function residues at any position of the (hypothetical) pole is the Wodzicki residue [4]. The Wodzicki (or noncommutative) residue [10, 11, 13] is the only extension of the Dixmier trace to ΨDOs which are not in $L^{1,\infty}$. Even more, it is the only trace at all one can
define in the algebra of ΨDOs up to a multiplicative constant. It is explicitly given by the integral

$$\text{res } A = \int_{S^* M} \text{tr } a_n(x, \xi) \, d\xi,$$

with $S^* M \subset T^* M$ the co-sphere bundle on $M$ (some authors put a coefficient in front of the integral). If $\dim M = n = - \ord A$ ($M$ compact Riemann, $A$ elliptic, $n \in \mathbb{N}$) it coincides with the Dixmier trace, and one has:

$$\text{Res}_{s=1} \zeta_A(s) = \frac{1}{n} \text{res } A^{-1}.$$  

An interesting property of the Wodzicki functional is that it is also the Cauchy residue for the zeta function [4]. Then we can express our condition of absence a pole in an integer position in the following simple way:

$$\int_{S^* M} \text{tr } a_n(j, \xi) \, d\xi = 0,$$

with $j = 1, 2, ...$ for the uniqueness of the trace of the heat kernel and $j = 0, -1, -2, ...$ for the density of states. It is clear that a sufficient condition to satisfy this requirement is that $a_n(j, \xi) = 0$ for the respective values of $j$. Furthermore, in noncommutative geometry we define a geometric space by a spectral triple [10],[11],[14] :

$$(A, H, D),$$

where $A$ is a concrete algebra of coordinates represented on a Hilbert space $H$ and the operator $D$ is the inverse of the line element. This is a completely spectral definition, where the elements of the algebra are operators and the points come from the joint spectrum of operators and the line element is an operator. More precisely, in this framework the operator $D$ gives the inverse of the length element $ds = D^{-1}$. The basic properties of spectral triples are simple to state, and do not make any reference to the commutativity of the algebra $A$ (see [10],[11],[14] for details). For our purposes, the following result for the case of spectral triples is noticeable:

$$\int |D|^{-n} \neq 0,$$

where $n$ is the dimension of the spectral triple. This amounts to saying that the residue of the zeta function associated with the operator $D$, $\zeta(s) = Tr \left(|D|^{-s}\right)$ at $s = n$ cannot vanish. Being $n$ an integer, we see clearly that this important case does not fulfill our conditions leading to determinacy for the heat-kernel.

8. Conclusions and outlook

The important result in this paper is the proof that the spectral zeta function gives all the moments associated with the density of states as well as those
coming from the partition function, which are the two fundamental quantities always studied in a quantum mechanical context. The moments of the density of states are obtained from the zeta function at negative integers and at the origin while zeta at the positive integers yields all the moments of the partition function. Interestingly enough, this observation provides also a clear physical motivation for the functional equation satisfied by the spectral zeta function. Namely the functional equation relates the moments of these two physical quantities, that are in fact connected through a Laplace transform. This leads us, in fact, to a functional equation of the type \( \zeta(-s) = \varphi[\Gamma(s+1)\zeta(s+1)] \). The functional equation gives the analytical continuation of the zeta function, and in this context it is very clear why it is important to know it, not only in a quantum field theory context, but as a fundamental object.

These considerations lead to an exact comparison with the classical moment problem, to arrive at the important formal result that, under the natural conditions stated, both the partition function as well as the density of states are uniquely determined by their respective moments: the corresponding zeta values. As already emphasized in the paper, only with the information encoded in the integer values of the zeta function we have determined both the density of states as well as the partition function. In the absence of the poles in the key positions, this is a clear and direct consequence of the boundedness of the values of the zeta function (that are in fact decreasing, due to the increasing nature of the spectral sequence) and of the existence of a functional equation for the zeta function.

In addition, the consideration of inversion questions, related to practical implementations of this result— that lie usually beyond the scope of the classical moment problem— has lead us to interesting observations regarding the commutation of series and the role and influence of the non-integer poles, studied in the context of the integral transform of the partition function.

Appendix A. The classical moment problem: some results and considerations

We have discussed essentially two different aspects of the classical moment problem. The proposition, that gives a sufficient condition through a bound on the sequence of moments, in order to prove determinacy, and Krein’s proposition, that relies on an integral criterion for the measure itself, in order to show indeterminacy. In fact, taking into account the two propositions and observing that

\[
\int_{-\infty}^{\infty} x^{2n} \exp(-|x|^\alpha) dx = 2\alpha^{-1}\Gamma\left(\frac{2n+1}{\alpha}\right) \sim \left(\frac{2n}{\alpha}\right)!
\]

and that Krein’s proposition holds for \( \exp(-|x|^\alpha) \) if \( \alpha < 1 \), then we see that there are examples of Hamburger indeterminate moment problems with growth just slightly faster than the \( n! \) growth (the determinate case). The same applies for the Stieltjes case but with \( \alpha < 1/2 \) and the \( (2n)! \) factorial growth.

It is explicitly stated in [3] and wrongly assumed, for example in [15], that from the first proposition one might hope that just as the condition of not too
great growth implies determinacy, there might be a condition of rapid growth that implies indeterminacy. This is false, since there are moments of essentially arbitrary rates of growth which lead to determinate moment problems. This is important both from the theoretical and from the practical point of view. In fact, it can be related to an analogous situation in Quantum Field Theory, when studying the role of power expansions in QFT (perturbative QFT) and can be, to begin with, related with resummation \[6\][8]. We will comment on this later.

Given a set of moments \( \{\gamma_n\}_{n=0}^{\infty} \) and \( c \in \mathbb{R} \), one can define a new set of moments:

\[
\gamma_n(c) = \sum_{j=0}^{\infty} c^j \gamma_{n-j},
\]

(33)

For the Hamburger problem, the solutions of the \( \{\gamma_n\}_{n=0}^{\infty} \) and each of the \( \{\gamma_n(c)\}_{n=0}^{\infty} \) are in one-to-one correspondence. The Stieltjes case is much more involved in this respect, due essentially to the fact that its associated interval \((0, \infty)\) gets modified under the change to a new set of moments (see \[3\] for details). Another well-known and useful condition on the moments is the Carleman criterion, which states that: (i) if

\[
\sum_{n=1}^{\infty} \gamma_{2n}^{-1/2n} = \infty,
\]

then the Hamburger problem is determinate, and (ii) if:

\[
\sum_{n=1}^{\infty} \gamma_n^{-1/2n} = \infty,
\]

for a set of Stieltjes moments, that problem is both Stieltjes and Hamburger determinate.

These few results already convey the idea that the classical moment problem, in spite of the simplicity of its formulation (common to many inverse problems) is highly nontrivial and deserves careful study. One important aspect that we have not dealt with here is its tight relationship with the theory of orthogonal polynomials. Since orthogonal polynomials can be constructed from the set of moments, many of the conditions can be stated in terms of the associated orthogonal polynomials, and these exhibit profound mathematical properties depending on whether they come from a determinate or from an undetermined measure.

The kind of mathematical concepts and arguments used here, as well as the information presented regarding the theory of the classical moment problem is clearly reminiscent to a fundamental problem in Quantum Field Theory, namely the role of the perturbative expansion and its relationship with the full theory. A huge amount of work has been devoted to clarify this issue, since the early criticisms and observations on the drawbacks of the perturbative expansion \[5\]. The literature on this problems is extense, and we just point out here some
conceptual remarks that can appear in a natural way in the context of our problem. In view of the probable divergence of QFT, the resummation of the perturbation series is necessary for obtaining finite answers to physical problems. It is believed that divergent expansions probably constitute asymptotic series, but the main point is that it is not yet well known if a unique answer is implied by the perturbation theory. This is a fundamental issue. Namely, the main question is not that of the convergence or divergence of the series, but whether the expansion uniquely determines the answer or not. This is, of course, the aim of the renormalization program. There, one source of problems, at the level of resummation, are the infrared renormalons that are the responsible, for example, for the non-summability of QED or QCD (see [6][8] for details and references to the literature). A point to be stressed is that the resummation of divergent series can be especially ambiguous if the Carleman theorem, which guarantees that there is a one-to-one correspondence between a function and its associated asymptotic series, is not satisfied (see [8] and references therein).

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