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Regularization of functional determinants using boundary perturbations

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Abstract. The formalism which has been developed to give general expressions for the determinants of differential operators is extended to the physically interesting situation where these operators have a zero mode which has been extracted. In the approach adopted here, this mode is removed by a novel regularization procedure, which allows remarkably simple expressions for these determinants to be derived.

1. Introduction

The increasing use of path integrals as a calculational tool has led to a corresponding increase in interest in the evaluation of functional determinants. This is simply because the evaluation of Gaussian path integrals typically gives such determinants. The first results were obtained over thirty years ago: Gel'fand and Yaglom [1] derived expressions for the functional determinants obtained from evaluating path integrals with the simplest type of quadratic action. In subsequent years the results have become more general and the formalism more elaborate [2, 3], culminating with the work of Forman [4] who has given a remarkably simple prescription which can be applied to a rather general operator and boundary conditions.

However, in many calculations involving Gaussian integrals which are currently carried out, these results are not directly applicable. The reason is that the Gaussian nature of the integral is frequently a consequence of expanding about some non-trivial 'classical' solution of the model (e.g. a soliton or instanton). Typically this results in a particular point (in space or time) being selected, which breaks the translational invariance of the theory, and so gives rise to a Goldstone mode. There are other possible ways that such a zero mode could come about, but in all cases the Gaussian approximation breaks down. The remedy is to first extract this mode as a collective coordinate [5] and to treat only the non-zero modes in the Gaussian approximation. Therefore, it is not the functional determinant which is required in these cases—it will in any case be identically zero—but the functional determinant with the zero mode extracted.

In this paper we present a systematic method to calculate this quantity. The most obvious way to proceed is to 'regularize' the theory in some way, so that the eigenvalue of the operator under consideration which was previously zero, is now non-zero. The determinant is now also non-zero and the pseudo-zero eigenvalue can be factored out, the regularization removed, and a finite result obtained. Previous approaches have been rather *ad hoc*, being performed on a case by case basis as the need arose. For example, it may be possible in certain cases to modify the form of the operator in such a way that the zero mode is regularized, but also that the calculation may still be performed [6, 7]. In other cases, it may be possible to move the boundaries to achieve the same end [8, 9]. Here we adopt an approach which applies to very general situations and which, we believe, is the simplest and most systematic regularization and calculational procedure. This is because the method is the least intrusive—the operator and the position of the boundaries are left unchanged—and only the form of the boundary conditions are modified in the regularization procedure. We use the notation and general approach of Forman to calculate the regularized functional determinant, since it is ideally suited to this form of regularization, emphasizing as it does the separation of the boundary conditions from the solutions of a homogeneous differential equation.

The outline of the paper is as follows. In section 2 we develop our method in one of the simplest situations, in order to clearly illustrate it. The calculation of the regularized expression for the formerly zero eigenvalue is derived, for the most general case that will interest us, in section 3 and the general procedure for finding the functional determinant with the zero mode extracted is described in section 4. In section 5 we apply the method to certain specific cases and we conclude in section 6 with some general remarks.

2. A simple example

In this section we explain the method by carrying out an explicit calculation on what is perhaps the simplest example. Suppose that we wish to calculate the determinant of an operator of the form

$$L = \frac{\mathrm{d}^2}{\mathrm{d}t^2} + P(t) \qquad t \in [a, b] \tag{2.1}$$

where $P(t)$ is a known real function. We suppose that the boundary conditions on the functions on which L operates is $u(a) = u(b) = 0$. In particular, the eigenfunctions of L have to satisfy these conditions.

We now give Forman's prescription for calculating $\det L$. A more detailed discussion is given in section 4, where our approach is explained in greater generality. The recipe has two ingredients.

(i) Write the boundary conditions on L in the form

$$\mathbf{M}\begin{bmatrix} u(a) \\ \dot{u}(a) \end{bmatrix} + \mathbf{N}\begin{bmatrix} u(b) \\ \dot{u}(b) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{2.2}$$

where $\mathbf{M}$ and $\mathbf{N}$ are 2×2 matrices and $\dot{u} = \mathrm{d}u/\mathrm{d}t$. These two matrices are not unique; for the case of our boundary conditions $u(a) = u(b) = 0$ we choose them to be

$$\mathbf{M} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \mathbf{N} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}. \tag{2.3}$$

(ii) Now consider a different problem. Let $y_1(t)$ and $y_2(t)$ be two independent solutions of the homogeneous differential equation $Lh = 0$. Construct

$$\mathbf{H}(t) = \begin{bmatrix} y_1(t) & y_2(t) \\ \dot{y}_1(t) & \dot{y}_2(t) \end{bmatrix} \tag{2.4}$$

and the 2×2 matrix $\mathbf{Y}(b) \equiv \mathbf{H}(b)\mathbf{H}^{-1}(a)$.

Forman then proves that [4]

$$\frac{\det L}{\det \hat{L}} = \frac{\det(\mathbf{M} + \mathbf{N}\mathbf{Y}(b))}{\det(\mathbf{M} + \mathbf{N}\hat{\mathbf{Y}}(b))}. \tag{2.5}$$

We would expect that $\det L$ itself is divergent, being a product of an infinite number of eigenvalues of increasing magnitude. Therefore it is only when it is defined relative to the determinant of an operator of a similar type (denoted here by $\hat{L}$), that it has any meaning. In applications to path integrals, ratios of determinants such as the one on the left-hand side of (2.5) naturally arise from the normalization of the path integral itself. In general, they will relate to a simple quantum system or stochastic process, such as the harmonic oscillator or Ornstein–Uhlenbeck process. In these cases, $\hat{P}(t)$ is independent of t and will not, in general, have a zero mode.

For the matrices $\mathbf{M}$ and $\mathbf{N}$ of our simple example,

$$\begin{aligned}\det(\mathbf{M} + \mathbf{N}\mathbf{Y}(b)) &= Y_{12}(b)\\ &= \frac{y_1(a)y_2(b) - y_2(a)y_1(b)}{y_1(a)\dot{y}_2(a) - y_2(a)\dot{y}_1(a)}.\end{aligned} \tag{2.6}$$

The denominator of this expression is the Wronskian, which does not vanish since the two solutions $y_1(t)$ and $y_2(t)$ are presumed independent. If we take $y_1(t)$ to be a solution for which $y_1(a) = 0$, then (2.6) can be simplified to $y_1(b)/\dot{y}_1(a)$, so that, if $\hat{y}_1(a) = 0$ also,

$$\frac{\det L}{\det \hat{L}} = \frac{y_1(b)\dot{\hat{y}}_1(b)}{\dot{y}_1(b)\hat{y}_1(b)}. \tag{2.7}$$

This simple expression is particularly useful, since it only involves y_1, $\hat{y}_1$ and their first derivatives at one of the boundaries. We should stress that results such as these have been known since the work of Gel'fand and Yaglom [1]—our purpose here is to introduce the formalism required to describe our approach, in as simple a way as possible.

Now suppose that $y_1(b) = 0$ (as well as $y_1(a) = 0$). Then $y_1(t)$ is an eigenvalue of L with zero eigenvalue. This is the situation of interest to us in this paper. To extract this zero mode, we first regularize the problem by modifying it so that the operator is unchanged, but the boundary conditions $u(a) = u(b) = 0$ become

$$u^{(\epsilon)}(a) = 0 \qquad u^{(\epsilon)}(b) = \epsilon \dot{u}^{(\epsilon)}(b) \tag{2.8}$$

where ϵ is some small number. So now $y_1(t)$ is no longer an eigenfunction of L with zero eigenvalue. Let $y_1^{(\epsilon)}(t)$ be the corresponding eigenfunction (i.e. the one which reduces to $y_1(t)$ when $\epsilon \to 0$) and let it have eigenvalue $\lambda^{(\epsilon)}$. To find $\det L$ with these boundary conditions we first note that $\mathbf{Y}(b)$ is unchanged, since it does not involve boundary conditions at all; it only depends on two independent solutions to the homogeneous differential equation $Lh = 0$. Modifying the boundary conditions as in (2.8) only changes $\mathbf{M}$ and $\mathbf{N}$ to

$$\mathbf{M}^{(\epsilon)} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \mathbf{N}^{(\epsilon)} = \begin{bmatrix} 0 & 0 \\ 1 & -\epsilon \end{bmatrix}. \tag{2.9}$$

This gives $\det(\mathbf{M}^{(\epsilon)} + \mathbf{N}^{(\epsilon)}\mathbf{Y}(b)) = Y_{12}(b) - \epsilon Y_{22}(b)$. But since $y_1(a) = y_1(b) = 0$, $Y_{12}(b) = 0$, and so

$$\begin{aligned}\det(\mathbf{M}^{(\epsilon)} + \mathbf{N}^{(\epsilon)}\mathbf{Y}(b)) &= -\epsilon Y_{22}(b)\\ &= -\epsilon\frac{\dot{y}_1(b)}{\dot{y}_1(a)}.\end{aligned} \tag{2.10}$$

This is the regularized form of the determinant. In the next section we will give a general method for finding $\lambda^{(\epsilon)}$. In this simple problem it turns out that, to lowest order,

$$\lambda^{(\epsilon)} = -\epsilon \frac{\dot{y}_1^2(b)}{\langle y_1 | y_1 \rangle} \tag{2.11}$$

where $\langle y_1 | y_1 \rangle$ is the norm of the zero mode:

$$\langle y_1 | y_1 \rangle = \int_a^b \mathrm{d}t \, y_1^2(t). \tag{2.12}$$

From (2.10) and (2.11) we have that

$$\lim_{\epsilon \to 0} \frac{\det(\mathbf{M}^{(\epsilon)} + \mathbf{N}^{(\epsilon)}\mathbf{Y}(b))}{\lambda^{(\epsilon)}} = \frac{\langle y_1 | y_1 \rangle}{\dot{y}_1(a)\dot{y}_1(b)}. \tag{2.13}$$

This remarkably simple result is the one which we sought. Note that, apart from the norm, it is only involves $\dot{y}_1$ at the boundaries. In applications, it will usually be the case that the norm in (2.13) will cancel with an identical factor coming from the lowest order form of the Jacobian of the transformation to collective coordinates. Therefore $\langle y_1 | y_1 \rangle$ need not be calculated. Denoting the determinant of L with the zero mode extracted by $\det' L$ and normalizing by $\det \hat{L}$, we finally obtain

$$\frac{\det' L}{\det \hat{L}} = \frac{\langle y_1 | y_1 \rangle}{\dot{y}_1(a)\dot{y}_1(b)} \frac{\dot{\hat{y}}_1(b)}{\hat{y}_1(b)}. \tag{2.14}$$

The method we have described to find the regularized form of $\det(\mathbf{M}+\mathbf{N}\mathbf{Y}(b))$ is hardly more complicated than finding the unregularized form. The key to achieving this happy state of affairs was first the decision to modify only the boundary conditions, and second, the choice of regularized boundary conditions which gave simple forms for $\mathbf{M}^{(\epsilon)}$ and $\mathbf{N}^{(\epsilon)}$. We shall now show that these choices also allow $\lambda^{(\epsilon)}$ to be determined in a very simple and elegant way.

3. The regularization of the eigenvalue

While the regularized form of the determinant could be found by use of Forman's method, a new technique for calculating the previously vanishing eigenvalue, $\lambda^{(\epsilon)}$, has to be developed. It is natural to attempt to calculate it perturbatively in ϵ, but it is not at all obvious that a general procedure can be set up. Fortunately, it will turn out that choosing the regularized boundary conditions in the manner illustrated in section 2 on a simple example, enables $\lambda^{(\epsilon)}$ to be found to lowest order almost without calculation.

Let us begin describing the method where the operator is of the simple form (2.1); we will generalize to more complicated operators later in this section. There is no need to specify the boundary conditions at this stage, since, as we will see, a useful formula for $\lambda^{(\epsilon)}$ can be derived without having to make any choices of boundary conditions. Using the notation introduced in the last section

$$L y_1^{(\epsilon)} = \lambda^{(\epsilon)} y_1^{(\epsilon)} \tag{3.1}$$

where $y_1^{(\epsilon)}(t) \to y_1(t)$ and $\lambda^{(\epsilon)} \to 0$ as $\epsilon \to 0$. From (3.1)

$$\begin{aligned} \int_a^b \mathrm{d}t \, y_1 L y_1^{(\epsilon)} &= \lambda^{(\epsilon)} \int_a^b \mathrm{d}t \, y_1 y_1^{(\epsilon)} \\ &= \lambda^{(\epsilon)} \langle y_1 | y_1 \rangle \end{aligned} \tag{3.2}$$

to lowest order in ϵ. Integrating by parts gives, again to leading order,

$$\lambda^{(\epsilon)} = \frac{[\dot{y}_1^{(\epsilon)}(t)y_1(t) - \dot{y}_1(t)y_1^{(\epsilon)}(t)]_a^b}{\langle y_1|y_1\rangle}. \tag{3.3}$$

This result is true for operators of the form (2.1) with arbitrary boundary conditions. As an example, suppose we impose the regularized boundary conditions (2.8). Then the eigenfunction $y_1^{(\epsilon)}(t)$ will satisfy them: $y_1^{(\epsilon)}(a) = 0$, $y_1^{(\epsilon)}(b) = \epsilon\dot{y}_1^{(\epsilon)}(b)$. In addition $y_1(a) = y_1(b) = 0$, so that to lowest order

$$\begin{aligned}\lambda^{(\epsilon)} &= -\frac{\dot{y}_1(b)y_1^{(\epsilon)}(b)}{\langle y_1|y_1\rangle}\\ &= -\epsilon\frac{\dot{y}_1(b)\dot{y}_1(b)}{\langle y_1|y_1\rangle}\end{aligned} \tag{3.4}$$

as given in section 2. Note that the ϵ dependence simply comes from the requirement that $y_1^{(\epsilon)}(b) = \epsilon\dot{y}_1(b)$, to lowest order.

Analogous results to (3.3) hold for more general operators. For example, suppose that

$$L_{ij} = \delta_{ij}\frac{\mathrm{d}^2}{\mathrm{d}t^2} + P_{ij}(t) \qquad i, j = 1, \ldots, r \tag{3.5}$$

where $\mathbf{P}(t)$ is a complex matrix, and suppose that the operator (3.5) has a single zero mode $y_{i,1}$, that is, $\sum_{j=1}^r L_{ij}y_{j,1} = 0$. In matrix notation, the zero mode is the column vector $\boldsymbol{y}_1 = (y_{1,1}, \ldots, y_{r,1})^{\mathrm{T}}$. Let $\boldsymbol{y}_1^{(\epsilon)}(t)$ be the corresponding eigenfunction of the regularized problem with eigenvalue $\lambda^{(\epsilon)}$. Then to lowest order

$$\int_a^b \mathrm{d}t \sum_{i,j} y_{i,1}^* L_{ij} y_{j,1}^{(\epsilon)} = \lambda^{(\epsilon)} \sum_i \langle y_{i,1}|y_{i,1}\rangle \tag{3.6}$$

where now

$$\langle \boldsymbol{y}_1|\boldsymbol{y}_1\rangle \equiv \sum_i \langle y_{i,1}|y_{i,1}\rangle = \int_a^b \mathrm{d}t \sum_i |y_{i,1}(t)|^2. \tag{3.7}$$

Integrating the left-hand side of (3.6) by parts gives the leading order result

$$\lambda^{(\epsilon)} = \frac{\sum_{i=1}^r [y_{i,1}^*(t)\dot{y}_{i,1}^{(\epsilon)}(t) - \dot{y}_{i,1}^*(t)y_{i,1}^{(\epsilon)}(t)]_a^b}{\langle \boldsymbol{y}_1|\boldsymbol{y}_1\rangle} + \frac{\int_a^b \mathrm{d}t \sum_{i,j} y_{i,1}^*(t)\{P_{ij} - P_{ji}^*\}y_{j,1}^{(\epsilon)}(t)}{\langle \boldsymbol{y}_1|\boldsymbol{y}_1\rangle}. \tag{3.8}$$

In most cases of interest to us L will be formally self-adjoint, and so the second term in (3.8) will vanish. The self-adjoint nature of L is expected from its origin as the second functional derivative of the action in the path integral with respect to the fields:

$$L(t, t')_{ij} = \frac{\delta^2 S}{\delta u_i^*(t)\delta u_j(t')}. \tag{3.9}$$

The most general operator which we will study in this paper takes the form

$$L_{ij} = [\mathbf{P}_0(t)]_{ij}\frac{\mathrm{d}^2}{\mathrm{d}t^2} + [\mathbf{P}_1(t)]_{ij}\frac{\mathrm{d}}{\mathrm{d}t} + [\mathbf{P}_2(t)]_{ij} \tag{3.10}$$

where $\mathbf{P}_0(t)$, $\mathbf{P}_1(t)$ and $\mathbf{P}_2(t)$ are complex $r \times r$ matrices. We begin by making the transformation

$$p_{ij}(t) = \exp\left\{\tfrac{1}{2}\int^t \mathrm{d}t\, (\mathbf{P}_0)^{-1}(\mathbf{P}_1)\right\}_{ij} \qquad P_{ij}(t) = [p(\mathbf{P}_0)^{-1}(\mathbf{P}_2)(p)^{-1}]_{ij} - [\ddot{p}(p)^{-1}]_{ij} \tag{3.11}$$

so that

$$L_{ij} = (P_0)_{ik}(p^{-1})_{kl}\mathcal{L}_{lm}(p)_{mj} \tag{3.12}$$

where

$$\mathcal{L}_{ij} = \delta_{ij}\frac{\mathrm{d}^2}{\mathrm{d}t^2} + P_{ij}(t). \tag{3.13}$$

Now if $\hat{L}$ is such that $\hat{\mathbf{P}}_0(t) = \mathbf{P}_0(t)$, then

$$\frac{\det L}{\det \hat{L}} = \frac{\det \mathcal{L}}{\det \hat{\mathcal{L}}} \tag{3.14}$$

where $\hat{\mathcal{L}}$ is as in (3.13), but with P replaced by $\hat{P}$. Therefore the problem has been reduced to that considered earlier in this section (see (3.5) *et seq*). In fact, as regards determining the ratio of the determinants, Forman gives a general expression for the left-hand side of (3.14) (see next section), and so there is no need to implement the transformation (3.11). To find the eigenvalue $\lambda^{(\epsilon)}$, however, this transformation is useful. It is easy to see that $\mathcal{L}$ has a zero mode if, and only if, L does, and that, in particular, if $y_i(t)$ is an eigenfunction of L_{ij} with zero eigenvalue, then $z_i(t) = \sum_j p_{ij}(t)y_j(t)$ is an eigenfunction of $\mathcal{L}_{ij}$ with zero eigenvalue. The results (3.6)–(3.8) now hold, but with L and y replaced by $\mathcal{L}$ and z, respectively. As in all of the examples discussed in this section, a judicious choice for the boundary conditions on the regularized eigenfunction $y_1^{(\epsilon)}$ will yield an explicit regularized form for $\lambda^{(\epsilon)}$ with the minimum of calculational effort.

4. General procedure

There are two aspects to our approach to the calculation of $\det' L/\det \hat{L}$. One is the operation of finding $\lambda^{(\epsilon)}$ to leading order, which was explored for the general case in the last section. The other aspect concerns the application of Forman's method for the calculation of $\det L/\det \hat{L}$, but with the regularized boundary matrices $\mathbf{M}^{(\epsilon)}$ and $\mathbf{N}^{(\epsilon)}$. This was illustrated with a simple example in section 2; in this section we discuss Forman's method in more detail and explain how to apply it to the general operator (3.10). We end the section with a summary of the general procedure which we have developed in this paper.

We suppose, following Forman [4], that the boundary conditions on (3.10) may be expressed as

$$\mathbf{M}\begin{bmatrix} u(a) \\ \dot{u}(a) \end{bmatrix} + \mathbf{N}\begin{bmatrix} u(b) \\ \dot{u}(b) \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \tag{4.1}$$

where $\mathbf{M}$ and $\mathbf{N}$ are $2r \times 2r$ matrices. This equation is simply the r-dimensional analogue of (2.2). So for instance, if the boundary conditions are $u(a) = u(b) = 0$, then

$$\mathbf{M} = \begin{bmatrix} \mathbf{I}_r & 0 \\ 0 & 0 \end{bmatrix} \qquad \mathbf{N} = \begin{bmatrix} 0 & 0 \\ \mathbf{I}_r & 0 \end{bmatrix}. \tag{4.2}$$

where $\mathbf{I}_r$ is the $r \times r$ identity matrix.

Now suppose that $h_i(t)$; $i = 1, \ldots, r$, is a solution of the homogeneous differential equation $\sum_j L_{ij}h_j = 0$, and define the $2r \times 2r$ matrix $\mathbf{Y}(t)$, which describes the evolution of a solution and its first derivative with respect to t, by

$$\begin{bmatrix} h(t) \\ \dot{h}(t) \end{bmatrix} = \mathbf{Y}(t)\begin{bmatrix} h(a) \\ \dot{h}(a) \end{bmatrix}. \tag{4.3}$$

If $y_1(t), y_2(t), \ldots, y_{2r}(t)$, are $2r$ solutions of $Lh = 0$, (4.3) will apply to each solution separately, that is, $\mathbf{H}(t) = \mathbf{Y}(t)\mathbf{H}(a)$, where

$$\mathbf{H}(t) = \begin{bmatrix} y_1(t) & y_2(t) & \cdots & y_{2r}(t) \\ \dot{y}_1(t) & \dot{y}_2(t) & \cdots & \dot{y}_{2r}(t) \end{bmatrix}. \tag{4.4}$$

So, in particular, $\mathbf{H}(b) = \mathbf{Y}(b)\mathbf{H}(a)$, or, if the solutions are independent so that $\det \mathbf{H} \neq 0$,

$$\mathbf{Y}(b) = \mathbf{H}(b)\mathbf{H}^{-1}(a). \tag{4.5}$$

This explains the second construction (labelled (ii)) in section 2.

The formula for the ratio of determinants for operators of the type (3.10) is [4]

$$\frac{\det L}{\det \hat{L}} = \frac{\exp(\frac{1}{2}\int_a^b dt \ \mathrm{tr}\, \mathbf{P}_1(t)\mathbf{P}_0^{-1}(t)) \det(\mathbf{M} + \mathbf{N}\mathbf{Y}(b))}{\exp(\frac{1}{2}\int_a^b dt \ \mathrm{tr}\, \hat{\mathbf{P}}_1(t)\mathbf{P}_0^{-1}(t)) \det(\mathbf{M} + \mathbf{N}\hat{\mathbf{Y}}(b))} \tag{4.6}$$

For this result to be applicable, the matrices $\mathbf{P}_1(t)$ and $\hat{\mathbf{P}}_1(t)$, and also $\mathbf{P}_2(t)$ and $\hat{\mathbf{P}}_2(t)$ need not be equal, however the matrix $\mathbf{P}_0(t)$, multiplying the second derivative, must be the same for both operators. In most applications L will be normalized by a $\hat{L}$ which has a different, and simpler, matrix $\mathbf{P}_2$, but is otherwise the same. In these situations $\hat{\mathbf{P}}_1 = \mathbf{P}_1$, the exponential factors in (4.6) cancel out, and the simple formula given by (2.5) holds (except, of course, that $\mathbf{M}$, $\mathbf{N}$ and $\mathbf{Y}(b)$ are now $2r \times 2r$, not 2×2, matrices). We also note that, although the formula seems to be asymmetric with respect to the two points a and b, one could just as well define a matrix $\tilde{\mathbf{Y}}(t)$ by

$$\begin{bmatrix} h(t) \\ \dot{h}(t) \end{bmatrix} = \tilde{\mathbf{Y}}(t) \begin{bmatrix} h(b) \\ \dot{h}(b) \end{bmatrix} \tag{4.7}$$

so that $\mathbf{H}(a) = \tilde{\mathbf{Y}}(a)\mathbf{H}(b)$. Then $\det(\mathbf{M} + \mathbf{N}\mathbf{Y}(b)) = \det(\mathbf{N} + \mathbf{M}\tilde{\mathbf{Y}}(a))$. Therefore, alternative formulae to (2.5) and (4.6) exist, with $\mathbf{M}$ and $\mathbf{N}$ interchanged and $\mathbf{Y}(b)$ replaced by $\tilde{\mathbf{Y}}(a)$.

All of the formalism discussed so far in this section also applies to the problem with regularized boundary conditions—the only difference is that $\mathbf{M}$ and $\mathbf{N}$ are replaced by $\mathbf{M}^{(\epsilon)}$ and $\mathbf{N}^{(\epsilon)}$ respectively. We are now in a position to summarize the whole procedure.

(i) Modify the boundary conditions of the original problem by a small amount (ϵ), so that $y_1(t)$ is no longer a zero mode. Let $y_1^{(\epsilon)}(t)$ be the eigenfunction of the new problem with an eigenvalue $\lambda^{(\epsilon)}$ which tends to zero as $\epsilon \to 0$. Express the modified boundary conditions in the form (4.1) so that they are characterized by two matrices $\mathbf{M}^{(\epsilon)}$ and $\mathbf{N}^{(\epsilon)}$.

(ii) Calculate $\mathbf{Y}(b) = \mathbf{H}(b)\mathbf{H}^{-1}(a)$, where $\mathbf{H}(t)$ is given by (4.4).

(iii) Calculate $\det(\mathbf{M}^{(\epsilon)} + \mathbf{N}^{(\epsilon)}\mathbf{Y}(b))$.

(iv) Calculate $\lambda^{(\epsilon)}$ from (3.8).

(v) Hence determine

$$\lim_{\epsilon \to 0} \frac{\det(\mathbf{M}^{(\epsilon)} + \mathbf{N}^{(\epsilon)}\mathbf{Y}(b))}{\lambda^{(\epsilon)}}. \tag{4.8}$$

(vi) Calculate the denominator factor $\det(\mathbf{M} + \mathbf{N}\hat{\mathbf{Y}}(b))$.

(vii) The ratio of the results of the last two steps gives $\det' L / \det \hat{L}$.

We will now study various specific examples where this procedure is applied.

5. Specific examples

The algorithm given at the end of the last section gives a method for determining the ratio $\det' L / \det \hat{L}$. In this section we will give explicit results for a few examples with commonly met boundary conditions and also discuss one example in some detail to show how the method we have developed works in practice. We will only give results for the quantity given by (4.8), since the final result is found by normalizing this by $\det \hat{L}$, which can be found from the formulae given in, for example, Forman's paper [4].

For simplicity we only consider the single component ($r = 1$) case where the operator has the form (2.1), for a variety of boundary conditions.

(a) With the boundary conditions $Au(a) + B\dot{u}(a) = 0$; $Cu(b) + D\dot{u}(b) = 0$,

$$\frac{\det' L}{\langle y_1|y_1\rangle} = \begin{cases} +AC/\dot{y}_1(a)\dot{y}_1(b) & \text{if } A, C \neq 0 \\ -BC/y_1(a)\dot{y}_1(b) & \text{if } B, C \neq 0 \\ -AD/\dot{y}_1(a)y_1(b) & \text{if } A, D \neq 0 \\ +BD/y_1(a)y_1(b) & \text{if } B, D \neq 0 \end{cases} . \tag{5.1}$$

If all four constants A, B, C, D are non-zero it is easy to see that all four expressions are equivalent. Similarly, if only three of the constants are non-zero, then the two applicable expressions are equivalent. If only two constants are non-zero, one involved in the boundary condition at a and the other at b, then only one of the above applies. The simple example given in section 2 falls into this class: the boundary conditions there correspond to $A = 1$, $B = 0$, $C = 1$, $D = 0$, and in this case (5.1) reduces to (2.13).

(b) With periodic boundary conditions $u(a) = u(b)$; $\dot{u}(a) = \dot{u}(b)$,

$$\frac{\det' L}{\langle y_1|y_1\rangle} = \frac{y_2(b) - y_2(a)}{y_1(a)\det \mathbf{H}(a)} \tag{5.2}$$

where $\det \mathbf{H}(a) = \dot{y}_2(a)y_1(a) - \dot{y}_1(a)y_2(a)$ is the Wronskian.

(c) With anti-periodic boundary conditions $u(a) = -u(b)$; $\dot{u}(a) = -\dot{u}(b)$,

$$\frac{\det' L}{\langle y_1|y_1\rangle} = -\frac{y_2(b) + y_2(a)}{y_1(a)\det \mathbf{H}(a)}. \tag{5.3}$$

As an example of the application of these results, we use one of the most well known situations where instantons exist: imaginary time quantum mechanics with a potential $V(x) = \frac{1}{2}x^2 - \frac{1}{4}x^4$ [6]. As shown in the appendix, this problem leads one to consider operators of the form

$$L = -\frac{\mathrm{d}^2}{\mathrm{d}t^2} + 1 - 3\beta^2 \mathrm{dn}^2(u|m) \tag{5.4}$$

where dn is an elliptic function [10], $u = \beta(t - t_0)/\sqrt{2}$ and $\beta = 2(1 - m)/(2 - m)$. The constants t_0 and m originate from the integration of the second-order ordinary differential equation which is satisfied by the instanton. The parameter t_0 reflects the breaking of the time-translational invariance of the original theory and m is related to the energy of the classical particle in the mechanical analogy. The spectral properties of the system can be studied by imposing periodic boundary conditions on the path integral [11], which dictates that we use (5.2) to find the required functional determinant. A straightforward calculation, outlined in the appendix, yields

$$\frac{\det' L}{\langle y_1|y_1\rangle} = -\frac{2(2 - m)^{7/2}}{m^2}\left[\frac{K(m)}{2 - m} - \frac{E(m)}{2(1 - m)}\right] \tag{5.5}$$

where $K(m)$ and $E(m)$ are the complete elliptic integrals of the first and second kind, respectively.

This result simplifies considerably in the limit where the energy of the particle in the mechanical energy is zero and consequently the period of the instanton, T, becomes infinite.

In the appendix it is shown that the asymptotic forms of (5.5), $\det(\mathbf{M}+\mathbf{N}\hat{\mathbf{Y}}(b))$ and $\langle y_1|y_1\rangle$, for T large are, respectively, $e^T/16$, $-e^T$ and $\frac{4}{3}$. Combining all of these results gives

$$\lim_{T\to\infty} \frac{\det' L}{\det \hat{L}} = -\frac{1}{12}. \tag{5.6}$$

This is in agreement with previous calculations (e.g. equation (29) of [6]). It also illustrates the extra complication that may occur if the range (a, b) is infinite. In these cases the numerator (4.8) and the denominator $\det(\mathbf{M}+\mathbf{N}\hat{\mathbf{Y}}(b))$ may separately diverge as $T \equiv (b-a) \to \infty$. One can avoid these divergences in various ways, but the most obvious way to proceed in these cases is to use T as a regulator and to perform all calculations with T large, but finite, cancelling out the potential divergences between numerator and denominator before taking the $T \to \infty$ limit.

6. Conclusions

In this paper we have developed a simple and effective way of regularizing operators which have zero modes. The method allows the functional determinants for these kinds of operators, with the zero modes extracted, to be calculated. The main advantage of the method, and the reason for its power, is that it leaves much of the structure of the unregularized problem intact. This means that much of the formalism originally developed in this case can be taken over with very little change. The approach which we have adopted has not emphasized rigor; it would be very interesting to put this work on a rigorous footing. In particular, we have not proved that the results are independent of the precise method of regularization adopted. Until this is done, the results obtained using our method, especially for $r > 1$, should be treated with caution. On the other hand, we have also kept the number of examples of the application of the technique to a minimum, preferring instead to give a clear and explicit discussion of the methodology.

Although we have tried to be quite general, describing most aspects of the formalism which may arise in practice, there are, inevitably, situations that have not been covered. One is the case where there is more than one zero mode present—an example is the model studied in [7]. The procedure in cases such as this is a simple extension of our previous discussion: regularizing parameters $\epsilon_1, \epsilon_2, \ldots$ are introduced for every broken symmetry, and hence for every zero mode. This symmetry may be external (spatial or temporal) or internal (global or local). The boundary conditions are then modified along the directions of breaking by an amount ϵ_α, and the prescription given in section 5 followed.

Our motivation for carrying out this work has been the increasing need to evaluate determinants of this kind in many areas of the physical sciences. We hope that the ideas presented here are sufficiently straightforward and easily implemented so that they will find wide application.

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Appendix

In this appendix we give details of the calculation of the functional determinant of (5.4). The motivation for studying an operator of this type is that it arises in the investigation of fluctuations about the instanton in one-dimensional quantum mechanics with the potential $V(x) = \frac{1}{2}x^2 - \frac{1}{4}x^4$ [6]. The instanton satisfies the equation $-\ddot{x} + V'(x) = 0$, which may be integrated once to give $\frac{1}{2}\dot{x}^2 - V(x) = E$, where E is a constant. Solutions to this equation are those of a classical particle of unit mass and energy E moving in the potential $-V(x)$. Bounded motion is allowed for $E < 0$, corresponding to the existence of real instantons.

Let the values of x at which the particle in this mechanical analogy has zero velocity be denoted by α and β ($0 < \alpha < \beta$). Then $-V(\alpha) = -V(\beta) = E$ which implies $\alpha^2 + \beta^2 = 2$ and $E = -\alpha^2\beta^2/4$. The once integrated equation of motion now reads

$$\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 = \tfrac{1}{2}(x^2 - \alpha^2)(\beta^2 - x^2) \tag{A1}$$

$$\Rightarrow \int_\beta^x \frac{\mathrm{d}x}{\sqrt{(x^2-\alpha^2)(\beta^2-x^2)}} = -\frac{1}{\sqrt{2}}(t - t_0) \tag{A2}$$

where t_0 is the time at which the particle was at $x = \beta$. This may be integrated in terms of elliptic functions [10]:

$$x_c(t; t_0, m) = \beta\,\mathrm{dn}(u|m) \tag{A3}$$

where $u = \beta(t - t_0)/\sqrt{2}$ and $m = 1 - (\alpha^2/\beta^2)$. The subscript 'c' denotes 'classical' and simply indicates that this is a solution of the classical equation of motion $\delta S/\delta x(t) = 0$, where $S[x] = \int_a^b \mathrm{d}t\left[\frac{1}{2}\dot{x}^2 + V(x)\right]$ is the action. The physical significance of the integration constant t_0 is clear: since the particle can start at any x ($\alpha \leqslant x \leqslant \beta$), the time at which it reaches β (defined to be t_0) is arbitrary. The constant m, on the other hand, is directly related to the energy of the particle, since $E = -(1-m)/2(2-m)^2$. An alternative to m, which also specifies the energy of the particle, is the period T defined by

$$\frac{T}{2}\frac{1}{\sqrt{2}} = \int_\alpha^\beta \frac{\mathrm{d}x}{\sqrt{(x^2-\alpha^2)(\beta^2-x^2)}}$$

$$= \beta^{-1}\int_0^{\pi/2} \frac{\mathrm{d}\theta}{\sqrt{1 - m\sin^2\theta}} \tag{A4}$$

$$= \left(\frac{2-m}{2}\right)^{1/2} K(m) \tag{A5}$$

where $K(m)$ is the complete elliptic integral of the first kind [10].

As explained in the main part of the text, we are interested in evaluating the expression (5.2), and therefore need to determine the values of the functions y_1 and y_2 at the endpoints a and b. These two functions are solutions of the homogeneous differential equation $Lh = 0$, where

$$L\delta(t - t') = \left.\frac{\delta^2 S}{\delta x(t)\delta x(t')}\right|_{x=x_c} = \left[-\frac{\mathrm{d}^2}{\mathrm{d}t^2} + 1 - 3x_c^2(t; t_0, m)\right]\delta(t - t'). \tag{A6}$$

Using the explicit form for x_c given by (A3) we obtain (5.4). But two independent solutions of $Lh = 0$ can be found by differentiating x_c with respect to t_0 and m [12], so we define y_1 and y_2 by

$$y_1(t; t_0, m) \equiv \frac{\partial x_c(t; t_0, m)}{\partial t_0} \tag{A7}$$

$$y_2(t;t_0,m) \equiv \frac{\partial x_c(t;t_0,m)}{\partial m}. \tag{A8}$$

It is a straightforward exercise in elliptic functions to find from (A3) that

$$y_1(t;t_0,m) = \frac{m\beta^2}{\sqrt{2}}\mathrm{sn}(u|m)\mathrm{cn}(u|m) \tag{A9}$$

$$\dot{y}_1(t;t_0,m) = \frac{m\beta^3}{2}\mathrm{dn}(u|m)\{\mathrm{cn}^2(u|m) - \mathrm{sn}^2(u|m)\}. \tag{A10}$$

One can now check using (A5) that $y_1(a) = y_1(b)$ and that $\dot{y}_1(a) = \dot{y}_1(b)$ for any initial and final times satisfying $b - a = T$. Therefore, since y_1 is a solution of $Lh = 0$ satisfying the correct boundary conditions, it is the zero mode for this problem, as expected.

A slightly longer calculation gives

$$\begin{aligned} y_2(t;t_0,m) = {} & \frac{\mathrm{d}\beta}{\mathrm{d}m}\mathrm{dn}(u|m) - \left\{um\frac{\mathrm{d}\beta}{\mathrm{d}m} - \frac{\beta E(u|m)}{2(1-m)} + \frac{\beta u}{2}\right\}\mathrm{sn}(u|m)\mathrm{cn}(u|m) \\ & - \frac{\beta\,\mathrm{sn}^2(u|m)\mathrm{dn}(u|m)}{2(1-m)} \end{aligned} \tag{A11}$$

where $E(u|m)$ is the elliptic integral of the second kind. Using the periodicity of the elliptic functions

$$\begin{aligned} \frac{y_2(b) - y_2(a)}{y_1(a)} &= -2\left\{K(m)m\frac{\mathrm{d}\beta}{\mathrm{d}m} - \frac{\beta E(m)}{2(1-m)} + \frac{\beta}{2}K(m)\right\}\left\{\frac{\beta^2 m}{\sqrt{2}}\right\}^{-1} \\ &= -2\frac{(2-m)^{1/2}}{m}\left\{\frac{K(m)}{2-m} - \frac{E(m)}{2(1-m)}\right\} \end{aligned} \tag{A12}$$

since $\beta^2 = 2(2-m)^{-1}$. Here $E(m)$ is the complete elliptic integral of the second kind.

The Wronskian $\det \mathsf{H}(t)$ is a constant, and so can be calculated for any convenient t. Choosing $t = t_0$, which implies $u = 0$ and so $y_1(t_0) = 0$,

$$\begin{aligned} \det \mathsf{H}(t) &= \dot{y}_2(t_0)y_1(t_0) - \dot{y}_1(t_0)y_2(t_0) \\ &= -\left(\frac{\beta^3 m}{2}\right)\left(\frac{\mathrm{d}\beta}{\mathrm{d}m}\right) \\ &= -\frac{m}{(2-m)^3}. \end{aligned} \tag{A13}$$

Substituting (A12) and (A13) into (5.2), and taking into account the extra minus sign which comes about because the operator (5.4) is *minus* the definition of operators as given in the text, gives (5.5).

Following the discussion of the most natural form for $\hat{L}$ given in section 2, we take it to be the second functional derivative of the action for the harmonic oscillator with the potential $\hat{V}(x) = \frac{1}{2}x^2$. Then

$$\hat{L} = -\frac{\mathrm{d}^2}{\mathrm{d}t^2} + 1. \tag{A14}$$

Choosing $\hat{y}_1(t) = \mathrm{e}^t$ and $\hat{y}_2(t) = \mathrm{e}^{-t}$ to be the two independent solutions of the homogeneous equation $\hat{L}h = 0$,

$$\hat{\mathbf{Y}}(b) = \begin{bmatrix} \cosh(b-a) & \sinh(b-a) \\ \sinh(b-a) & \cosh(b-a) \end{bmatrix}. \tag{A15}$$

Using the same periodic boundary conditions which gave (5.2),

$$\det(\mathbf{M} + \mathbf{N}\hat{\mathbf{Y}}(b)) = 2 - \hat{\mathbf{Y}}_{11}(b) - \hat{\mathbf{Y}}_{22}(b)$$
$$= 2(1 - \cosh T) \tag{A16}$$
$$= -4\sinh^2([2-m]^{1/2}K(m)). \tag{A17}$$

Dividing (5.5) by (A17) gives the required expression for

$$\frac{1}{\langle y_1|y_1\rangle}\frac{\det' L}{\det \hat{L}}. \tag{A18}$$

As a check on the results let us look at the limit $E \to 0_-$, i.e. $m \to 1$ or $T \to \infty$. In this case $K(m) \sim \frac{1}{2}\ln(1-m)$, which from (A5) gives $m \sim 1 - 16\mathrm{e}^{-T}$. Using $E(m) \to 1$ as $m \to 1$, we have

$$\frac{\det' L}{\langle y_1|y_1\rangle} \sim \frac{\mathrm{e}^T}{16} \qquad \text{as } T \to \infty \tag{A19}$$

Since from (A16), $\det \hat{L} \sim -\mathrm{e}^T$ as $T \to \infty$,

$$\lim_{T\to\infty} \frac{1}{\langle y_1|y_1\rangle}\frac{\det' L}{\det \hat{L}} = -\frac{1}{16}. \tag{A20}$$

The sign is the expected one: the zero mode which has been extracted, y_1, has a single node, which leads us to deduce that L has only one eigenfunction with a negative eigenvalue; all the other eigenvalues are non-negative. The signs of (A17) and (A19) are not those that we might naively expect, but these signs have no meaning separately—both the magnitude and sign of these terms can be changed at will by the replacement $\mathbf{M} \to \lambda\mathbf{M}, \mathbf{N} \to \lambda\mathbf{N}$, where λ is any real number.

The ratio (A20) agrees with the calculation of [6]. To see this we note that $\alpha \to 0, \beta \to \sqrt{2}$ as $m \to 1$, hence the instanton becomes

$$x_c(t; t_0, m = 1) = \sqrt{2}\,\mathrm{sech}(t - t_0) \tag{A21}$$
$$\Rightarrow y_1(t; t_0, m = 1) = \sqrt{2}\,\mathrm{sech}(t - t_0)\tanh(t - t_0) \tag{A22}$$
$$\Rightarrow \lim_{T\to\infty}\langle y_1|y_1\rangle = \tfrac{4}{3}. \tag{A23}$$

Combining (A20) and (A23) gives (5.6), as required.

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