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by

Klaus Kirsten and Alan J. McKane

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Klaus Kirsten

Max Planck Institute for Mathematics in the Sciences,
Inselstrasse 22-26, 04103 Leipzig, Germany
and
Mathematics Department, Baylor University,
Waco TX 76798, USA

Alan J. McKane

Department of Theoretical Physics,
University of Manchester, Manchester M13 9PL,
England

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Abstract

We present a simple and accessible method which uses contour integration methods to derive formulae for functional determinants. To make the presentation as clear as possible, the general idea is first illustrated on the simplest case: a second order differential operator with Dirichlet boundary conditions. The method is applicable to more general situations, and we discuss the way in which the formalism has to be developed to cover these cases. In particular, we also show that simple and elegant formulae exist for the physically important case of determinants where zero modes exist, but have been excluded.

1 Introduction

The need to calculate functional determinants, usually of second order differential operators, arises in many different fields. For example, the leading order contribution to path-integrals often involves the integration of the exponential of a quadratic form, which can be carried out exactly, and yields a functional determinant [1, 2]. The explicit formulae for one-dimensional functional determinants of this kind are not simply of interest because of their utility, but also because rather general results may be obtained. For instance, the functional determinant of an operator L can often be given explicitly in terms of the solutions of the homogeneous equation $Ly = 0$. The elegance and generality of the results that can be obtained has attracted mathematicians, especially in the last decade or so. However, many researchers who are simply searching for an explicit form for a particular differential operator may find these treatments rather abstract, and, in addition, some will be interested in the value of these determinants with the zero modes extracted. These zero modes will usually exist whenever a quadratic form in a path-integral is the result of performing a linearisation about a solution with non-trivial spatial or temporal dependence. By Goldstone's theorem, this symmetry breaking will give rise to zero modes, which must be excluded from the quadratic form if this is to be a consistent leading order approximation [3]. Thus the functional determinant obtained by evaluating the path-integral is as before, but with these modes absent.

This paper is designed to give a simple, and easily accessible, derivation of the main formulae for functional determinants, and also to show how these results may be modified to give analogous expressions for determinants with the zero mode (or modes) extracted. We will avoid unnecessary mathematical abstraction, concentrate on the most straightforward results and give examples to illustrate the methods; a forthcoming paper will discuss some of the technical points in more detail [4]. Specifically, we will use only contour integration methods and elementary facts concerning the solutions of differential equations and concentrate on second order differential operators. An earlier study of determinants with the zero modes extracted [5] obtained results by invoking a regularisation procedure in which the zero modes became non-zero, extracting them, and then removing the regularisation. The problem with this approach is that it is not clear that the result is independent of the regularisation. Within the contour integration adopted here, the zero modes are not included from the beginning, and there is no need to introduce any regularisation procedure for them.

An early review of functional integrals and their evaluation [6] gives a prescription for finding the functional determinant of a second order differential operator with no first order derivative and with Dirichlet boundary conditions. The method consists of discretising the functional integral, explicitly carrying out the resulting multidimensional Gaussian integral, and showing that, on return to the continuum, the determinant satisfies the homogeneous equation with given boundary conditions. This method is also clearly presented in Schulman's book on path-integrals [2]. During the 1970's quantum field theory in general, and functional integral techniques in particular, became very popular and many studies of non-trivial field configurations such as solitons

and instantons appeared. In some cases [7] the calculation of the determinants involved in these studies were carried out by explicitly determining the eigenvalues of the Sturm-Liouville problem and calculating their product. This had the advantage that the omission of the zero mode required in these cases could be carried out explicitly. On the other hand, Coleman, in an appendix to his 1977 lectures on instantons at Erice [8], gives the outline of a rather straightforward demonstration of the result for Dirichlet boundary conditions mentioned above. The method, which depends on the result being known a priori, consists of shifting the eigenvalues by a parameter z, and arguing that both sides of the result to be proved are analytic in z and have the same zeros. Standard results from the theory of complex variables then allows the result to be proved.

The first published studies devoted to obtaining formulae for functional determinants of this kind were by Levit and Smilansky [9] and Dreyfus and Dym [10]. They extended the known results to more general kinds of operators, for example those of higher order, but continued to assume Dirichlet boundary conditions. While Dreyfus and Dym used a method of proof similar to Coleman's, Levit and Smilansky proved the result by showing that the logarithmic derivatives of both sides of the required result were equal. This was also the approach adopted by Forman [11], who extended the known results to situations with more general boundary conditions. These results were rederived by yet another method a few years later [12]. Burghelea *et al* investigated these and closely related questions using more abstract language [13, 14] (see also [15]); Ref [16] contains an accessible discussion of some of their results. In particular unknown prefactors are determined in these articles. Other authors [17]-[20] were concerned with defining generalised forms of determinants (the "p-determinant" or the "Δ-determinant") which act as regularised versions of the conventional determinant, and may be useful in cases where the usual determinant does not exist. Recent work has extended some of this rigorous work to regular singular potentials [21] and to more general kinds of boundary conditions [22]. Also explicit formulae that relate quotients of determinants with the corresponding Green function have been given [23].

In contrast to the many different techniques devised to prove these rather mathematically attractive results, the task of obtaining analogs for functional determinants with the zero mode extracted has been neglected. Apart from the paper by McKane and Tarlie already mentioned [5], the only published articles to address this point have been by Kleinert and Chervyakov [24, 25]. They base their approach on the Wronski method for constructing Green functions, but they do not discuss cases where there is more than one variable, and again introduce an explicit regularisation as an intermediate step in the calculation. In this article we will use the contour integration methods developed in [26, 27] to avoid introducing ad hoc regularisation procedures for the zero modes. For a recent review of these methods see Kirsten [28]. This will allow us to easily obtain the formulae for functional determinants we seek in terms of solutions of the associated homogeneous equation and the boundary data of the problem. The results generalise known answers where the absence of zero modes was assumed.

The outline of the paper is as follows. In Section 2 we describe the method in the most straightforward case: obtaining the functional determinant of a second order dif-

ferential operator with Dirichlet boundary conditions. Having illustrated the method, in Section 3 we discuss how the formalism has to be modified to give results when any zero mode which exists has been omitted. In sections 4 and 5 we extend the treatment of sections 2 and 3 respectively, to general boundary conditions. The extension to systems of differential equations will be briefly discussed in section 6 but, for simplicity, we will limit ourselves to an outline and give results which for the most part apply to a specific example. We conclude in section 7. Two appendices contain technical results pertaining to the development of some aspects of the formalism described in sections 5 and 6.

2 Dirichlet boundary conditions

We begin by considering the simplest class of differential operators:

$$L_j = -\frac{d^2}{dx^2} + R_j(x) \tag{1}$$

on the interval $I = [0, 1]$. Since the determinant of any such operator will diverge, it is usual to calculate ratios of determinants both of which involve operators having similar structure, for instance, defined on the same interval and having the same leading order term. The index $j = 1, 2$ labels these two determinants. We will adopt the convention that the $j = 1$ operator is the one for which we wish to calculate the determinant and the other, $j = 2$ one, will be some standard reference operator, in terms of which our result can be given. As long as the interval in the problem of interest is finite, we can shift and scale x so that $x \in [0, 1]$. The operators in this section will have no first derivative term and no non-trivial function of x multiplying the second derivative term. We will factor out any constant terms from the L_j so that the coefficients of the second derivatives is -1. The functions $R_j(x)$ will be assumed to be continuous and all the eigenvalues will be assumed to be positive.

In applications which involve the evaluation of functional integrals, ratios of determinants frequently arise, as do Dirichlet boundary conditions. So it is natural that the first results which were obtained should have been for this case. As we have already mentioned in Section 1, the result involves the solutions of the associated homogeneous equation. In fact it is given in terms of the solution which satisfies given initial conditions:

$$\frac{\det L_1}{\det L_2} = \frac{y_1(1)}{y_2(1)}, \tag{2}$$

where $y_j(x)$ is the unique solution of

$$L_j y_j(x) = 0, \quad y_j(0) = 0, \quad y_j'(0) = 1.$$

The main purpose of this section is to rederive this result by a direct contour integration method.

To do this let $u_{j,k}(x)$ be the unique solution of

$$(L_j - k^2)u_{j,k}(x) = 0$$

satisfying

$$u_{j,k}(0) = 0, \quad u'_{j,k}(0) = 1, \tag{3}$$

k being a complex parameter. The eigenvalues are then fixed by imposing

$$u_{j,k}(1) = 0. \tag{4}$$

The second condition in (3) is simply a choice of normalisation for the eigenfunction $u_{j,k}(x)$; we will indicate at the end of this section what happens if we make a more general choice. In what follows we will assume that $u_{j,k}(1)$ is analytic in k for $\Re k \geq 0$. The definition of this eigenvalue problem allows the zeta function of L_j to be written as

$$\zeta_{L_j}(s) = \frac{1}{2\pi i}\int_\gamma dk k^{-2s}\frac{d}{dk}\ln u_{j,k}(1).$$

The contour γ is counterclockwise and encloses all eigenvalues on the positive (by assumption) real axis. As given, the representation is valid for $\Re s > 1/2$. Clearly

$$\zeta_{L_1}(s) - \zeta_{L_2}(s) = \frac{1}{2\pi i}\int_\gamma dk k^{-2s}\frac{d}{dk}\ln\frac{u_{1,k}(1)}{u_{2,k}(1)}. \tag{5}$$

The next step is to deform the contour to the imaginary axis. In the case being considered here there are no negative or zero modes, this means $u_{j,0}(1) \neq 0$, and so no contribution arises from the origin. The leading $|k| \to \infty$ behaviour is independent of $R_j(x)$ and is governed by [29]

$$u_{j,k}(x) \sim \sin(kx)\left(1 + \mathcal{O}(k^{-1})\right), \tag{6}$$

$j = 1, 2$, so that for $|k| \to \infty$ we have

$$\frac{d}{dk}\ln\frac{u_{1,k}(1)}{u_{2,k}(1)} = \mathcal{O}(k^{-2}).$$

With $\epsilon > 0$ a small real number introduced to indicate that the contour approaches the imaginary axis from the right, this allows us to write

$$\zeta_{L_1}(s) - \zeta_{L_2}(s) = \frac{1}{2\pi i}\int_\infty^{-\infty} dk(ik + \epsilon)^{-2s}\frac{d}{dk}\ln\frac{u_{1,ik}(1)}{u_{2,ik}(1)}, \tag{7}$$

which is valid for $\Re s > -1/2$.

The next relevant observation is that $u_{j,ik}(x)$ and $u_{j,-ik}(x)$ satisfy the same differential equation, and since they are the unique solution one has $u_{j,ik}(x) = u_{j,-ik}(x)$.

The integral in (7) may be broken up into two contributions, $k > 0$ and $k < 0$. The two contributions combine to give

$$\zeta_{L_1}(s) - \zeta_{L_2}(s) = \frac{\sin(\pi s)}{\pi} \int_0^\infty dk k^{-2s} \frac{d}{dk} \ln \frac{u_{1,ik}(1)}{u_{2,ik}(1)},$$

which is valid for $-1/2 < \Re s < 1/2$. The upper restriction comes from the lower integration bound $k = 0$, whereas the lower restriction is from the upper integration limit as discussed.

From here it is immediate that

$$\zeta'_{L_1}(0) - \zeta'_{L_2}(0) = \int_0^\infty dk \frac{d}{dk} \ln \frac{u_{1,ik}(1)}{u_{2,ik}(1)} = -\ln \frac{u_{1,0}(1)}{u_{2,0}(1)} = -\ln \frac{y_1(1)}{y_2(1)},$$

which reproduces eq. (2) using the definition

$$\det(L_1 L_2^{-1}) = \exp -(\zeta'_{L_1}(0) - \zeta'_{L_2}(0)). \tag{8}$$

If we do not normalise $u'_{j,k}(0) = 1$ but instead ask that $u'_{j,k}(0) = c_j$, the above integral will give a contribution at infinity:

$$\zeta'_{L_1}(0) - \zeta'_{L_2}(0) = \ln \frac{u_{1,i\infty}(1)}{u_{2,i\infty}(1)} - \ln \frac{u_{1,0}(1)}{u_{2,0}(1)} = -\ln \frac{c_2 u_{1,0}(1)}{c_1 u_{2,0}(1)},$$

because now

$$\frac{u_{1,i\infty}(1)}{u_{2,i\infty}(1)} = \frac{c_1}{c_2}.$$

This is consistent with the answer expected:

$$\det(L_1 L_2^{-1}) = \frac{c_2 y_1(1)}{c_1 y_2(1)} = \frac{y_1(1) y_2'(0)}{y_1'(0) y_2(1)}. \tag{9}$$

The strength of the method is that, as discussed later, it can be applied with very little modification to more complicated operators and boundary conditions. However, just as important, we can use it to determine the analogous result to (9) for the situation where a zero mode is present and has been extracted.

3 Omitting the zero mode

To explain how the procedure discussed in the last section can be modified to deal with a situation in which a zero mode is present, but has been omitted from the evaluation of the determinant, we stay with the simple operator (1) and Dirichlet boundary conditions. However, as before, we will see that the method generalises to more complicated situations. In addition to (3) we now also suppose that $u_{1,0}(1) = 0$, that is, L_1 has an eigenfunction with zero eigenvalue, and all the other eigenvalues

are assumed to be positive. The integrand in (5) will now have a pole at $k = 0$ and therefore the contour γ can no longer be deformed along the imaginary axis. Our approach will be to consider a modified form of the integrand which has no pole, and which still gives us the determinant of L_1, but now with the zero eigenvalue extracted.

We first need to determine the behaviour of $u_{1,k}(1)$ for small k in order to eliminate the pole. To do this, we note that integrating the left-hand side of

$$\int_0^1 dx\, u_{1,0}(x)^* L_1 u_{1,k}(x) = k^2 \int_0^1 dx\, u_{1,0}(x)^* u_{1,k}(x),$$

by parts gives

$$\Big[u'_{1,0}(x)^* u_{1,k}(x) - u'_{1,k}(x)^* u_{1,0}(x)\Big]_0^1 + \int_0^1 dx\, u_{1,k}(x)(L_1 u_{1,0}(x))^* = k^2 \langle u_{1,0}|u_{1,k}\rangle.$$

Here $*$ denotes complex conjugation and we have introduced the Hilbert space product $\langle\ |\ \rangle$ on $\mathcal{L}^2(I)$ by

$$\langle u|v\rangle = \int_0^1 dx\ u(x)^*\ v(x).$$

Although we will be mostly concerned with real functions in this paper, the generalisation to complex functions will be required in section 6, and so it is useful to allow for this possibility in the development of the formalism.

Using the boundary conditions this gives

$$u_{1,k}(1) = \frac{k^2 \langle u_{1,0}|u_{1,k}\rangle}{u'_{1,0}(1)^*} \equiv -k^2 f_{1,k}. \tag{10}$$

Since $f_{1,k}$ is finite and non-zero as $k \to 0$, we have the desired behaviour of $u_{1,k}(1)$. The minus sign has been included in the definition of $f_{1,k}$ for later convenience. It is important to note that (10) is true for any k — no small k assumption was made to derive it.

We can now modify the discussion of section 2 to cover the case when a zero mode is present, by using the following two observations:

(i) The function $f_{1,k}$, defined by (10), vanishes at all values of k for which k^2 is a positive eigenvalue, as $u_{1,k}(1)$ does. Only in the case of the zero eigenvalue do we have the situation where $f_{1,0} \neq 0$, but $u_{1,0}(1) = 0$. Therefore if we use $f_{1,k}$ instead of $u_{1,k}(1)$ in (5), and choose the contour so as to surround the positive eigenvalues, the formalism developed in section 2 can be used to obtain the required result.

(ii) The notion that $u_{1,k}(1)$ may be straightforwardly substituted by $f_{1,k}$ has to be amended slightly, since these functions have different behaviours as $k \to \infty$. This is because the method of proof we used in the last section relies on $u_{1,ik}(1)$ and $u_{2,ik}(1)$ having the same behaviour in this limit. This difference in behaviour is accounted for if we replace $u_{1,k}(1)$ not by $f_{1,k}$, but by $(1 - k^2)f_{1,k}$, since then $u_{1,ik}(1) \sim k^2 f_{1,ik}$ as $k \to \infty$, while $(1 - k^2)f_{1,k}$ remains non-zero at $k = 0$.

These remarks lead us to consider the contour integral

$$\frac{1}{2\pi i}\int_\gamma dk k^{-2s}\frac{d}{dk}\ln(1-k^2)f_{1,k}, \tag{11}$$

where the contour surrounds all of the eigenvalues on the positive k axis. This integral equals

$$\zeta_{L_1}(s)+\frac{1}{2\pi i}\int_\gamma dk k^{-2s}\frac{d}{dk}\ln(1-k^2), \tag{12}$$

where it is understood that the zero mode has been omitted from the definition of the zeta-function. The second term in (12) is equal to 1 if the contour surrounds $k=1$, and zero if it does not. Our final result does not depend on this choice so, for definiteness, we choose the contour to surround this point.

The results (11) and (12) can now be combined with the conventional result for the zeta function of L_2 (the eigenvalues of L_2 are assumed to be all positive). The contour can safely be deformed to the imaginary axis and the contribution from infinity in the right-half plane shown to vanish. Using $f_{1,ik}=f_{1,-ik}$ and proceeding as before we find

$$\zeta_{L_1}(s)-\zeta_{L_2}(s)=\frac{\sin(\pi s)}{\pi}\int_0^\infty dk k^{-2s}\frac{d}{dk}\ln\frac{(1+k^2)f_{1,ik}}{u_{2,ik}(1)}-1. \tag{13}$$

The conditions on s for this representation to be valid are the same as those given in section 2, and therefore we may differentiate with respect to s and set $s=0$. If we impose the condition $u'_{j,k}(0)=1$, then the argument of the logarithm in (13) equals $u_{1,i\infty}(1)/u_{2,i\infty}(1)=1$ in the limit $k\to\infty$. Therefore the contribution from the upper limit of integration is zero. So only the contribution from the lower limit remains and we obtain

$$\zeta'_{L_1}(0)-\zeta'_{L_2}(0)=-\ln\frac{f_{1,0}}{u_{2,0}(1)}.$$

Using (8) and (10) this gives

$$\frac{\det' L_1}{\det L_2}=\frac{f_{1,0}}{u_{2,0}(1)}=-\frac{\langle y_1|y_1\rangle}{y'_1(1)^* y_2(1)}, \tag{14}$$

where we have denoted the determinant of L_1 with the zero mode extracted by $\det' L_1$.

This result should be compared to (2), rather than (9), since we have imposed the normalisation condition $y'_j(0)=1$. If we had not imposed normalisation conditions, an extra factor of c_1/c_2 would be present as in (9). We see that the modification required when a zero mode is extracted gives a final result which is still very simple, involving only the derivative of the zero mode at an end-point (both end-points if the function is not normalised) and its norm. It agrees with the result derived in Ref. [5], once typographical errors in eqns. (2.7) and (2.14) of that paper have been corrected. However, when making the comparison it should be borne in mind that the operators

used in that paper are minus those used here, and so the extraction of a mode gives a result which differs from ours by a sign. We can check that our result has the correct sign by noting that the lowest eigenfunction should have no nodes, so $y_1'(0)$ and $y_1'(1)$ should have opposite signs. In particular, if we impose the condition $y_1'(0) = 1$, then $y_1'(1) < 0$. Therefore, (14) should be positive, which is correct, since all eigenvalues are positive.

In applications it may not even be necessary to calculate $\langle y_1|y_1\rangle$. This is because, if the zero mode has been extracted using the method of collective coordinates [3], a Jacobian appears due to the transformation to new coordinates which, to lowest order, is proportional to the norm of the zero mode, and cancels it out. A little care is required with this cancellation, since the zero mode appearing in the Jacobian function will have a definite normalisation associated with it, which it inherited from the classical solution (for instance, the zero mode will be the spatial derivative of the classical solution if translational invariance has been broken). Therefore an overall constant may have to be factored out of the zero mode to get y_1, and similarly from the Jacobian to get $\langle y_1|y_1\rangle$, but these are purely algebraic procedures — no integration will be required.

To illustrate the ideas presented so far in this paper, let us give an example. A rich source of operators of the type (1) are Hamiltonian operators in one-dimensional quantum mechanics. The functions $R_j(x)$ will be the potentials; we will take as our example the linear potential [30] $R_1(x) = x - x_0$ and normalise it with respect to the case $R_2(x) = 0$. This potential has been chosen purely on grounds of simplicity; it has not to our knowledge occurred in a calculation of fluctuations about a nontrivial solution as described in the Introduction. As a consequence, if we wish the lowest eigenvalue to be zero, the constant x_0 has to be appropriately tuned.

The general solution of the equation $u_1'' = (x - x_0 - k^2)u_1$ which satisfies $u_{1,k}(0) = 0$ is, up to normalisation,

$$u_{1,k}(x) = \mathrm{Ai}(-z)\,\mathrm{Bi}(x-z) - \mathrm{Bi}(-z)\,\mathrm{Ai}(x-z), \quad z \equiv x_0 + k^2, \tag{15}$$

where Ai and Bi are Airy functions [31]. Implementation of the second boundary condition, $u_{1,k}(1) = 0$, fixes the condition for k^2 to be an eigenvalue. This condition takes the form of a transcendental equation involving Airy functions, however a good approximation to the allowed values of k^2 may be obtained by using the asymptotic form for Airy functions, valid when the argument of the function is large [31]. One finds $z^{3/2} = (z-1)^{3/2} + 3n\pi/2$, $n = 1, 2, \ldots$, which implies that $z \approx n^2\pi^2 + 1/2$. Although this result has been formally derived under the assumption that z is large, it turns out to be an excellent approximation even for quite small n: correct to 0.01%. For the $n = 1$ case, which is the least accurate, the true result is $10.3685\ldots$ and the above approximation gives $\pi^2 + 0.5 = 10.3696\ldots$. Note that for large n the eigenvalue condition becomes $z \approx n^2\pi^2$, which is the result which would be found in the case $R_2(x) = 0$. Thus it is at least plausible that the ratio of the product of eigenvalues converges. However, the whole point of the formalism we have been developing is to bypass the determination of the eigenvalues, and simply work with the solutions of the corresponding homogeneous equation.

The relevant solution of the homogeneous equation for this particular example is $y_1(x) = \lim_{k\to 0} u_{1,k}(x)$, where $u_{1,k}(x)$ is given by (15), but subject to the normalisation condition $u'_{1,k}(0) = 1$, as in (3). Thus

$$\begin{aligned} y_1(x) &= \frac{\mathrm{Ai}(-x_0)\,\mathrm{Bi}(x-x_0) - \mathrm{Bi}(-x_0)\,\mathrm{Ai}(x-x_0)}{\mathrm{Ai}(-x_0)\,\mathrm{Bi}'(-x_0) - \mathrm{Bi}(-x_0)\,\mathrm{Ai}'(-x_0)} \\ &= \pi\left[\mathrm{Ai}(-x_0)\mathrm{Bi}(x-x_0) - \mathrm{Bi}(-x_0)\mathrm{Ai}(x-x_0)\right], \end{aligned} \tag{16}$$

where we used the result for the Wronskian determinant [31]

$$W\left\{\mathrm{Ai}(z), \mathrm{Bi}(z)\right\} = \frac{1}{\pi}.$$

Similarly,

$$y_2(x) = x. \tag{17}$$

Therefore using (5),

$$\frac{\det L_1}{\det L_2} = \pi\left[\mathrm{Ai}(-x_0)\mathrm{Bi}(1-x_0) - \mathrm{Bi}(-x_0)\mathrm{Ai}(1-x_0)\right]. \tag{18}$$

If $x_0 = 0$, the result simplifies considerably [31]:

$$\frac{\det L_1}{\det L_2} = \frac{\Gamma(1/3)}{2\,3^{1/6}}\left[\mathrm{Bi}(1) - \sqrt{3}\mathrm{Ai}(1)\right] = 1.085. \tag{19}$$

Now suppose that we artificially fix x_0 to be $x_0^* = 10.3685\ldots$ — the smallest value of z for which $u_{1,k}(x)$ given by (15) satisfies $u_{1,k}(1) = 0$. Then $k^2 = 0$ is an eigenvalue, $y_1(1) = 0$ and the expression in (18) is identically zero. To find the ratio of functional determinants with the zero mode extracted from the determinant in the numerator, we use (14) and (16) to find

$$\frac{\det' L_1}{\det L_2} = -\frac{\langle y_1|y_1\rangle}{\pi(\mathrm{Ai}(-x_0^*)\mathrm{Bi}'(1-x_0^*) - \mathrm{Bi}(-x_0^*)\mathrm{Ai}'(1-x_0^*))} = 0.050666. \tag{20}$$

Let us mention that $\langle y_1|y_1\rangle$ can be expressed as a combination of Airy functions and their derivatives. However, no simplifications occur and we do not display the resulting answer.

4 General boundary conditions

In the last two sections we have illustrated how an expression for the ratio of functional determinants can be derived in the simple case of a single differential equation of the type (1) and Dirichlet boundary conditions. In the remainder of the paper we will extend this treatment to more general situations. Those parts of the proof involving zeta-functions and contour integration will remain essentially unchanged; the novel

aspects arise from setting up the problem so that the method naturally generalises. Since the main aim of this paper is to provide a transparent discussion available to a wide readership, we will limit our discussion to more general boundary discussions, leaving the topic of more complicated second order operators to a future paper [4]. We will, however, briefly discuss a system of two coupled operators of type (1) in section 6, in order to provide some indication of how the procedure generalises in that direction.

The boundary conditions on the functions on which L_j operates fall into two classes: separated and non-separated. Separated boundary conditions are defined as those which do not mix conditions on $u_{j,k}(x)$ and $u'_{j,k}(x)$ at the boundary $x = 0$ with conditions at the boundary $x = 1$. Robin boundary conditions $Au_{j,k}(0) + Bu'_{j,k}(0) = 0, Cu_{j,k}(1) + Du'_{j,k}(1) = 0$, where A, B, C, D are given real constants, are the generic case. Non-separated conditions can involve $u_{j,k}(x)$ and its derivative at different boundaries in the same equation. Periodic boundary conditions $u_{j,k}(0) = u_{j,k}(1), u'_{j,k}(0) = u'_{j,k}(1)$ are a common example. In previous sections, where Dirichlet boundary conditions were imposed, initial conditions were specified at $x = 0$ which guaranteed a unique $u_{j,k}(x)$ on which to impose boundary conditions. The imposition of more complicated types of boundary conditions, and in particular those of the non-separated type, does not permit us to proceed in the same way, and we need to set up a more systematic approach.

The first modification consists of no longer working with the second order differential equation

$$\frac{d^2u_{j,k}}{dx^2} = \left(R_j(x) - k^2\right) u_{j,k}, \tag{21}$$

but going over to the first order formalism where we define $v_{j,k}(x) \equiv u'_{j,k}(x)$, and view the column vector

$$\mathbf{u}_{j,k}(x) = \begin{pmatrix} u_{j,k}(x) \\ v_{j,k}(x) \end{pmatrix} \tag{22}$$

as the basic element of the theory. Then (21) may be written as

$$\frac{d}{dx}\begin{pmatrix} u_{j,k}(x) \\ v_{j,k}(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ R_j - k^2 & 0 \end{pmatrix} \begin{pmatrix} u_{j,k}(x) \\ v_{j,k}(x) \end{pmatrix}. \tag{23}$$

The general form for the boundary conditions can then be expressed in terms of $\mathbf{u}_{j,k}(x)$, using the notation of Ref. [11], as

$$M\begin{pmatrix} u_{j,k}(0) \\ v_{j,k}(0) \end{pmatrix} + N\begin{pmatrix} u_{j,k}(1) \\ v_{j,k}(1) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \tag{24}$$

where M and N are 2×2 matrices. For example, in the case of Dirichlet boundary conditions

$$M = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad N = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{25}$$

Now let $\mathbf{u}_{j,k}^{(1)}(x)$ and $\mathbf{u}_{j,k}^{(2)}(x)$ be two independent solutions of the differential equation (23). We will not impose the boundary condition (24) on these solutions, instead they will be uniquely specified by the imposition of initial conditions. They may then be thought of as basis functions from which a general solution can be constructed:

$$\begin{aligned}\begin{pmatrix} u_{j,k}(x) \\ v_{j,k}(x) \end{pmatrix} &= \begin{pmatrix} \alpha u_{j,k}^{(1)}(x) + \beta u_{j,k}^{(2)}(x) \\ \alpha v_{j,k}^{(1)}(x) + \beta v_{j,k}^{(2)}(x) \end{pmatrix} \\ &= \begin{pmatrix} u_{j,k}^{(1)}(x) & u_{j,k}^{(2)}(x) \\ v_{j,k}^{(1)}(x) & v_{j,k}^{(2)}(x) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \end{aligned} \tag{26}$$

In the special case when k^2 is an eigenvalue, the constants α and β can then be chosen so that $\mathbf{u}_{j,k}(x)$ satisfies the boundary conditions (24).

Now

$$H_{j,k}(x) = \begin{pmatrix} u_{j,k}^{(1)}(x) & u_{j,k}^{(2)}(x) \\ v_{j,k}^{(1)}(x) & v_{j,k}^{(2)}(x) \end{pmatrix} \tag{27}$$

is a fundamental solution to (23). Since $\det H_{j,k}(x) \neq 0$,

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = H_{j,k}^{-1}(0) \begin{pmatrix} u_{j,k}(0) \\ v_{j,k}(0) \end{pmatrix}.$$

So, in summary,

$$\begin{pmatrix} u_{j,k}(x) \\ v_{j,k}(x) \end{pmatrix} = H_{j,k}(x) H_{j,k}^{-1}(0) \begin{pmatrix} u_{j,k}(0) \\ v_{j,k}(0) \end{pmatrix}$$

is the unique solution of (23) with initial value $(u_{j,k}(0), v_{j,k}(0))$ at $x = 0$. This allows us to rewrite the boundary condition (24) as

$$(M + N H_{j,k}(1) H_{j,k}^{-1}(0)) \begin{pmatrix} u_{j,k}(0) \\ v_{j,k}(0) \end{pmatrix} = 0. \tag{28}$$

Nontrivial solutions only exist if

$$\det \left(M + N H_{j,k}(1) H_{j,k}^{-1}(0) \right) = 0, \tag{29}$$

and this gives the condition for k^2 to be an eigenvalue.

Although we could in principle work with any set of $\{\mathbf{u}_{jk}^{(1)}(x), \mathbf{u}_{jk}^{(2)}(x)\}$, a particularly suitable choice is

$$H_{j,k}(0) = \begin{pmatrix} u_{j,k}^{(1)}(0) & u_{j,k}^{(2)}(0) \\ v_{j,k}^{(1)}(0) & v_{j,k}^{(2)}(0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{30}$$

This has a number of simplifying features. For instance, $\det H_{j,k}(x) = 1$ for all x, $\alpha = u_{j,k}(0), \beta = v_{j,k}(0)$ and the eigenvalue condition becomes $\det(M + N H_{j,k}(1)) = 0$.

A simple example of a set of functions satisfying (30) are those for the equation with $R_j = 0$. They are given by $u^{(1)}_{j,k}(x) = \cos kx$ and $u^{(2)}_{j,k}(x) = k^{-1}\sin kx$.

The solution $\mathbf{u}_{j,k}(x)$, by contrast, depends on the nature of the boundary conditions. For Robin boundary conditions, for example, $A\alpha + B\beta = 0$, and we may take $\alpha = -B$ and $\beta = A$, $u_{j,k}(x)$ being only defined up to a constant as usual. Thus

$$\mathbf{u}_{jk}(x) = -B\mathbf{u}^{(1)}_{j,k}(x) + A\mathbf{u}^{(2)}_{j,k}(x). \tag{31}$$

It is now straightforward to calculate $\det(M+NH_{j,k}(1))$ using the matrices appropriate for Robin conditions:

$$M = \begin{pmatrix} A & B \\ 0 & 0 \end{pmatrix}, \quad N = \begin{pmatrix} 0 & 0 \\ C & D \end{pmatrix}, \tag{32}$$

to find that

$$\det(M + NH_{j,k}(1)) = Cu_{j,k}(1) + Dv_{j,k}(1),$$

so that imposing the boundary conditions at the "final" point gives the eigenvalue condition (29).

For non-separated boundary conditions, initial and final conditions are mixed together and the appropriate linear combination (26) is determined by imposing either one of the boundary conditions. For example in the case of periodic boundary conditions, $u_{j,k}(0) = u_{j,k}(1)$ implies that $\alpha(1 - u^{(1)}_{j,k}(1)) = \beta u^{(2)}_{j,k}(1)$, so that we may take

$$u_{j,k}(x) = u^{(2)}_{j,k}(1)u^{(1)}_{j,k}(x) + \left(1 - u^{(1)}_{j,k}(1)\right) u^{(2)}_{j,k}(x). \tag{33}$$

The other boundary condition then gives the eigenvalue condition. Explicitly calculating $\det(M + NH_{j,k}(1))$ using (33) and $M = -N = I_2$, where I_2 is the 2×2 unit matrix, one finds

$$\det(M + NH_{j,k}(1)) = v_{j,k}(0) - v_{j,k}(1).$$

It is now possible to see how the approach adopted to investigate the case of Dirichlet boundary conditions fits into this more general structure. The solution $\mathbf{u}_{j,k}(x)$ which satisfies (23) is simply equal to $u^{(2)}_{j,k}(x)$ introduced in this section, that is, $\alpha = 0, \beta = 1$. Using (25), $\det(M + NH_{j,k}(1)) = u^{(2)}_{j,k}(1)$, so that the eigenvalues are fixed by imposing $u_{j,k}(1) = 0$, just as in (4). For Neumann boundary conditions $\alpha = 1, \beta = 0$; for other cases both of the fundamental solutions $u^{(1)}_{j,k}(x)$ and $u^{(2)}_{j,k}(x)$ will be required to construct a solution $u_{j,k}(x)$ which has the correct properties.

The discussion presented in this section so far indicates how our earlier proof can be extended to more general types of boundary conditions. Assuming suitable analyticity properties in k, the eigenvalue condition (4) is now replaced by the more general condition (29), and so the analogue of (5) becomes

$$\zeta_{L_1}(s) - \zeta_{L_2}(s) = \frac{1}{2\pi i}\int_\gamma dk k^{-2s}\frac{d}{dk}\ln\frac{\det(M + NH_{1,k}(1))}{\det(M + NH_{2,k}(1))}. \tag{34}$$

We next perform the same steps as in section 2. The leading $|k| \to \infty$ behaviour of $u^{(2)}_{j,k}(x)$ is governed by eq. (6), whereas for $u^{(1)}_{j,k}(x)$ we have [29]

$$u^{(1)}_{j,k}(x) \sim \cos(kx)(1 + \mathcal{O}(k^{-1})).$$

This shows

$$\frac{d}{dk} \ln \frac{\det(M + NH_{1,k}(1))}{\det(M + NH_{2,k}(1))} = \mathcal{O}(k^{-2})$$

and all goes through as before. Thus, with the definition

$$Y_j(x) \equiv \begin{pmatrix} y^{(1)}_j(x) & y^{(2)}_j(x) \\ y^{(1)\prime}_j(x) & y^{(2)\prime}_j(x) \end{pmatrix} = \lim_{k\to 0} H_{j,k}(x)$$

the formalism immediately provides the answer for the quotient of determinants

$$\frac{\det L_1}{\det L_2} = \frac{\det(M + NY_1(1))}{\det(M + NY_2(1))}. \tag{35}$$

From a practical point of view, in order to calculate (35) only the matrices M and N, which specify the boundary conditions, and the two independent solutions $\{y^{(1)}_j(x), y^{(2)}_j(x)\}$ of the homogeneous equation $L_j y_j = 0$ are needed. These fundamental solutions also satisfy the initial conditions (30) inherited from the solutions $\{u^{(1)}_{j,k}(x), u^{(2)}_{j,k}(x)\}$:

$$Y_j(0) = \begin{pmatrix} y^{(1)}_j(0) & y^{(2)}_j(0) \\ y^{(1)\prime}_j(0) & y^{(2)\prime}_j(0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{36}$$

For instance, in the example introduced in section 3 where $R_1(x) = x$, the fundamental solutions are

$$\begin{aligned} y^{(1)}_1(x) &= \frac{3^{-1/3}\,\pi}{\Gamma(1/3)} \left[\mathrm{Bi}(x) + \sqrt{3}\mathrm{Ai}(x)\right] \\ y^{(2)}_1(x) &= \frac{\Gamma(1/3)}{2\,3^{1/6}} \left[\mathrm{Bi}(x) - \sqrt{3}\mathrm{Ai}(x)\right]. \end{aligned} \tag{37}$$

For Dirichlet boundary conditions $y_1(x)$ is simply $y^{(2)}_1(x)$ (compare with (19)), and for Neumann boundary conditions it is $y^{(1)}_1(x)$.

Let us end this section by giving an alternative, slightly simpler, form for (35) which will be useful in the next section. We have seen in the case of Robin and periodic boundary conditions, that if we implement one of the boundary conditions, then $\det(M+NH_{j,k}(1))$ is proportional (equal, with the correct choice of normalisation) to the other condition. This will be true in general. To explicitly show this, let us write the condition (24) out in full:

$$\begin{pmatrix} m_{11}u_{j,k}(0) + m_{12}v_{j,k}(0) + n_{11}u_{j,k}(1) + n_{12}v_{j,k}(1) \\ m_{21}u_{j,k}(0) + m_{22}v_{j,k}(0) + n_{21}u_{j,k}(1) + n_{22}v_{j,k}(1) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{38}$$

We ask that $u_{j,k}(x)$ satisfy only one boundary condition. This could be either one, but one choice gives

$$m_{11}u_{j,k}(0) + m_{12}v_{j,k}(0) + n_{11}u_{j,k}(1) + n_{12}v_{j,k}(1) = 0. \tag{39}$$

We now want to construct a $u_{j,k}(x)$ which explicitly satisfies the condition (39). To do so we expand $u_{j,k}(x)$ as in (26) and implement (39). This gives (with an appropriate choice of normalisation)

$$\begin{aligned} u_{j,k}(x) &= -\left[m_{12} + n_{11}u^{(2)}_{j,k}(1) + n_{12}v^{(2)}_{j,k}(1)\right] u^{(1)}_{j,k}(x) \\ &+ \left[m_{11} + n_{11}u^{(1)}_{j,k}(1) + n_{12}v^{(1)}_{j,k}(1)\right] u^{(2)}_{j,k}(x). \end{aligned} \tag{40}$$

Using the expression (40) to calculate an explicit expression for the second row of the left-hand side of (38) gives

$$\begin{aligned} \det M + \det N &+ u^{(1)}_{j,k}(1)(n_{11}m_{22} - n_{21}m_{12}) + u^{(2)}_{j,k}(1)(m_{11}n_{21} - m_{21}n_{11}) \\ &+ v^{(1)}_{j,k}(1)(n_{12}m_{22} - n_{22}m_{12}) + v^{(2)}_{j,k}(1)(m_{11}n_{22} - m_{21}n_{12}), \end{aligned}$$

which is simply $\det(M + NH_{j,k}(1))$ expanded out and simplified using $\det H_{j,k}(1) = 1$. Therefore we have shown that

$$\det(M + NH_{j,k}(1)) = m_{21}u_{j,k}(0) + m_{22}v_{j,k}(0) + n_{21}u_{j,k}(1) + n_{22}v_{j,k}(1). \tag{41}$$

The fact that the constant of proportionality between the two sides of this equation is 1 is a consequence of the judicious choice of normalisation of (40). If we had chosen to implement the second row of (38) instead of (39), we would simply have obtained a different $u_{j,k}(x)$, which, when substituted into the first row of (38), would have again given $\det(M + NH_{j,k}(1))$.

As a result of (41) we find for the quotient of functional determinants

$$\frac{\det L_1}{\det L_2} = \frac{m_{21}y_1(0) + m_{22}y_1'(0) + n_{21}y_1(1) + n_{22}y_1'(1)}{m_{21}y_2(0) + m_{22}y_2'(0) + n_{21}y_2(1) + n_{22}y_2'(1)}, \tag{42}$$

which is the alternative form to (35) mentioned above. It is now possible to immediately write down the required formulae for any boundary condition. For instance, in the case of Robin boundary conditions defined by (32),

$$\frac{\det L_1}{\det L_2} = \frac{Cy_1(1) + Dy_1'(1)}{Cy_2(1) + Dy_2'(1)}, \tag{43}$$

and for periodic boundary conditions defined by $M = -N = I_2$,

$$\frac{\det L_1}{\det L_2} = \frac{y_1'(0) - y_1'(1)}{y_2'(0) - y_2'(1)}. \tag{44}$$

5 Omitting the zero mode: general case

In this section we will derive the result for the ratio of functional determinants when a zero mode has been extracted, in the case when general boundary conditions of the type (24) have been imposed on operators of the type (1). As before, we will assume that the operator L_j with the boundary conditions imposed defines a self-adjoint operator. This requires that the elements of the matrices M and N satisfy certain conditions, as described in Appendix A. The main result which we will require will be the nature of the generalisation of (10), where $u_{1,k}(1)$ will presumably be replaced by $\det(M+NH_{j,k}(1))$. As in section 3, the starting point of the analysis is

$$[v_{1,0}(x)^* u_{1,k}(x) - v_{1,k}(x)u_{1,0}(x)^*]_0^1 = k^2\langle u_{1,0}|u_{1,k}\rangle. \tag{45}$$

We implement both boundary conditions on the $k = 0$ solution, but only one of the boundary conditions on the solution for general k, since we wish to keep k arbitrary, and not restrict it so that k^2 is an eigenvalue.

To gain some insight, we first look at particular boundary conditions before we outline the procedure for general boundary conditions. For Robin boundary conditions we have $Au_{1,0}(0) + Bv_{1,0}(0) = 0, Cu_{1,0}(1) + Dv_{1,0}(1) = 0$ and $Au_{1,k}(0) + Bv_{1,k}(0) = 0$. The left-hand side of (45) then gives zero for the contribution at $x = 0$ (both functions satisfy the boundary conditions there) and at $x = 1$ gives

$$-\frac{C}{D}u_{1,0}(1)^* u_{1,k}(1) - v_{1,k}(1)u_{1,0}(1)^* = -\left(\frac{u_{1,0}(1)^*}{D}\right)\left[Cu_{1,k}(1) + Dv_{1,k}(1)\right].$$

Therefore

$$Cu_{1,k}(1) + Dv_{1,k}(1) = -\left(\frac{D}{u_{1,0}(1)^*}\right) k^2\langle u_{1,0}|u_{1,k}\rangle. \tag{46}$$

For periodic boundary conditions we have $u_{1,0}(0) = u_{1,0}(1), v_{1,0}(0) = v_{1,0}(1)$ and $u_{1,k}(0) = u_{1,k}(1)$. The left-hand side of (45) then gives

$$-v_{1,k}(1)u_{1,0}(0)^* + v_{1,k}(0)u_{1,0}(0)^*$$

which leads to

$$v_{1,k}(0) - v_{1,k}(1) = \frac{1}{u_{1,0}(0)^*}\, k^2\langle u_{1,0}|u_{1,k}\rangle. \tag{47}$$

For all special examples considered, the result takes the form (see eqs. (10), (46), (47))

$$\det(M + NH_{1,k}(1)) = \mathcal{B}k^2\langle u_{1,0}|u_{1,k}\rangle, \tag{48}$$

where $\mathcal{B}$ depends on the zero mode data at the boundary and on the boundary condition imposed.

In fact, the procedure described above can be extended to the case of general boundary conditions and the analogous results will always have the form (48). To see

this recall from the last section that implementing one boundary condition only leads, in the case of general boundary conditions, to (see (39) and (41))

$$\begin{aligned} m_{11}u_{1,k}(0) + m_{12}v_{1,k}(0) + n_{11}u_{1,k}(1) + n_{12}v_{1,k}(1) &= 0 \\ m_{21}u_{1,k}(0) + m_{22}v_{1,k}(0) + n_{21}u_{1,k}(1) + n_{22}v_{1,k}(1) &= \det(M + NH_{1,k}(1)). \end{aligned} \tag{49}$$

When $k = 0$, $u_{1,k}(x)$ is the zero mode and so (49) holds, but with $\det(M + NH_{1,0}(1))$ replaced by 0.

We wish to obtain expressions for $u_{1,k}(x), u_{1,0}(x)$, and their derivatives, at the boundaries in order to substitute them into the left-hand side of (45), and ultimately obtain an expression for $\det(M + NH_{1,k}(1))$. To do this we have to proceed by cases, which depend on the particular boundary conditions prescribed. Suppose that, for instance, the boundary conditions are such that $m_{12}n_{22} - n_{12}m_{22} \neq 0$. Then in this case we rewrite (49) as

$$\begin{pmatrix} m_{12} & n_{12} \\ m_{22} & n_{22} \end{pmatrix} \begin{pmatrix} v_{1,k}(0) \\ v_{1,k}(1) \end{pmatrix} = \begin{pmatrix} 0 \\ \det(M + NH_{1,k}(1)) \end{pmatrix} - \begin{pmatrix} m_{11} & n_{11} \\ m_{21} & n_{21} \end{pmatrix} \begin{pmatrix} u_{1,k}(0) \\ u_{1,k}(1) \end{pmatrix}. \tag{50}$$

The condition on the elements of M and N that we have imposed implies that the matrix on the extreme left of (50) is invertible and so we may solve for $v_{1,k}(0)$ and $v_{1,k}(1)$. These intermediate results are of no intrinsic interest and are given in the Appendix A. Obviously the equations for $v_{1,0}(0)$ and $v_{1,0}(1)$ are identical to those for general k, except that $\det(M + NH_{1,k}(1))$ is replaced by $\det(M + NH_{1,0}(1)) = 0$. We may now eliminate $v_{1,k}(0), v_{1,k}(1), v_{1,0}(0)$ and $v_{1,0}(1)$ from (45) using these equations. The basic steps are outlined in Appendix A. We obtain

$$\det(M + NH_{1,k}(1)) = \frac{n_{12}m_{22} - m_{12}n_{22}}{m_{12}u_{1,0}(1)^* + n_{12}u_{1,0}(0)^*}\langle u_{1,0}|u_{1,k}\rangle, \quad n_{12}m_{22} - m_{12}n_{22} \neq 0. \tag{51}$$

Expressing $\{v_{1,k}(0), v_{1,k}(1)\}$ in terms of $\{u_{1,k}(0), u_{1,k}(1)\}$ is just one possibility; there are five more ways to express two boundary data by the complementary ones. Proceeding as described gives the list of results presented in Appendix A. It is seen that the precise form that $\mathcal{B}$ takes depends on which combination of elements of M and N are non-zero. The formulae in Appendix A, together with (51), cover all possible cases. If more than one of the results is appropriate, then they are, of course, equivalent.

Having established that (48) holds in general, we may simply replace (10) by

$$\det(M + NH_{1,k}(1)) = -k^2 f_{1,k}; \quad f_{1,k} \equiv -\mathcal{B}\langle u_{1,0}|u_{1,k}\rangle, \tag{52}$$

and repeat the steps in section 3. One finds

$$\zeta'_{L_1}(0) - \zeta'_{L_2}(0) = -\ln \frac{f_{1,0}}{\det(M + NY_2(1))},$$

which using (8) gives

$$\frac{\det' L_1}{\det L_2} = -\frac{\mathcal{B}\,\langle y_1|y_1\rangle}{\det(M + NY_2(1))}, \tag{53}$$

where $\mathcal{B}$ takes on the following values:

$$\begin{aligned}
&\frac{n_{12}m_{22}-m_{12}n_{22}}{m_{12}y_1(1)^*+n_{12}y_1(0)^*}, && \text{if } n_{12}m_{22}-m_{12}n_{22} \neq 0,\\
&\frac{m_{11}n_{21}-m_{21}n_{11}}{m_{11}y_1'(1)^*+n_{11}y_1'(0)^*}, && \text{if } m_{11}n_{21}-m_{21}n_{11} \neq 0,\\
&\frac{m_{11}m_{22}-m_{12}m_{21}}{m_{12}y_1'(0)^*+m_{11}y_1(0)^*}, && \text{if } m_{11}m_{22}-m_{12}m_{21} \neq 0,\\
&\frac{m_{12}n_{21}-m_{22}n_{11}}{m_{12}y_1'(1)^*-n_{11}y_1(0)^*}, && \text{if } m_{12}n_{21}-m_{22}n_{11} \neq 0,\\
&\frac{n_{12}n_{21}-n_{22}n_{11}}{n_{12}y_1'(1)^*+n_{11}y_1(1)^*}, && \text{if } n_{12}n_{21}-n_{22}n_{11} \neq 0,\\
&\frac{m_{11}n_{22}-m_{21}n_{12}}{n_{12}y_1'(0)^*-m_{11}y_1(1)^*}, && \text{if } m_{11}n_{22}-m_{21}n_{12} \neq 0.
\end{aligned} \tag{54}$$

As an example, for periodic boundary conditions when $M = I_2$, the third of the above results is applicable, and therefore $\mathcal{B} = 1/y_1(0)^*$. Equivalently the fifth result may be used, since $N = -I_2$, to give $\mathcal{B} = 1/y_1(1)^*$. Furthermore $\det(M + NY_2(1)) = y_2'(0) - y_2'(1)$ (see (44)), so that

$$\frac{\det' L_1}{\det L_2} = -\frac{\langle y_1|y_1\rangle}{y_1(0)^*\,[y_2'(0)-y_2'(1)]}. \tag{55}$$

Let us end this section by showing that (55) is in agreement with the result obtained by a different method [5]. In order to show that the two results are identical, we need to establish a correspondence between the solutions utilised in the two approaches. In this paper we have taken $u^{(1)}_{j,k}(x)$ and $u^{(2)}_{j,k}(x)$ — which in the $k \to 0$ limit become $y^{(1)}(x)$ and $y^{(2)}(x)$ — as the two independent solutions (to facilitate comparisons with the formulae given in Ref. [5], we will drop the j subscript for the rest of this section). In Ref. [5] the two independent solutions were denoted by $y_1(x)$ and $y_2(x)$, but we will denote them here by $y^{(\mathrm{I})}(x)$ and $y^{(\mathrm{II})}(x)$. The solution $y^{(\mathrm{I})}(x)$ is simply what we have called $y(x)$ in this paper, that is, the solution which is the zero mode if one exists, and which satisfies only one of the boundary conditions, if a zero mode does not exist. Thus from (26), when $k \to 0$,

$$\begin{pmatrix} y^{(\mathrm{I})}(x) & y^{(\mathrm{II})}(x) \\ y^{(\mathrm{I})\prime}(x) & y^{(\mathrm{II})\prime}(x) \end{pmatrix} = \begin{pmatrix} y^{(1)}(x) & y^{(2)}(x) \\ y^{(1)\prime}(x) & y^{(2)\prime}(x) \end{pmatrix} \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix}, \tag{56}$$

where $y^{(\mathrm{II})}(x) = \gamma y^{(1)}(x) + \delta y^{(2)}(x)$ is any solution which is independent of $y^{(\mathrm{I})}(x)$. Since $\det Y(x) = 1$ in our formalism, the Wronskian of the two solutions $y^{(\mathrm{I})}(x)$ and $y^{(\mathrm{II})}(x)$ is

$$y^{(\mathrm{I})}(x)y^{(\mathrm{II})\prime}(x) - y^{(\mathrm{II})}(x)y^{(\mathrm{I})\prime}(x) = \alpha\delta - \beta\gamma. \tag{57}$$

All of this holds whatever the nature of the boundary conditions — they will correspond to particular choices for α and β. Specifically, for periodic boundary conditions,

(33) shows that $\alpha = y^{(2)}(1)$ and $\beta = 1 - y^{(1)}(1)$, so that the Wronskian, W, is given by $W = \delta y^{(2)}(1) - \gamma\left(1 - y^{(1)}(1)\right)$. It is straightforward to show that $y^{(\mathrm{II})}(1) - y^{(\mathrm{II})}(0)$ is also equal to this quantity. So, for periodic boundary conditions, and $y^{(\mathrm{I})}(x)$ given by the $k \to 0$ version of (33), $W = y^{(\mathrm{II})}(1) - y^{(\mathrm{II})}(0)$. This verifies that eq. (5.2) of Ref. [5] reduces to (55) above, up to a minus sign which originates from an overall sign difference in the definition of the operators L_j.

6 Systems of differential operators

As we have stressed several times already, our main aim in this paper is to present results and proofs in such a way as to be as free of technical details as possible. So, while the results for a second order differential operator of the type (1) presented in the earlier sections of the paper generalise to systems of differential operators, we will only give a brief outline of the formalism here, leaving the details to a forthcoming publication [4]. In particular, we will, for definiteness, discuss most of the results in the context of a specific example, encountered in the study of transition rates between metastable states in superconducting rings [32, 33]. The differential operator in this problem is defined on the interval $[-l/2, l/2]$ and has the form

$$L_1 = \begin{pmatrix} -\frac{d^2}{dx^2} + (1-2\mu^2) & (1-\mu^2)e^{2i\mu x} \\ (1-\mu^2)e^{-2i\mu x} & -\frac{d^2}{dx^2} + (1-2\mu^2) \end{pmatrix} \equiv -I_2\,\frac{d^2}{dx^2} + Q_1(x). \tag{58}$$

In the actual problem this example is taken from, μ is a wavevector, which is small (so that $\mu^2 < 1$), and l is the circumference of the ring divided by the temperature-dependent correlation length. The solutions of $(L_j - k^2)\,\mathbf{u}_{j,k}(x) = 0$ will be denoted explicitly by

$$\mathbf{u}_{j,k}(x) = \begin{pmatrix} u_{j,k,1}(x) \\ u_{j,k,2}(x) \end{pmatrix}. \tag{59}$$

The sole purpose of the operator L_2 is to render the ratio $\det L_1 / \det L_2$ finite, and it is chosen on grounds of simplicity and convenience.

In the completely general case $\mathbf{u}_{j,k}(x)$ will have r components $u_{j,k,a}(x); a = 1, \ldots, r$, and L_j will take the form of an $r \times r$ matrix containing second order derivatives along the diagonal. It is again convenient to go over to the equivalent problem containing only first order derivatives, which will have the form (23), but with the column vectors having entries $u_{j,k,a}(x)$ and $v_{j,k,a}(x); a = 1, \ldots, r$, and with the square matrix having the structure

$$\left(\begin{array}{c|c} 0 & I_r \\ \hline Q_j(x) - k^2 I_r & 0 \end{array}\right), \tag{60}$$

where I_r is the $r \times r$ unit matrix and $Q_j(x)$ contains the non-derivative terms in L_j, as in our specific example (58). The boundary conditions can again be expressed as (24), but now with M and N being $2r \times 2r$ matrices. The advantage of defining the structure in this way is that much of the formalism described in section 4 goes through unchanged. For instance, the fundamental solution consists of $2r$ independent solutions of L_1 and their derivatives:

$$H_{j,k}(x) = \begin{pmatrix} u^{(1)}_{j,k,1}(x) & \dots & \dots & u^{(2r)}_{j,k,1}(x) \\ \dots & \dots & \dots & \dots \\ u^{(1)}_{j,k,r}(x) & \dots & \dots & u^{(2r)}_{j,k,r}(x) \\ \\ v^{(1)}_{j,k,1}(x) & \dots & \dots & v^{(2r)}_{j,k,1}(x) \\ \dots & \dots & \dots & \dots \\ v^{(1)}_{j,k,r}(x) & \dots & \dots & v^{(2r)}_{j,k,r}(x) \end{pmatrix}, \tag{61}$$

and the eigenvalue condition is again (29). We again choose the solutions so that $H_{j,k}(-l/2) = I_4$, just as we did in the one-component case (30). When no zero modes are present, the representation (34) then leads to the final result (35) as before. To calculate the right-hand side of (35) we only need solutions of the homogeneous equations $L_j \mathbf{y}_j = 0$ and the matrices M and N.

In the particular example we are considering here, we will impose "twisted boundary conditions" [32, 33] $M = -\mathrm{diag}\left\{e^{i\mu l}, e^{-i\mu l}, e^{i\mu l}, e^{-i\mu l}\right\}$ and $N = I_4$. It is easy to check that

$$\mathbf{y}_1(x) = \begin{pmatrix} e^{i\mu x} \\ -e^{-i\mu x} \end{pmatrix}, \tag{62}$$

is an eigenfunction of the problem with zero eigenvalue and so $\det(M + NH_{1,0}(l/2)) = 0$.

Since a zero mode is present we have to proceed in the general way indicated in section 5, but suitably generalised to this particular two-component case. The analog of (45) is

$$\sum_{a=1}^{2} \left[v^*_{1,0,a}(x) u_{1,k,a}(x) - v_{1,k,a}(x) u^*_{1,0,a}(x) \right]^{l/2}_{-l/2} = k^2 \langle \mathbf{u}_{1,0} | \mathbf{u}_{1,k} \rangle. \tag{63}$$

Now we assume that $\mathbf{u}_{1,0}(x)$ satisfies all of the boundary conditions, so it is a zero mode, but $\mathbf{u}_{1,k}(x)$ satisfies only 3 of the 4 — for instance, those used in Appendix B, see (B.1). This means that k is not restricted to values for which k^2 is an eigenvalue. Substituting in these conditions, (63) becomes

$$-\left[v_{1,k,2}(l/2) - e^{-i\mu l} v_{1,k,2}(-l/2) \right] u^*_{1,0,2}(l/2) = k^2 \langle \mathbf{u}_{1,0} | \mathbf{u}_{1,k} \rangle. \tag{64}$$

Only the component of $\mathbf{u}_{1,k}(x)$ that does not satisfy the boundary condition survives on the left-hand side of the equation. If $\mathbf{u}_{1,k}(x)$ is appropriately normalised, the term in square brackets on the left-hand side of (64) is $\det(M + NH_{1,k}(l/2))$, and we find

$$\det(M + NH_{1,k}(l/2)) = -\frac{k^2}{u^*_{1,0,2}(l/2)} \langle \mathbf{u}_{1,0} | \mathbf{u}_{1,k} \rangle \equiv -k^2 f_{1,k}, \tag{65}$$

where $f_{1,k} = -\mathcal{B}\langle \mathbf{u}_{1,0}|\mathbf{u}_{1,k}\rangle$ and $\mathcal{B} = -\left\{y^*_{1,2}(l/2)\right\}^{-1}$. The only remaining task is the calculation of the appropriately normalised function $\mathbf{y}_1(x)$. The method used to obtain it is outlined in Appendix B. Using this procedure we find

$$\mathbf{y}_1(x) = -\frac{4l(1-\mu^2)\sinh^2\left(\frac{l\nu}{2}\right)e^{il\mu/2}}{\nu^2}\begin{pmatrix} e^{i\mu x} \\ -e^{-i\mu x}\end{pmatrix}, \tag{66}$$

which should be contrasted with the unnormalised result (62). Therefore

$$f_{1,0} = \frac{\langle \mathbf{y}_1|\mathbf{y}_1\rangle}{y^*_{1,2}(l/2)} = \frac{8l^2(1-\mu^2)\sinh^2\left(\frac{l\nu}{2}\right)}{\nu^2}, \tag{67}$$

which agrees with the result calculated in Ref. [33] using a different method. This result gives $\det' L_1$, provided that we divide by $\det L_2$. The most convenient choice for L_2 is to take it to be of the form $L_2 = -I_2(d^2/dx^2)$. The calculation of $\det L_2$ then decouples into the calculation of the determinant of two identical operators of the kind studied in the earlier sections of this paper.

7 Conclusion

The two main objectives of this paper have been firstly to present a simple, yet rigorous, way of determining the now well-established formulae for ratios of functional determinants, and secondly to extend the results to the situation where a zero mode exists, but is omitted, in one of the determinants. We have stressed clarity, preferring to study the simplest types of operators, and leaving the most general case to a later publication [4].

The main idea behind the method of proof which we have adopted involved defining two solutions of the eigenvalue equation $L_j u_{j,k}(x) = k^2 u_{j,k}(x)$, denoted by $u^{(1)}_{j,k}(x)$ and $u^{(2)}_{j,k}(x)$. Here L_1 is the second order differential operator of interest, and L_2 is a similar, typically simpler, operator used for normalisation. Although $u^{(1)}_{j,k}(x)$ and $u^{(2)}_{j,k}(x)$ satisfy the eigenvalue equation, they are not, in general, eigenfunctions since they do not satisfy the boundary conditions (simple boundary conditions such as Dirichlet and Neumann are exceptions). Instead we impose "initial" conditions on these two solutions — conditions on the functions and their first derivatives at $x = 0$ — so that they are uniquely defined. The particular choice we made in this paper was (30), but obviously other choices are permissible.

Once two unique and independent solutions of the eigenvalue equation have been defined, any other solution may be expressed as a linear combination of these by specifying the two constants α and β, as in (26). In particular, if we wish to determine eigenfunctions we would first apply one of the boundary conditions to find the ratio of α to β. Since the overall normalisation of eigenfunctions is irrelevant, this application of only one of the boundary conditions determines the functional form of the

eigenfunction $u_{j,k}(x)$. The imposition of the second boundary condition has the effect of restricting values of k^2 to those which are eigenvalues — which are real, since the operators considered here are all taken to be self-adjoint.

The proof of the results begins from the observation that the quantity $\det(M + NH_{j,k}(1))$ is zero only when k^2 is an eigenvalue. It follows that its logarithmic derivative has poles with unit residue at values of k such that k^2 is an eigenvalue. Therefore a zeta-function can be defined through a contour integration, where the contour is chosen to surround these values of k. Since these poles are restricted to the non-negative real axis, the contour may be deformed to lie on the imaginary k axis, and then evaluated to give the required result (35). The only other information which is required during this process relates to the nature of the solutions of the differential equation for large $|k|$ [29].

An alternative result, which is slightly more explicit than (35), can be obtained by using the solution $y_j(x) \equiv \lim_{k\to 0} u_{j,k}(x)$ rather than $y_j^{(1)}(x) \equiv \lim_{k\to 0} u_{j,k}^{(1)}(x)$ and $y_j^{(2)}(x) \equiv \lim_{k\to 0} u_{j,k}^{(2)}(x)$, to express the result. Here one has to be careful with questions of normalisation. The solution $u_{j,k}(x)$ satisfies only one of the boundary conditions, but is unnormalised. However if its normalisation is chosen appropriately, then $\det(M + NH_{j,k}(1))$ can be made to exactly equal the second boundary condition (that is, with a constant of proportionality equal to 1). The effect of this, after the $k \to 0$ limit has been taken, is to allow $\det(M + NH_{j,0}(1))$ in (35) to be replaced by the second boundary condition, where the function appearing in this boundary condition is simply $y_j(x)$, appropriately normalised. In the case of the generalised boundary conditions considered in section 4, the appropriately normalised $u_{j,k}(x)$ satisfying the first part of the boundary conditions is given by (40), the expression of $\det(M + NH_{j,k}(1))$ in terms of the second boundary condition is given by (41), and the final result, in which the ratios of functional determinants are expressed in terms of $y_j(x)$, is (42).

One of the advantages of the above method of proof is that it can be relatively simply adapted to the case when $k = 0$ is an eigenvalue of L_1 which is excluded from the determinant. This is achieved by noting that in these cases $\det(M + NH_{1,k}(1)) = -k^2 f_{1,k}$, where $f_{1,0} \neq 0$. Since $f_{1,k}$ will, like $\det(M + NH_{1,k}(1))$, vanish at all the non-zero eigenvalues, the proof we have described can be repeated but with $\det(M + NH_{1,k}(1))$ replaced by $f_{1,k}$ — or rather, by $(1 - k^2)f_{1,k}$, so that the large $|k|$ behaviour remains unchanged. The result will be a formula for the ratio of functional determinants, but with the zero mode omitted in the determinant in the numerator. It is given by (53), and although it depends on a constant $\mathcal{B}$ whose form depends on the nature of the boundary conditions, it is nonetheless simple, in the sense that it only depends on (i) the zero mode $y_1(x)$, and (ii) the matrices M and N which define the boundary conditions. Furthermore, we expect that in many applications the norm $\langle y_1|y_1\rangle$ will cancel with a similar factor resulting from the transformation to a set of coordinates which allows easy extraction of the zero mode. So, once again, only the values of solutions of the homogeneous equation at the boundary are required.

In the examples given in this paper, we have been able to obtain the solutions of the homogeneous equations analytically, and so determine their values, and/or those of

their derivatives, at the boundaries. In most cases of interest this will not be possible, but this does not create any real difficulty: it is straightforward enough to determine the solutions $y_j^{(1)}(x)$ and $y_j^{(2)}(x)$ numerically and so calculate the required result from either (35) or (42). Since functional determinants of this sort are often perceived as being the most difficult quantities to evaluate in calculations of fluctuations about classical field configurations, we hope that the results presented in this paper will prove useful in this context.

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A Determinants in the presence of zero modes for general boundary conditions

In this section we give details of some of the algebraic manipulations used in section 5 and collect together the results for the different cases.

Let us first consider the case discussed in the main part of the text, that is, boundary conditions which are such that $m_{12}n_{22}-m_{22}n_{12} \neq 0$. This condition allows us to rewrite (50) as

$$\begin{aligned}\begin{pmatrix} v_{1,k}(0) \\ v_{1,k}(1) \end{pmatrix} &= \begin{pmatrix} m_{12} & n_{12} \\ m_{22} & n_{22} \end{pmatrix}^{-1} \begin{pmatrix} 0 \\ \det(M+NH_{1,k}(1)) \end{pmatrix} \\ &- \begin{pmatrix} m_{12} & n_{12} \\ m_{22} & n_{22} \end{pmatrix}^{-1} \begin{pmatrix} m_{11} & n_{11} \\ m_{21} & n_{21} \end{pmatrix} \begin{pmatrix} u_{1,k}(0) \\ u_{1,k}(1) \end{pmatrix}.\end{aligned}$$

Multiplying this out yields

$$\begin{aligned} v_{1,k}(0) &= \frac{1}{[m_{12}n_{22}-n_{12}m_{22}]} \left\{-n_{12}\det(M+NH_{1,k}(1))\right. \\ &- \left.[m_{11}n_{22}-n_{12}m_{21}]\,u_{1,k}(0)-[n_{11}n_{22}-n_{12}n_{21}]\,u_{1,k}(1)\right\}\end{aligned}$$

and

$$\begin{aligned} v_{1,k}(1) &= \frac{1}{[m_{12}n_{22}-n_{12}m_{22}]} \left\{m_{12}\det(M+NH_{1,k}(1))\right. \\ &- \left.[m_{12}m_{21}-m_{11}m_{22}]\,u_{1,k}(0)-[m_{12}n_{21}-n_{11}m_{22}]\,u_{1,k}(1)\right\}.\end{aligned}$$

Two similar equations hold for $v_{1,0}(0)$ and $v_{1,0}(1)$, but with $\det(M+NH_{1,k}(1))$ replaced by 0. Using these four equations we find

$$\begin{aligned}[v_{1,0}(x)^* u_{1,k}(x) - v_{1,k}(x)u_{1,0}(x)^*]_0^1 &= -\frac{[m_{12}u_{1,0}(1)^* + n_{12}u_{1,0}(0)^*]}{[m_{12}n_{22}-n_{12}m_{22}]}\det(M+NH_{1,k}(1)) \\ &+u_{1,k}(1)u_{1,0}(0)^*\left\{-\frac{\det N}{m_{12}n_{22}-n_{12}m_{22}}+\frac{(\det M)^*}{(m_{12}n_{22}-n_{12}m_{22})^*}\right\} \\ &+u_{1,k}(0)u_{1,0}(1)^*\left\{-\frac{\det M}{m_{12}n_{22}-n_{12}m_{22}}+\frac{(\det N)^*}{(m_{12}n_{22}-n_{12}m_{22})^*}\right\} \\ &+u_{1,k}(1)u_{1,0}(1)^*\left\{\frac{m_{12}n_{21}-n_{11}m_{22}}{m_{12}n_{22}-n_{12}m_{22}}-\frac{(m_{12}n_{21}-n_{11}m_{22})^*}{(m_{12}n_{22}-n_{12}m_{22})^*}\right\} \\ &+u_{1,k}(0)u_{1,0}(0)^*\left\{\frac{(m_{11}n_{22}-n_{12}m_{21})^*}{(m_{12}n_{22}-n_{12}m_{22})^*}-\frac{(m_{11}n_{22}-n_{12}m_{21})}{(m_{12}n_{22}-n_{12}m_{22})}\right\}\end{aligned}$$

If k is an eigenvalue, the first term in the above expression vanishes. Therefore, in the case that k is an eigenvalue, in order to have a self-adjoint problem the sum of the last

four terms must vanish. But this can only happen for general $u_{1,k}$ if each of the four terms in curly brackets is separately zero. This gives conditions on the entries of the matrices M and N for the problem to be self-adjoint. We will leave the discussion of these to a subsequent paper [4], although let us note that in the case where M and N are real, these reduce to $\det M = \det N$.

Therefore, for general k, we have using (45),

$$k^2\langle u_{1,0}|u_{1,k}\rangle = \frac{[m_{12}u_{1,0}(1)^* + n_{12}u_{1,0}(0)^*]}{[n_{12}m_{22} - m_{12}n_{22}]}\,\det(M + NH_{1,k}(1)),$$

which yields (51).

If, for the particular boundary conditions under consideration, $m_{12}n_{22} - n_{12}m_{22} = 0$, then (49) should be expressed not as (50), but in an alternative way that allows the above derivation to be repeated. For example, if $m_{11}n_{21} - n_{11}m_{21} \neq 0$,

$$\begin{pmatrix} m_{11} & n_{11} \\ m_{21} & n_{21} \end{pmatrix}\begin{pmatrix} u_{1,k}(0) \\ u_{1,k}(1) \end{pmatrix} = \begin{pmatrix} 0 \\ \det(M + NH_{1,k}(1)) \end{pmatrix} - \begin{pmatrix} m_{12} & n_{12} \\ m_{22} & n_{22} \end{pmatrix}\begin{pmatrix} v_{1,k}(0) \\ v_{1,k}(1) \end{pmatrix},$$

and we can solve for $u_{1,k}(0)$ and $u_{1,k}(1)$. Proceeding in this way we obtain the following results:

$$\begin{aligned}
\det(M + NH_{1,k}(1)) &= \frac{m_{11}n_{21} - m_{21}n_{11}}{m_{11}v_{1,0}(1)^* + n_{11}v_{1,0}(0)^*}k^2\langle u_{1,0}|u_{1,k}\rangle, \quad m_{11}n_{21} - m_{21}n_{11} \neq 0, \\
\det(M + NH_{1,k}(1)) &= \frac{m_{11}m_{22} - m_{12}m_{21}}{m_{12}v_{1,0}(0)^* + m_{11}u_{1,0}(0)^*}k^2\langle u_{1,0}|u_{1,k}\rangle, \quad m_{11}m_{22} - m_{12}m_{21} \neq 0, \\
\det(M + NH_{1,k}(1)) &= \frac{m_{12}n_{21} - m_{22}n_{11}}{m_{12}v_{1,0}(1)^* - n_{11}u_{1,0}(0)^*}k^2\langle u_{1,0}|u_{1,k}\rangle, \quad m_{12}n_{21} - m_{22}n_{11} \neq 0, \\
\det(M + NH_{1,k}(1)) &= \frac{n_{12}n_{21} - n_{22}n_{11}}{n_{12}v_{1,0}(1)^* + n_{11}u_{1,0}(1)^*}k^2\langle u_{1,0}|u_{1,k}\rangle, \quad n_{12}n_{21} - n_{22}n_{11} \neq 0, \\
\det(M + NH_{1,k}(1)) &= \frac{m_{11}n_{22} - m_{21}n_{12}}{n_{12}v_{1,0}(0)^* - m_{11}u_{1,0}(1)^*}k^2\langle u_{1,0}|u_{1,k}\rangle, \quad m_{11}n_{22} - m_{21}n_{12} \neq 0.
\end{aligned}$$

Together with (51) these equations cover all possible cases.

B Explicit calculations for the two-component problem

In this appendix we will give details of the calculation required to calculate the functional determinant of the problem defined by (58) on the interval $[-l/2, l/2]$ with boundary conditions given by the matrices $M = -\mathrm{diag}\left\{e^{i\mu l}, e^{-i\mu l}, e^{i\mu l}, e^{-i\mu l}\right\}$ and $N = I_4$.

The evaluation of the functional determinant $\det' L_1$ is based on the evaluation of suitably normalised solutions. In particular we need to find $\mathbf{u}_{1,k}(x) = (u_{1,k,1}(x), u_{1,k,2}(x),$

$v_{1,k,1}(x), v_{1,k,2}(x)$) such that all but one boundary condition are satisfied. We choose a normalisation such that

$$(M + NH_{1,k}(l/2)) \begin{pmatrix} u_{1,k,1}(-l/2) \\ u_{1,k,2}(-l/2) \\ v_{1,k,1}(-l/2) \\ v_{1,k,2}(-l/2) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \det(M + NH_{1,k}(l/2)) \end{pmatrix}. \tag{B.1}$$

This should be compared with the analogous choices (39) and (41) in section 4. For the twisted boundary condition under consideration, this implies

$$\det(M + NH_{1,k}(l/2)) = v_{1,k,2}(l/2) - e^{-i\mu l} v_{1,k,2}(-l/2), \tag{B.2}$$

which is used in the main text to derive (64). In order to derive a solution satisfying the condition (B.1) we first note that when k is not an eigenvalue (so that, in particular, $k \neq 0$), we can invert this equation to find

$$\begin{pmatrix} u_{1,k,1}(-l/2) \\ u_{1,k,2}(-l/2) \\ v_{1,k,1}(-l/2) \\ v_{1,k,2}(-l/2) \end{pmatrix} = (M + NH_{1,k}(l/2))^{-1} \begin{pmatrix} 0 \\ 0 \\ 0 \\ \det(M + NH_{1,k}(l/2)) \end{pmatrix}. \tag{B.3}$$

Given the fundamental matrix $H_{1,k}(l/2)$, (B.3) can be used to find the initial conditions that have to be imposed on $\mathbf{u}_{1,k}(x)$ for (B.2) to hold. However, what actually enters into the final answer is $f_{1,0}$, the $k \to 0$ value of $f_{1,k}$ defined by (65). Therefore we only need to evaluate (B.3) in the limit $k \to 0$. Although $(M + NH_{1,0}(l/2))^{-1}$ does not exist (because $k = 0$ is an eigenvalue) the right-hand side does exist in the limit, because the determinant cancels between the inverse and the entry in the column vector leaving only the cofactors of the matrix which are perfectly well defined in the $k \to 0$ limit. To calculate these cofactors we only need the entries of the fundamental matrix $H_{1,k}(l/2)$ at $k = 0$. Thus we only need to construct the normalised fundamental matrix for $k = 0$. Defining, as in section 4, $Y_j(x) \equiv \lim_{k\to 0} H_{j,k}(x)$, this means we have to construct

$$Y_1(x) \equiv \begin{pmatrix} y^{(1)}_{1,1}(x) & y^{(2)}_{1,1}(x) & y^{(3)}_{1,1}(x) & y^{(4)}_{1,1}(x) \\ y^{(1)}_{1,2}(x) & y^{(2)}_{1,2}(x) & y^{(3)}_{1,2}(x) & y^{(4)}_{1,2}(x) \\ y^{(1)\prime}_{1,1}(x) & y^{(2)\prime}_{1,1}(x) & y^{(3)\prime}_{1,1}(x) & y^{(4)\prime}_{1,1}(x) \\ y^{(1)\prime}_{1,2}(x) & y^{(2)\prime}_{1,2}(x) & y^{(3)\prime}_{1,2}(x) & y^{(4)\prime}_{1,2}(x) \end{pmatrix},$$

where the 4 fundamental solutions are chosen to satisfy $Y_1(-l/2) = I_4$. The explicit form of these solutions is

$$\mathbf{y}^{(1)}_1(x) = \frac{e^{i\mu l/2}}{\nu^2} \begin{pmatrix} \left[\frac{\nu^2}{2} + i\mu(1-\mu^2)z + \frac{\nu^2}{2}\cosh\nu z - \frac{i\mu}{\nu}(3-7\mu^2)\sinh\nu z\right] e^{i\mu x} \\ \\ (1-\mu^2)\left[-1 - i\mu z + \cosh\nu z + \frac{i\mu}{\nu}\sinh\nu z\right] e^{-i\mu x} \end{pmatrix}$$

$$\mathbf{y}_1^{(2)}(x) = \frac{e^{-i\mu l/2}}{\nu^2}\begin{pmatrix} (1-\mu^2)\left[-1+i\mu z+\cosh\nu z-\frac{i\mu}{\nu}\sinh\nu z\right]e^{i\mu x} \\ \left[\frac{\nu^2}{2}-i\mu(1-\mu^2)z+\frac{\nu^2}{2}\cosh\nu z+\frac{i\mu}{\nu}(3-7\mu^2)\sinh\nu z\right]e^{-i\mu x}\end{pmatrix}$$

$$\mathbf{y}_1^{(3)}(x) = \frac{e^{i\mu l/2}}{\nu^2}\begin{pmatrix} \left[2i\mu+(1-\mu^2)z-2i\mu\cosh\nu z+\frac{1}{\nu}(1-5\mu^2)\sinh\nu z\right]e^{i\mu x} \\ (1-\mu^2)\left[-z+\frac{1}{\nu}\sinh\nu z\right]e^{-i\mu x}\end{pmatrix}$$

$$\mathbf{y}_1^{(4)}(x) = \frac{e^{-i\mu l/2}}{\nu^2}\begin{pmatrix} (1-\mu^2)\left[-z+\frac{1}{\nu}\sinh\nu z\right]e^{i\mu x} \\ \left[-2i\mu+(1-\mu^2)z+2i\mu\cosh\nu z+\frac{1}{\nu}(1-5\mu^2)\sinh\nu z\right]e^{-i\mu x}\end{pmatrix},$$

where $\nu^2 = 2(1-3\mu^2)$ and $z = x + l/2$.

Due to the condition $Y_1(-l/2) = I_4$, it is easy to see that the solution with initial conditions (B.3) reads

$$\mathbf{y}_1(x) = u_{1,0,1}(-l/2)\mathbf{y}_1^{(1)}(x) + u_{1,0,2}(-l/2)\mathbf{y}_1^{(2)}(x) + v_{1,0,1}(-l/2)\mathbf{y}_1^{(3)}(x) + v_{1,0,2}(-l/2)\mathbf{y}_1^{(4)}(x).$$

Therefore by finding the relevant initial conditions from (B.3) in the $k \to 0$ limit, we can determine the correct normalisation for $\mathbf{y}_1(x)$. The result is given by (66).

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