Computation of determinants using contour integrals

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Abstract

It is shown how the pre-exponential factor of the Feynman propagator for a large class of potentials can be computed using contour integrals. This is of direct relevance in the context of tunnelling processes in quantum theories. The prerequisites for this analysis are accessible to advanced undergraduate students and involve only introductory courses in ordinary differential equations and complex variables.

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I. INTRODUCTION

The spectrum of certain differential operators encodes fundamental properties of different physical systems. Various functions of the spectrum, the so-called spectral functions, are needed to decode these properties. One of the most prominent spectral functions is the zeta function, which relates for example to partition sums, the heat-kernel and the functional determinant; see, e.g., Ref. 16. Zeta functions are often associated with suitable sequences of real numbers $\{\lambda_k\}_{k\in\mathbb{N}}$, which, for many applications, are eigenvalues of Laplace-type operators. In generalization to the zeta function of Riemann,

$$\zeta_R(s) = \sum_{k=1}^{\infty} k^{-s}, \tag{1}$$

one defines

$$\zeta(s) = \sum_{k=1}^{\infty} \lambda_k^{-s}, \tag{2}$$

where s is a complex parameter whose real part is assumed to be sufficiently large such as to make the series convergent.

To indicate how zeta functions relate to other spectral functions, let us use the functional determinant as an example because it is going to be the focus of the article. For the purpose of relating zeta functions and determinants assume for the moment that we talk about a sequence of *finitely* many numbers $\{\lambda_k\}_{k=1}^n$. Considering them as eigenvalues of a matrix L, we have

$$\det L = \prod_{k=1}^{n} \lambda_k,$$

which implies

$$\ln \det L = \sum_{k=1}^{n} \ln \lambda_k = -\frac{d}{ds}\Big|_{s=0} \sum_{k=1}^{n} \lambda_k^{-s}.$$

In the notation of Eq. (2) this shows

$$\ln \det L = -\zeta'(0) \quad \text{or} \quad \det L = e^{-\zeta'(0)}. \tag{3}$$

When the finite dimensional matrix is replaced by a differential operator L having infinitely many eigenvalues, in general $\prod_{k=1}^{\infty} \lambda_k$ will not be defined. However, as it

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turns out for many situations of relevance, definition (3) makes perfect sense and has found important applications in mathematics and physics; for the first appearance of definition (3) see Refs. 10, 13, and 24.

In recent years a contour integral method has been developed for the analysis of zeta functions,[2,16] which, although applicable in any dimension and to a variety of spectral functions, shows its full elegance and simplicity when applied in one dimension, and when applied to functional determinants. One of the main reasons for the relevance of determinants is the fact that the evaluation of the Feynman propagator involves this quantity. The probably most important field of application of functional determinants deals with tunnelling processes in quantum mechanics, quantum field theory and quantum statistics.[20,25] Because of its relevance a considerable number of articles in American Journal of Physics have been devoted to this topic; see, e.g., Refs. 1, 5, 7, 14, and 15, and so we decided to also concentrate on this topic. Our aim is to show how and why a contour integral method is extremely well adapted for the evaluation of *in particular* functional determinants. By demonstrating an additional way by which results may be obtained we enlarge the arsenal of techniques by a component already proven useful in recent research, see, e.g., Refs. 17 and 19. The probably most attractive feature of our approach is that all prerequisites are known to advanced undergraduate students of physics and mathematics. Namely, we only assume some working knowledge with Cauchy's residue theorem[6] and some elementary facts about ordinary differential equations.[23]

The outline of this article is as follows. We explain the basic ideas of our approach by looking at the zeta function of Riemann, and by evaluating $\zeta_R'(0)$. This is identical to the evaluation of the functional determinant of a free particle in an interval with Dirichlet boundary conditions at the endpoints. We then will consider the case of particles in a harmonic oscillator potential previously considered in Refs. 1, 7, and 15. Results will be trivially rederived. Finally, we show how particles moving in any potential (satisfying reasonable conditions) and obeying quite general boundary conditions can be analyzed. The Conclusions highlight the most important points of our contribution.

II. FUNCTIONAL DETERMINANT OF A FREE PARTICLE IN AN INTERVAL

A free particle in an interval is described by the operator $\frac{d^2}{dt^2}$ together with some boundary condition. In the context of the Feynman propagator Dirichlet boundary conditions are quite common[15] and this is what we first concentrate on. It will be convenient to make a rotation in the complex t-plane and to define $t = -i\tau$. The resulting operator

$$P = -\frac{d^2}{d\tau^2}$$

in terms of τ has positive eigenvalues. This is the relevant setting in the context of quantum tunnelling,[8,9,20,21,22,25] cf. the last part of Section IV.

So in order to evaluate the functional determinant associated with this situation we consider the eigenvalue problem

$$-\frac{d^2}{d\tau^2}\phi_n(\tau) = \lambda_n\phi_n(\tau), \qquad \phi_n(0) = \phi_n(L) = 0.$$

The eigenfunctions have the form

$$\phi_n(\tau) = a\sin(\sqrt{\lambda_n}\,\tau) + b\cos(\sqrt{\lambda_n}\,\tau).$$

The appearance of the cosine is excluded by the boundary value $\phi_n(0) = 0$. The eigenvalues are then found from the equation

$$\sin(\sqrt{\lambda_n}L) = 0. \tag{4}$$

This condition is simple enough to be solved for analytically and one determines

$$\phi_n(\tau) = a\sin(\sqrt{\lambda_n}\tau), \qquad \lambda_n = \left(\frac{n\pi}{L}\right)^2, \quad n \in \mathbb{N},$$

with some normalization constant a.

Although in this particular case it is of course convenient to have an explicit expression for the eigenvalues, let us pretend the best we are able to obtain is an equation like (4), namely eigenvalues are determined as the zeroes of some function $F(\lambda)$. As we will see, actually this is as convenient as having explicit eigenvalues, but of much larger applicability.

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For the given setting the natural choice $F(\lambda) = \sin(\sqrt{\lambda}L)$ has to be modified as $\lambda = 0$ satisfies $F(0) = 0$. In order to avoid $F(\lambda)$ having more zeroes than there are actual eigenvalues we therefore define

$$F(\lambda) = \frac{\sin(\sqrt{\lambda}L)}{\sqrt{\lambda}}. \tag{5}$$

Note that $F(\lambda)$ is an entire function of λ. The next step in the contour integral formalism is to rewrite the zeta function using Cauchy's integral formula. Given that $F(\lambda) = 0$ defines the eigenvalues λ_n, then

$$\frac{d}{d\lambda} \ln F(\lambda) = \frac{F'(\lambda)}{F(\lambda)}$$

has poles exactly at those eigenvalues. Furthermore, expanding about $\lambda = \lambda_n$ we see for $F'(\lambda_n) \neq 0$ that

$$\frac{F'(\lambda)}{F(\lambda)} = \frac{F'(\lambda - \lambda_n + \lambda_n)}{F(\lambda - \lambda_n + \lambda_n)} = \frac{F'(\lambda_n) + (\lambda - \lambda_n)F''(\lambda_n) + \ldots}{(\lambda - \lambda_n)F'(\lambda) + (\lambda - \lambda_n)^2 F''(\lambda_n) + \ldots} = \frac{1}{\lambda - \lambda_n} + \ldots$$

and the residue at all eigenvalues is 1. (A variation of this argument shows that if m_n is the multiplicity of λ_n, the residue of $F'(\lambda)/F(\lambda)$ at λ_n is m_n.) This shows, noticing the appropriate behavior of $F(\lambda)$ at infinity, that for $\Re s > \frac{1}{2}$,

$$\zeta_P(s) = \frac{1}{2\pi i} \int_\gamma d\lambda \, \lambda^{-s} \frac{d}{d\lambda} \ln F(\lambda), \tag{6}$$

where the contour γ is shown in Figure 1.

As is typical for complex analysis, the next step in the evaluation of a line integral is a suitable deformation of the contour. Roughly speaking, deformations are allowed as long as one does not cross over poles or branch cuts of the integrand. For the integrand in (6), the poles are on the positive real axis, and there is a branch cut of λ^{-s} which we define to be on the negative real axis, as is customary. So as long as the bahavior at infinity is appropriate, we are allowed to deform the contour to the one given in Figure 2.

In order to better see the $|\lambda| \to \infty$ behavior of $F(\lambda)$, let us rewrite the sine in terms of exponentials. We then have

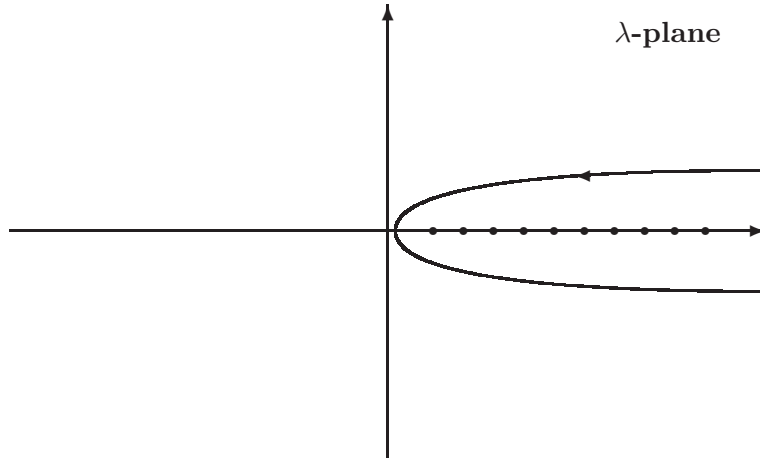$$F(\lambda) = \frac{1}{2i\sqrt{\lambda}} \left(e^{i\sqrt{\lambda}L} - e^{-i\sqrt{\lambda}L} \right),$$
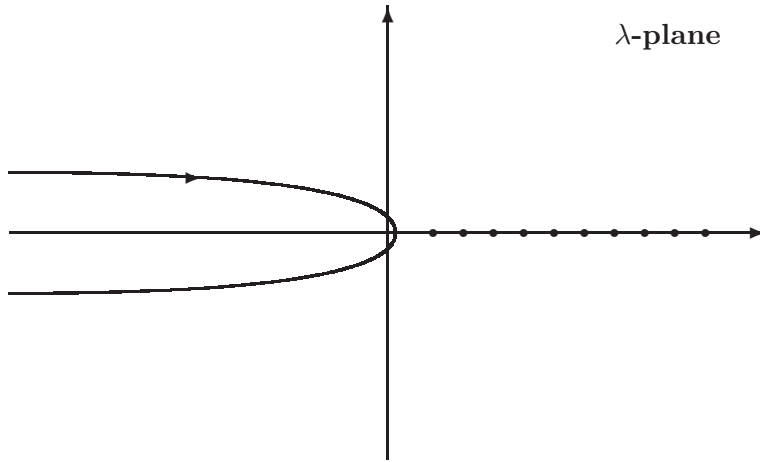
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FIG. 1: Contour γ

FIG. 2: Contour γ after deformation

and for $\Re s > \frac{1}{2}$ all deformations are indeed allowed. We next want to shrink the contour to the negative real axis as shown in Figure 3.

As λ approaches the negative real axis from above, λ^{-s} picks up a phase $(e^{i\pi})^{-s} = e^{-i\pi s}$, whereas the limit from below produces $(e^{-i\pi})^{-s} = e^{i\pi s}$. Given the opposite direction of the contour above and below the negative real axis, contributions add up to produce a $\sin(\pi s)$. Taking care of the same kind of argumentation in $F(\lambda)$ one
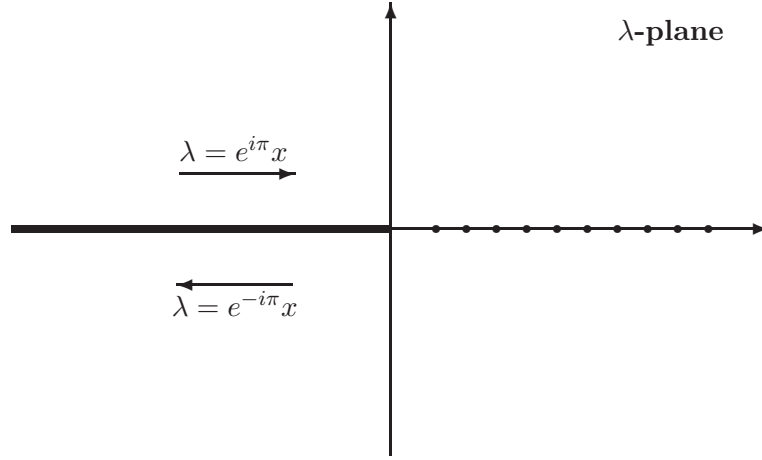
λ-plane

$\lambda = e^{i\pi}x$

$\lambda = e^{-i\pi}x$

FIG. 3: Contour γ

obtains

$$\zeta_P(s) = \frac{\sin \pi s}{\pi} \int\limits_0^\infty dx \; x^{-s} \frac{d}{dx} \ln \left(\frac{e^{\sqrt{x}L}}{2\sqrt{x}} \left[1 - e^{-2\sqrt{x}L} \right] \right). \tag{7}$$

Notice, that by shrinking the contour to the negative real axis a new condition for the integral to be well defined, namely $\Re s < 1$, has become necessary due to the behavior about $x = 0$.

Let us rest for a moment to stress the nice features of equation (7) for the evaluation of determinants. If the integral were finite at $s = 0$, an evaluation of the determinant would be trivial. From

$$\begin{aligned}
\zeta'_P(0) &= \left(\frac{d}{ds}\Big|_{s=0} \frac{\sin \pi s}{\pi} \right) \cdot \left(\int\limits_0^\infty dx \; x^{-s} \frac{d}{dx} \ln \left(\frac{e^{\sqrt{x}L}}{2\sqrt{x}} \left[1 - e^{-2\sqrt{x}L} \right] \right) \right) \Big|_{s=0} \\
&\quad + \left(\frac{\sin \pi s}{\pi} \right)\Big|_{s=0} \cdot \left(\frac{d}{ds}\Big|_{s=0} \int\limits_0^\infty dx \; x^{-s} \frac{d}{dx} \ln \left(\frac{e^{\sqrt{x}L}}{2\sqrt{x}} \left[1 - e^{-2\sqrt{x}L} \right] \right) \right) \\
&= \int\limits_0^\infty dx \; \frac{d}{dx} \ln \left(\frac{e^{\sqrt{x}L}}{2\sqrt{x}} \left[1 - e^{-2\sqrt{x}L} \right] \right) \tag{8}
\end{aligned}$$

it would amount to finding ln(...) at the limits of integration; even no integration needed to be done explicitly. Whereas this is exactly what occurs when considering *ratios* of determinants, see Section 4, for absolute determinants the situation is slightly more

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complicated. The reason is that (7) is only well defined for $\frac{1}{2} < \Re s < 1$ and a little more effort is needed. Notice, the problem is caused by the $x \to \infty$ behavior which enforces the condition $\frac{1}{2} < \Re s$. To analyze this further we therefore split the integral according to $\int_0^1 dx + \int_1^\infty dx$. Whereas from the above remarks it follows that $\int_0^1 dx$ can be considered to be in final form, the $\int_1^\infty dx$ needs further manipulation. The pieces needing extra attention are

$$\int_1^\infty dx \; x^{-s} \frac{d}{dx} \ln e^{\sqrt{x}L} = \frac{L}{2} \int_1^\infty dx \; x^{-s-\frac{1}{2}} = \frac{L}{2s-1},$$

$$\int_1^\infty dx \; x^{-s} \frac{d}{dx} \ln \left(\frac{1}{2\sqrt{x}}\right) = -\frac{1}{2} \int_1^\infty dx \; x^{-s-1} = -\frac{1}{2s}.$$

This shows

$$\zeta_P(s) = \frac{L \sin \pi s}{(2s-1)\pi} - \frac{\sin \pi s}{2s\pi} + \frac{\sin \pi s}{\pi} \int_1^\infty dx \; x^{-s} \frac{d}{dx} \ln \left(1 - e^{-2\sqrt{x}L}\right)$$

$$+ \frac{\sin \pi s}{\pi} \int_0^1 dx \; x^{-s} \frac{d}{dx} \ln \left(\frac{e^{\sqrt{x}L}}{2\sqrt{x}} \left[1 - e^{-2\sqrt{x}L}\right]\right),$$

a form perfectly suited for the evaluation of $\zeta_P'(0)$. We find

$$\zeta_P'(0) = -L - 0 - \ln \left(1 - e^{-2L}\right) + \ln \left(\frac{e^L}{2} \left[1 - e^{-2L}\right]\right) - \ln L = -\ln(2L).$$

This, of course, agrees with the answer found from the well known values $\zeta_R(0) = -\frac{1}{2}$, $\zeta_R'(0) = -\frac{1}{2} \ln(2\pi)$:

$$\zeta_P(s) = \sum_{n=1}^\infty \left(\frac{n\pi}{L}\right)^{-2s} = \left(\frac{L}{\pi}\right)^{2s} \zeta_R(2s)$$

$$\implies \zeta_P'(0) = 2 \ln \left(\frac{L}{\pi}\right) \zeta_R(0) + 2\zeta_R'(0) = -\ln \left(\frac{L}{\pi}\right) - \ln(2\pi) = -\ln(2L). \quad (9)$$

III.   FUNCTIONAL DETERMINANT FOR PARTICLES IN A HARMONIC OSCILLATOR POTENTIAL

Let ω be the frequency of the harmonic oscillator, then the relevant operator to be considered is

$$P_{ho} = -\frac{d^2}{d\tau^2} + \omega^2,$$

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with Dirichlet boundary conditions imposed at the endpoints $\tau = 0$ and $\tau = L$. Eigenvalues are then determined by the implicit equation

$$\sin(\sqrt{\lambda_n - \omega^2}L) = 0. \tag{10}$$

Instead of looking at the determinant of P_{ho} itself, let us now consider the ratio $\det(P_{ho})/\det(P)$, where as before $P = -\frac{d^2}{d\tau^2}$, that is we consider the difference of the associated zeta function. Using the same strategy as before in Section 2, we have

$$\zeta_{P_{ho}}(s) - \zeta_P(s) = \frac{1}{2\pi i} \int_\gamma d\lambda \, \lambda^{-s} \frac{d}{d\lambda} \ln \left(\frac{\sin(\sqrt{\lambda - \omega^2}L)}{\sin(\sqrt{\lambda}L)} \frac{\sqrt{\lambda}}{\sqrt{\lambda - \omega^2}} \right),$$

the contour γ still given by Figure 1. Deforming as before, we obtain

$$\zeta_{P_{ho}}(s) - \zeta_P(s) = \frac{\sin \pi s}{\pi} \int_0^\infty dx \, x^{-s} \frac{d}{dx} \ln \left(\frac{\sinh(\sqrt{x + \omega^2}L)}{\sinh(\sqrt{x}L)} \frac{\sqrt{x}}{\sqrt{x + \omega^2}} \right), \tag{11}$$

where $\sin(iy) = i \sinh y$ has been used. The technically simplifying consequence of considering ratios gets now apparent: as x tends to infinity, the behavior of the integrand has improved. In detail we have as $x \to \infty$

$$\frac{\sinh(\sqrt{x + \omega^2}L)}{\sinh(\sqrt{x}L)} \frac{\sqrt{x}}{\sqrt{x + \omega^2}} = e^{L(\sqrt{x+\omega^2}-\sqrt{x})} \frac{\sqrt{x}}{\sqrt{x + \omega^2}} \frac{1 - e^{-2L\sqrt{x+\omega^2}}}{1 - e^{-2L\sqrt{x}}} = 1 + \frac{1}{2} \frac{\omega^2 L}{\sqrt{x}} + ...$$

and the integrand behaves like $x^{-s-3/2}$. Noting that the $x \to 0$ behavior up to a proportionality constant is as before, we see that (11) is well defined for $-\frac{1}{2} < \Re s < 1$, in particular, it is well defined at $s = 0$. Thus, trivially, following along the lines leading to (8),

$$\zeta'_{P_{ho}}(0) - \zeta'_P(0) = -\ln \left(\frac{\sinh \omega L}{\omega L} \right),$$

or, switching back to real time, replacing $L = i(t_f - t_i)$,

$$\ln \frac{\det P_{ho}}{\det P} = \ln \frac{\sinh(i\omega(t_f - t_i))}{i\omega(t_f - t_i)} = \ln \frac{\sin(\omega(t_f - t_i))}{\omega(t_f - t_i)}, \tag{12}$$

the well known answer; see, e.g., Refs. 11 and 15.

Other boundary conditions can be dealt with basically with no extra effort. For example let us consider quasi-periodic boundary conditions as they have been analyzed for anyon-like oscillators.[3,4] In this case the boundary condition reads

$$\phi_n(L) = e^{i\theta} \phi_n(0), \qquad \phi'_n(L) = e^{i\theta} \phi'_n(0),$$

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with θ some real parameter; $\theta = 0$ corresponds to periodic boundary conditions, whereas $\theta = \pi$ gives antiperiodic boundary conditions typical for fermions. The general form of eigenfunctions is

$$\phi_n(\tau) = a \sin\left(\sqrt{\lambda_n - \omega^2}\tau\right) + b \cos\left(\sqrt{\lambda_n - \omega^2}\tau\right).$$

The boundary condition produces the equations, use $\mu_n = \sqrt{\lambda_n - \omega^2}$,

$$a \sin(\mu_n L) + b \cos(\mu_n L) = e^{i\theta}b, \qquad -\mu_n b \sin(\mu_n L) + \mu_n a \cos(\mu_n L) = e^{i\theta}\mu_n a.$$

Under the assumptions that $\mu_n \neq 0$, which excludes periodic boundary conditions, this system represents the matrix equation

$$\begin{pmatrix} \sin(\mu_n L) & \cos(\mu_n L) - e^{i\theta} \\ \cos(\mu_n L) - e^{i\theta} & -\sin(\mu_n L) \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = 0.$$

This has a nontrivial solution if and only if the determinant of the matrix is zero, which after some simple manipulations gives the condition for eigenvalues as

$$\cos(\mu_n L) - \cos\theta = 0.$$

Following the steps of the previous calculation, denoting the operator with quasi-periodic boundary conditions as P^{qp}_{ho} and P^{qp}, the answer can essentially be simply read off,

$$\zeta^{qp}_{P_{ho}}{}'(0) - \zeta^{qp\prime}_P(0) = -\ln\left(\frac{\cosh(\omega L) - \cos\theta}{1 - \cos\theta}\right),$$

and agrees with Ref. 3. So in real time,

$$\ln\frac{\det P^{qp}_{ho}}{\det P^{qp}} = \ln\frac{\cos(\omega(t_f - t_i)) - \cos\theta}{1 - \cos\theta}.$$

For periodic boundary conditions an eigenfunction with zero eigenvalue occurs, namely the constant, and we comment on this situation in the conclusions.

IV. FUNCTIONAL DETERMINANTS OF PARTICLES IN GENERAL PO-TENTIALS

As the previous section made clear, the answer was obtained without ever worrying what the actual eigenvalues of the operator in question might be. The only information

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that entered was the implicit eigenvalue equation (10). Is there any way an equation like (10) can be obtained for general potentials, such that the evaluation of determinants is similarly trivial as the previous one? The answer is yes and elementary knowledge of ordinary differential equations is all that is needed.[23]

So let us say we were interested in the ratio of determinants of operators of the type

$$P_j = -\frac{d^2}{d\tau^2} + R_j(\tau), \qquad j = 1, 2,$$

where for convenience again Dirichlet conditions are considered. In the previous sections $R_2(\tau) = 0$ was chosen, but no additional complication arises for this more general case. Such ratios arise, for example, in the evaluation of decay probabilities in the theory of quantum tunnelling.[8,9,21,22] Recall that if a quantum particle moves in a potential $V(x)$ for which classically a particle is at rest at $x = 0$, and if $\overline{x}$ denotes the, say only, stationary point of the Euclidean action, then to leading order in $\hbar$ the decay probability per unit time of the unstable state is a multiple of, see Eq. (2.25) of Ref. 9,

$$\left| \frac{\det\left(-\frac{d^2}{d\tau^2} + V''(\overline{x})\right)}{\det\left(-\frac{d^2}{d\tau^2} + V''(0)\right)} \right|^{-1/2}.$$

Our contour integration method can easily handle such ratios. Indeed, as suggested by the previous examples, in order to evaluate $\det P_1 / \det P_2$ in the general case, the contour integral to be written down should involve solutions to the equation

$$P_j \phi_{j,\lambda}(\tau) = \lambda \phi_{j,\lambda}(\tau),$$

where λ, for now, is an arbitrary complex parameter. As is well known, for continuous potentials $R_j(\tau)$ there will be two linearly independent solutions and every initial value problem $\phi_{j,\lambda}(0) = a$, $\phi'_{j,\lambda}(0) = b$, will have a unique solution. A contact with the original boundary value problem is established by imposing $\phi_{j,\lambda}(0) = 0$; the condition on the derivative is merely a normalization and for convenience we choose $\phi'_{j,\lambda}(0) = 1$. The eigenvalues for the boundary value problem are then discovered by imposing

$$\phi_{j,\lambda}(L) = 0, \tag{13}$$

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considered as a function of λ. To see a little better how this works, consider the case $R_2 = 0$. The unique solution of the initial value problem described is

$$\phi_{2,\lambda}(\tau) = \frac{\sin(\sqrt{\lambda}\tau)}{\sqrt{\lambda}}.$$

Eigenvalues follow precisely from the condition

$$\phi_{2,\lambda}(L) = 0.$$

But having the implicit eigenvalue equation (13) at our disposal, the calculation of the determinant is basically done! Arguing as below (5) we write

$$
\begin{aligned}
\zeta_{P_1}(s) - \zeta_{P_2}(s) &= \frac{1}{2\pi i} \int_\gamma d\lambda \ \lambda^{-s} \frac{d}{d\lambda} \ln \frac{\phi_{1,\lambda}(L)}{\phi_{2,\lambda}(L)} \\
&= \frac{\sin \pi s}{\pi} \int_0^\infty dx \ x^{-s} \frac{d}{dx} \ln \frac{\phi_{1,-x}(L)}{\phi_{2,-x}(L)},
\end{aligned}
$$

valid about $s = 0$ because the leading behavior as $x \to \infty$ of $\phi_{j,-x}(L)$ does not depend on the potential $R_j(\tau)$; as evidence see the analysis in Section 3. So as around (8)

$$\zeta'_{P_1}(0) - \zeta'_{P_2}(0) = -\ln \frac{\phi_{1,0}(L)}{\phi_{2,0}(L)}$$

and we obtain the Gel'fand-Yaglom formula[12]

$$\frac{\det P_1}{\det P_2} = \frac{\phi_{1,0}(L)}{\phi_{2,0}(L)}.$$

The ratio of determinants is determined by the boundary value of the solutions to the homogeneous initial value problem

$$\left(-\frac{d^2}{d\tau^2} + R_j(\tau)\right) \phi_{j,0}(\tau) = 0, \qquad \phi_{j,0}(0) = 0, \quad \phi'_{j,0}(0) = 1.$$

Even if no analytical knowledge about the boundary value might be available, they can easily be determined numerically.

V.   CONCLUSIONS

The main aim of this contribution was to show that the analysis of functional determinants for a large class of operators is accessible to advanced undergraduate students.

The only prerequisites are elementary ordinary differential equation theory and a basic course in complex variables. The beauty of the approach is that it is easily adapted to different situations. We have indicated how other boundary conditions than Dirichlet ones can be dealt with. Indeed, general boundary conditions can be considered along the same lines and generalizations of the Gel'fand-Yaglom formula can be obtained.[19]

We have mentioned that the presence of zero eigenvalues adds some extra complication. The reason is that when deforming the contour to the negative real axis, some contribution from the origin may result. But again, a minor modification of the procedure allows for a complete analysis.[18]

Even systems of differential equations can be considered with about the same effort.[19]

An example where all of the above generalizations need to be considered is the study of transition rates between metastables states in superconducting rings. For this case, a 2×2-system with twisted boundary conditions needs to be analyzed; see, e.g., Refs. 18 and 26.

The many advantages of this approach described show that it is optimally adapted to the evaluation of determinants. Instead of struggling with the needed mathematical manipulations the students should be able to easily get a grasp of this technique and to concentrate on the underlying physics.

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