Calculation of determinants using contour integrals

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We show how the preexponential factor of the Feynman propagator for a large class of potentials can be calculated using contour integrals. This factor is relevant in the context of tunneling processes in quantum systems. The prerequisites for this analysis involve only introductory courses in ordinary differential equations and complex variables. © 2008 American Association of Physics Teachers. [DOI: 10.1119/1.2794348]

I. INTRODUCTION

The spectrum of certain differential operators encodes the fundamental properties of the corresponding physical systems. Various functions of the spectrum, the spectral functions, are needed to decode these properties. One of the most prominent spectral functions is the zeta function, which is related, for example, to partition sums, the heat-kernel, and the functional determinant (see, for example, Ref. 1). Zeta functions are often associated with sequences of real numbers $\lambda_1, \lambda_2, \lambda_3, \ldots$, which, for many applications, are eigenvalues of Laplace-type operators. As a generalization of the Riemann zeta function,

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

we define

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

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

To indicate how the zeta function relates to other spectral functions, we discuss the example of a functional determinant. Consider a sequence of finitely many numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$. If we consider them as eigenvalues of the matrix *P*, we have

$$\det P = \prod_{k=1}^{n} \lambda_k, \tag{3}$$

which implies

$$\ln \det P = \sum_{k=1}^{n} \ln \lambda_{k} = -\frac{d}{ds} \sum_{k=1}^{n} \lambda_{k}^{-s} \bigg|_{s=0}.$$
 (4)

In the notation of Eq. (2), Eq. (4) shows that

$$\ln \det P = -\zeta'(0) \tag{5a}$$

or

$$\det P = e^{-\zeta'(0)}.$$
 (5b)

When the finite dimensional matrix is replaced by the differential operator *P* with infinitely many eigenvalues, $\prod_{k=1}^{\infty} \lambda_k$ will not be defined in general. However, as is the case for many physical situations, the definition (5) makes sense and has important applications in mathematics and physics. For the first appearance of the definition (5), see Refs. 2–4.

In recent years a contour integral method has been developed for the analysis of the zeta functions, ^{1,5} 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 that they are involved with the evaluation of the Feynman propagator. Important applications of functional determinants includes tunneling processes in quantum mechanics, quantum field theory, and quantum statistics.^{6,7} Because of its relevance, many articles have been devoted to the topic of functional determinants; see, for example, Refs. 8–12.

Our aim is to show how and why a contour integral method is well adapted for the evaluation of functional determinants in particular. An attractive feature of our approach is that the prerequisites are known to advanced undergraduate students of physics and mathematics. Namely, we assume only a working knowledge of Cauchy's residue theorem¹³ and some elementary properties of ordinary differential equations.¹⁴

The outline of this article is as follows. In Sec. II we explain the basic ideas of our approach by looking at the Riemann zeta function and evaluating $\zeta'_R(0)$. This analysis is identical to the evaluation of the functional determinant of a free particle in an interval with Dirichlet boundary conditions at the endpoints. In Sec. III we consider the case of a particle in a harmonic oscillator potential previously considered in Refs. 8, 10, and 12. Results will be trivially rederived. In Sec. IV we show how a particle in any potential (satisfying reasonable conditions) and obeying general boundary conditions can be analyzed. In Sec. V we summarize the main advantages of our approach.

II. FUNCTIONAL DETERMINANT OF A FREE PARTICLE IN AN INTERVAL

A free particle in an interval is described by the operator d^2/dt^2 together with some boundary conditions. Dirichlet boundary conditions are common in the context of the Feynman propagator,¹² and we first concentrate on this case. It will be convenient to make a rotation in the complex *t*-plane and define $t=-i\tau$. The resulting operator,

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$$P = -\frac{d^2}{d\tau^2},\tag{6}$$

in terms of τ has positive eigenvalues. This type of operator is relevant in the context of quantum tunneling^{6,7,15–18} (see the last part of Sec. IV).

To evaluate the functional determinant associated with this example we consider the eigenvalue problem

$$-\frac{d^2}{d\tau^2}\phi_n(\tau) = \lambda_n\phi_n(\tau), \quad \phi_n(0) = \phi_n(L) = 0.$$
(7)

The eigenfunctions have the form

$$\phi_n(\tau) = a \sin(\sqrt{\lambda_n}\tau) + b \cos(\sqrt{\lambda_n}\tau). \tag{8}$$

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

$$\sin(\sqrt{\lambda_n}L) = 0. \tag{9}$$

This condition can be solved for analytically, and we find

$$\phi_n(\tau) = A \sin(\sqrt{\lambda_n}\tau), \quad \lambda_n = \left(\frac{n\pi}{L}\right)^2,$$
 (10)

with some normalization constant A, and where n is an integer. Thus, for the operator P in Eq. (6), we have

$$\zeta_P(s) = \sum_{n=1}^{\infty} \lambda_n^{-s}.$$
(11)

The subscript *P* is used to emphasize that $\zeta_P(s)$ is the zeta function resulting from the operator *P*.

Although in this example it is convenient to have an explicit expression for the eigenvalues, let us pretend that the best we can do is to obtain a relation such as Eq. (9), namely, the eigenvalues are determined as the zeros of some function $F(\lambda)$. We will see that such a relation is as convenient as having explicit eigenvalues and is of much wider applicability.

For this example the natural choice for the function *F* is $F(\lambda) = \sin(\sqrt{\lambda}L)$. This choice has to be modified because $\lambda = 0$ satisfies F(0)=0. To avoid $F(\lambda)$ having more zeros than there are actual eigenvalues we define

$$F(\lambda) = \frac{\sin(\sqrt{\lambda L})}{\sqrt{\lambda}}.$$
(12)

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 the logarithmic derivative

$$\frac{d}{d\lambda}\ln F(\lambda) = \frac{F'(\lambda)}{F(\lambda)}$$
(13)

has poles at the same eigenvalues. If we expand the logarithmic derivative about $\lambda = \lambda_n$, we obtain for $F'(\lambda_n) \neq 0$ that



Fig. 1. Contour γ used in the representation of the zeta function $\zeta_P(s)$, Eq. (15).

$$\frac{F'(\lambda)}{F(\lambda)} = \frac{F'(\lambda - \lambda_n + \lambda_n)}{F(\lambda - \lambda_n + \lambda_n)}$$
$$= \frac{F'(\lambda_n) + (\lambda - \lambda_n)F''(\lambda_n) + \cdots}{(\lambda - \lambda_n)F'(\lambda_n) + (\lambda - \lambda_n)^2F''(\lambda_n) + \cdots}$$
$$= \frac{1}{\lambda - \lambda_n} + \cdots$$
(14)

and the residue at all the 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 .] Thus Eq. (14) and Cauchy's residue theorem¹³ show, given the appropriate behavior of $F(\lambda)$ at infinity, that for Re $s > \frac{1}{2}$,

$$\zeta_P(s) = \frac{1}{2\pi i} \int_{\gamma} d\lambda \lambda^{-s} \frac{d}{d\lambda} \ln F(\lambda), \qquad (15)$$

where the contour γ is shown in Fig. 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 poles or branch cuts of the integrand are not crossed. For the integrand in Eq. (15) 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. As long as the behavior at infinity is appropriate, we are allowed to deform the contour to the one given in Fig. 2.

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

$$F(\lambda) = \frac{1}{2i\sqrt{\lambda}} (e^{i\sqrt{\lambda}L} - e^{-i\sqrt{\lambda}L}), \qquad (16)$$

and for Re $s > \frac{1}{2}$ all deformations are allowed.

We next want to shrink the contour to the negative real axis as shown in Fig. 3. As λ approaches the negative real axis from above, λ^{-s} picks up the phase $(e^{i\pi})^{-s} = e^{-i\pi s}$; the limit from below produces $(e^{-i\pi})^{-s} = e^{i\pi s}$. Given the opposite



Fig. 2. The contour γ after deformation.

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

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

Fig. 3. The contour γ after shrinking it to the negative real axis. The parameterization of the upper and lower parts of the contour is depicted.

direction of the contour above and below the negative real axis, the contributions add to produce sin πs . If we make the same arguments for $F(\lambda)$, we obtain

$$\zeta_P(s) = \frac{\sin \pi s}{\pi} \int_0^\infty dx x^{-s} \frac{d}{dx} \ln\left(\frac{e^{\sqrt{xL}}}{2\sqrt{x}} [1 - e^{-2\sqrt{xL}}]\right).$$
(17)

Note that if we shrink the contour to the negative real axis, a new condition for the integral to be well defined, namely Re s < 1, becomes necessary due to the behavior of the integrand about x=0.

Let us stress the desirable features of Eq. (17) for the evaluation of determinants. If the integral were finite at s = 0, an evaluation of the determinant would be trivial. From

$$\begin{aligned} \zeta_P'(0) &= \left(\frac{d}{ds}\bigg|_{s=0} \frac{\sin \pi s}{\pi}\right) \left(\int_0^\infty dx x^{-s} \\ &\times \frac{d}{dx} \ln\left(\frac{e^{\sqrt{x}L}}{2\sqrt{x}} \left[1 - e^{-2\sqrt{x}L}\right]\right)\right)\bigg|_{s=0} + \left(\frac{\sin \pi s}{\pi}\right)\bigg|_{s=0} \\ &\times \left(\frac{d}{ds}\bigg|_{s=0} \int_0^\infty dx x^{-s} \frac{d}{dx} \ln\left(\frac{e^{\sqrt{x}L}}{2\sqrt{x}} \left[1 - e^{-2\sqrt{x}L}\right]\right)\right) \end{aligned}$$
(18a)

$$= \int_{0}^{\infty} dx \frac{d}{dx} \ln\left(\frac{e^{\sqrt{x}L}}{2\sqrt{x}} [1 - e^{-2\sqrt{x}L}]\right)$$
(18b)

calculating the determinant would amount to finding $\ln(...)$ at the limits of integration and no integration need to be done explicitly. This feature is what occurs when considering ratios of determinants (see Sec. IV).

For absolute determinants the situation is more complicated. The reason is that Eq. (17) is well defined only for $\frac{1}{2} < \text{Re } s < 1$ and a little more effort is needed. Note that the problem is caused by the $x \to \infty$ behavior, which enforces the condition $\frac{1}{2} < \text{Re } s$. To analyze Eq. (17) further we split the integral as $\int_0^1 dx + \int_1^\infty dx$. From our previous remarks it follows that $\int_0^1 dx$ can be considered to be in final form, but $\int_1^\infty dx$ needs further manipulation. The pieces needing extra attention are

$$\int_{1}^{\infty} dx x^{-s} \frac{d}{dx} \ln e^{\sqrt{x}L} = \frac{L}{2} \int_{1}^{\infty} dx x^{-s-1/2} = \frac{L}{2s-1}, \quad (19a)$$

$$\int_{1}^{\infty} dx x^{-s} \frac{d}{dx} \ln\left(\frac{1}{2\sqrt{x}}\right) = -\frac{1}{2} \int_{1}^{\infty} dx x^{-s-1} = -\frac{1}{2s}.$$
 (19b)

Equations (19a) and (19b) show

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

$$\zeta_P'(0) = -L - 0 - \ln(1 - e^{-2L}) + \ln\left(\frac{e^L}{2}[1 - e^{-2L}]\right) - \ln L$$
$$= -\ln(2L).$$
(21)

Equation (21) agrees with the answer found from the well known values¹⁹ $\zeta_R(0) = -\frac{1}{2}$, $\zeta'_R(0) = -\frac{1}{2} \ln (2\pi)$:

$$\zeta_P(s) = \sum_{n=1}^{\infty} \left(\frac{n\pi}{L}\right)^{-2s} = \left(\frac{L}{\pi}\right)^{2s} \zeta_R(2s), \qquad (22a)$$

which implies that

$$\begin{aligned} \zeta_P'(0) &= 2 \ln\left(\frac{L}{\pi}\right) \zeta_R(0) + 2\zeta_R'(0) \\ &= -\ln\left(\frac{L}{\pi}\right) - \ln\left(2\pi\right) \\ &= -\ln\left(2L\right). \end{aligned}$$
(22b)

III. FUNCTIONAL DETERMINANT FOR PARTICLES IN A HARMONIC OSCILLATOR POTENTIAL

Let ω be the frequency of the harmonic oscillator. The relevant operator to be considered is

$$P_{\rm ho} = -\frac{d^2}{d\tau^2} + \omega^2, \qquad (23)$$

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

$$\sin(\sqrt{\lambda_n - \omega^2}L) = 0.$$
⁽²⁴⁾

Instead of looking at the determinant of $P_{\rm ho}$ itself, we consider the ratio det $(P_{\rm ho})/\det(P)$, where as before $P = -d^2/d\tau^2$. That is, we consider the difference of the associated zeta functions. We use the same strategy as before in Sec. II and find

$$\zeta_{P_{ho}}(s) - \zeta_{P}(s) = \frac{1}{2\pi i} \int_{\gamma} d\lambda \lambda^{-s} \frac{d}{d\lambda} \\ \times \ln\left(\frac{\sin(\sqrt{\lambda - \omega^{2}}L)}{\sin(\sqrt{\lambda}L)} \frac{\sqrt{\lambda}}{\sqrt{\lambda - \omega^{2}}}\right), \quad (25)$$

with the contour γ given by Fig. 1. We deform the contour as before and obtain

$$\zeta_{P_{\text{ho}}}(s) - \zeta_{P}(s) = \frac{\sin \pi s}{\pi} \int_{0}^{\infty} dx x^{-s} \\ \times \frac{d}{dx} \ln\left(\frac{\sinh(\sqrt{x+\omega^{2}}L)}{\sinh(\sqrt{x}L)}\frac{\sqrt{x}}{\sqrt{x+\omega^{2}}}\right),$$
(26)

where sin(iy) = i sinh y has been used.

The simplifying consequence of considering ratios now becomes apparent: as x tends to infinity, the behavior of the integrand has improved. We have as $x \rightarrow \infty$

$$\frac{\sinh(\sqrt{x}+\omega^2 L)}{\sinh(\sqrt{x}L)} \frac{\sqrt{x}}{\sqrt{x}+\omega^2}$$
$$= e^{L(\sqrt{x}+\omega^2-\sqrt{x})} \frac{\sqrt{x}}{\sqrt{x}+\omega^2} \frac{1-e^{-2L\sqrt{x}+\omega^2}}{1-e^{-2L\sqrt{x}}}$$
$$= 1 + \frac{1}{2} \frac{\omega^2 L}{\sqrt{x}} + \cdots, \qquad (27)$$

and the integrand behaves like $x^{-s-3/2}$. Because the $x \rightarrow 0$ behavior is the same as before up to a proportionality constant, we see that Eq. (26) is well defined for $-\frac{1}{2} < \text{Re } s < 1$, and, in particular, it is well defined at s=0. Thus if we follow along the lines leading to Eq. (18b), we have

$$\zeta_{P_{\text{ho}}}'(0) - \zeta_{P}'(0) = -\ln\left(\frac{\sinh\omega L}{\omega L}\right).$$
(28)

If we switch back to real time and replace $L=i(t_f-t_i)$, we have

$$\ln \frac{\det P_{\text{ho}}}{\det P} = \ln \frac{\sinh(i\omega(t_f - t_i))}{i\omega(t_f - t_i)} = \ln \frac{\sin(\omega(t_f - t_i))}{\omega(t_f - t_i)}, \quad (29)$$

which is the well known answer; see, for example, Refs. 12 and 20.

Other boundary conditions can be considered with no extra effort. For example, consider quasi-periodic boundary conditions, which have been analyzed for anyon-like oscillators.^{21,22} In this case the boundary condition reads

$$\phi_n(L) = e^{i\theta}\phi_n(0), \quad \phi'_n(L) = e^{i\theta}\phi'_n(0), \tag{30}$$

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

$$\phi_n(\tau) = a \sin(\sqrt{\lambda_n - \omega^2}\tau) + b \cos(\sqrt{\lambda_n - \omega^2}\tau).$$
(31)

The boundary conditions produce the equations

$$a\sin(\mu_n L) + b\cos(\mu_n L) = e^{i\theta}b, \qquad (32a)$$

$$-\mu_n b \sin(\mu_n L) + \mu_n a \cos(\mu_n L) = e^{i\theta} \mu_n a, \qquad (32b)$$

with $\mu_n = \sqrt{\lambda_n - \omega^2}$. If we assume that $\mu_n \neq 0$, which excludes periodic boundary conditions, Eq. (32) can be represented by the matrix equation

$$\begin{pmatrix} \sin(\mu_n L) & \cos(\mu_n L) - e^{i\theta} \\ \cos(\mu_n L) - e^{i\theta} & -\sin(\mu_n L) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0.$$
(33)

Equation (33) has a nontrivial solution if and only if the determinant of the matrix is zero. After some simple manipu-

lations this condition for the eigenvalues gives

$$\cos(\mu_n L) - \cos \theta = 0. \tag{34}$$

If we follow the steps of the previous calculation and denote the operators for quasi-periodic boundary conditions as P_{ho}^{qp} and P^{qp} , we obtain

$$\zeta_{P_{\text{ho}}}^{\text{qp}}{}'(0) - \zeta_{P}^{\text{qp}}{}'(0) = -\ln\left(\frac{\cosh(\omega L) - \cos\theta}{1 - \cos\theta}\right),\tag{35}$$

and agrees with Ref. 21. So, in real time,

$$\ln \frac{\det P_{\text{ho}}^{\text{qp}}}{\det P^{\text{qp}}} = \ln \frac{\cos(\omega(t_f - t_i)) - \cos \theta}{1 - \cos \theta}.$$
(36)

For periodic boundary conditions an eigenfunction with zero eigenvalue occurs, namely a constant. We comment on this case in Sec. V.

IV. FUNCTIONAL DETERMINANTS OF PARTICLES IN GENERAL POTENTIALS

As we discussed in Sec. III, the answer for the functional determinant was obtained without worrying what the actual eigenvalues of the operator in question are. The only information that entered was the implicit eigenvalue equation (24). Is there any way an equation such as (24) can be obtained for general potentials so that the evaluation of determinants is as simple as the previous one? The answer is yes and elementary knowledge of ordinary differential equations is all that is needed.¹⁴

Suppose we are interested in the ratio of determinants of operators of the type

$$P_{j} = -\frac{d^{2}}{d\tau^{2}} + V_{j}(\tau) \quad (j = 1, 2),$$
(37)

where for convenience Dirichlet conditions are considered. In the previous sections $V_2(\tau)=0$ 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 tunneling.^{15–18} 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 \bar{x} denotes the 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 the quantity [see Ref. 16, Eq. (2.25)],

$$\left| \frac{\det\left(-\frac{d^2}{d\tau^2} + V''(\bar{x})\right)}{\det\left(-\frac{d^2}{d\tau^2} + V''(0)\right)} \right|^{-1/2} .$$
(38)

The contour integration method can easily handle such ratios. As suggested by the previous examples, in order to evaluate det P_1 /det P_2 in the general case, the contour integral should involve solutions to the equation

$$P_{j}\phi_{j,\lambda}(\tau) = \lambda\phi_{j,\lambda}(\tau), \tag{39}$$

where λ is an arbitrary complex parameter for now. For continuous potentials $V_j(\tau)$, there are two linearly independent solutions and every initial value problem $\phi_{j,\lambda}(0)=a$, $\phi'_{j,\lambda}(0)=b$, has a unique solution. 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 found by imposing the condition

$$\phi_{i,\lambda}(L) = 0, \tag{40}$$

considered as a function of λ . To understand better how Eq. (40) determines eigenvalues, consider the case $V_2=0$. The unique solution of the initial value problem is

$$\phi_{2,\lambda}(\tau) = \frac{\sin(\sqrt{\lambda}\,\tau)}{\sqrt{\lambda}}.\tag{41}$$

The eigenvalues follow from the condition

$$\phi_{2,\lambda}(L) = 0. \tag{42}$$

With the implicit eigenvalue equation (40) at our disposal, the calculation of the determinant is basically done. If we follow the same argument as the one following Eq. (12), we can write

$$\zeta_{P_1}(s) - \zeta_{P_2}(s) = \frac{1}{2\pi i} \int_{\gamma} d\lambda \lambda^{-s} \frac{d}{d\lambda} \ln \frac{\phi_{1,\lambda}(L)}{\phi_{2,\lambda}(L)}$$
$$= \frac{\sin \pi s}{\pi} \int_0^\infty dx x^{-s} \frac{d}{dx} \ln \frac{\phi_{1,-x}(L)}{\phi_{2,-x}(L)}, \qquad (43)$$

which is valid about s=0 because the leading behavior of $\phi_{j,-x}(L)$ as $x \to \infty$ does not depend on the potential $V_j(\tau)$. As evidence, see the analysis in Sec. III. So, arguing as we did to get Eq. (18b), we have

$$\zeta_{P_1}'(0) - \zeta_{P_2}'(0) = -\ln \frac{\phi_{1,0}(L)}{\phi_{2,0}(L)},\tag{44}$$

and we obtain the Gel'fand-Yaglom formula²³

$$\frac{\det P_1}{\det P_2} = \frac{\phi_{1,0}(L)}{\phi_{2,0}(L)}.$$
(45)

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

$$\left(-\frac{d^2}{d\tau^2} + V_j(\tau)\right)\phi_{j,0}(\tau) = 0, \quad \phi_{j,0}(0) = 0, \quad \phi'_{j,0}(0) = 1.$$
(46)

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

V. CONCLUSIONS

Our main aim was to describe the analysis of functional determinants for a large class of operators. The only prerequisites are knowledge of ordinary differential equations and a basic course in complex variables. The beauty of the approach is that it is easily adapted to different cases. We have indicated how boundary conditions other than Dirichlet can be treated. General boundary conditions can be considered along the same lines and generalizations of the Gel'fand-Yaglom formula can be obtained.²⁴

We have mentioned that the presence of zero eigenvalues adds an extra complication. The reason is that when deforming the contour to the negative real axis, a contribution from the origin may result. A minor modification of the procedure allows for a complete analysis.²⁵

Even systems of ordinary differential equations can be considered with about the same effort.²⁴

An example where all of these generalizations need to be considered is the study of transition rates between metastable states in superconducting rings. For this case, a 2×2 system with twisted boundary conditions needs to be analyzed as in, for example, Refs. 25 and 26.

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