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Calculation of the hidden symmetry operator for a $\mathcal{PT}$-symmetric square well

Carl M Bender[1] **and Barnabas Tan**[2]

[1] Department of Physics, Washington University, St Louis, MO 63130, USA
[2] Blackett Laboratory, Imperial College, London SW7 2BZ, UK

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Abstract
It has been shown that a Hamiltonian with an unbroken $\mathcal{PT}$ symmetry also possesses a hidden symmetry that is represented by the linear operator $\mathcal{C}$. This symmetry operator $\mathcal{C}$ guarantees that the Hamiltonian acts on a Hilbert space with an inner product that is both positive definite and conserved in time, thereby ensuring that the Hamiltonian can be used to define a unitary theory of quantum mechanics. In this paper it is shown how to construct the operator $\mathcal{C}$ for the $\mathcal{PT}$-symmetric square well using perturbative techniques.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

The discovery [1–3] that there were huge classes of $\mathcal{PT}$-symmetric non-Hermitian Hamiltonians of the form $H = p^2 + x^2(\mathrm{i}x)^\epsilon$ ($\epsilon \geqslant 0$) whose spectra were real and positive led to the investigation of many new kinds of $\mathcal{PT}$-symmetric model Hamiltonians. One particularly elegant model is the $\mathcal{PT}$-symmetric square well, whose Hamiltonian on the domain $0 < x < \pi$ is given by

$$H = p^2 + V(x), \tag{1}$$

where $V(x) = \infty$ for $x < 0$ and $x > \pi$ and

$$V(x) = \begin{cases} \mathrm{i}\epsilon & \text{for} \quad \frac{\pi}{2} < x < \pi, \\ -\mathrm{i}\epsilon & \text{for} \quad 0 < x < \frac{\pi}{2}. \end{cases} \tag{2}$$

This Hamiltonian reduces to the conventional Hermitian square well in the limit as $\epsilon \to 0$. For H in (1) the parity operator $\mathcal{P}$ performs a reflection about $x = \frac{\pi}{2}$: $\mathcal{P} : x \to \pi - x$. The $\mathcal{PT}$-symmetric square-well Hamiltonian was invented and first examined by Znojil [4] and it has been heavily studied by many other researchers [5–8].

The principal challenge in understanding non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians was to show that they describe unitary time evolution. This was accomplished by the discovery of a hidden symmetry operator called $\mathcal{C}$. This operator is used to define the Hilbert-space inner product with respect to which the Hamiltonian is self-adjoint [9]. In [9] the $\mathcal{C}$ operator in coordinate space was shown to have a representation as a sum over the eigenfunctions $\phi_n(x)$ of the Hamiltonian:

$$\mathcal{C}(x, y) = \sum_{n=0}^{\infty} \phi_n(x)\phi_n(y), \tag{3}$$

where the eigenfunctions are normalized so that they are eigenstates of the $\mathcal{PT}$ operator with eigenvalue 1,

$$\mathcal{PT}\phi_n(x) = \phi_n(x), \tag{4}$$

and the integral of the square of the nth eigenfunction oscillates in sign

$$\int \mathrm{d}x[\phi_n(x)]^2 = (-1)^n. \tag{5}$$

The discovery of the $\mathcal{C}$ operator led immediately to attempts to calculate it for various model Hamiltonians. For the elementary $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \mathrm{i}x$, the exact $\mathcal{C}$ operator is given by [10]

$$\mathcal{C} = \mathrm{e}^{-2p}\mathcal{P}. \tag{6}$$

However, for more complicated Hamiltonians the $\mathcal{C}$ operator cannot be obtained in closed form. It was shown in [11] how to use perturbative methods to evaluate the sum in (3) for the Hamiltonian

$$H = p^2 + x^2 + \mathrm{i}\epsilon x^3. \tag{7}$$

In [12] this perturbative procedure was extended to quantum-mechanical Hamiltonians having several degrees of freedom.

The perturbative methods used in [11] and [12] were not powerful enough to be used in quantum field theory, so a simple recipe for finding $\mathcal{C}$ was devised that can be used in systems having an infinite number of degrees of freedom [10]. The procedure was to solve the three simultaneous algebraic equations satisfied by $\mathcal{C}$:

$$\mathcal{C}^2 = 1, \qquad [\mathcal{C}, \mathcal{PT}] = 0, \qquad [\mathcal{C}, H] = 0. \tag{8}$$

This recipe gives the $\mathcal{C}$ operator as a product of the exponential of an antisymmetric Hermitian operator Q and the parity operator $\mathcal{P}$:

$$\mathcal{C} = \mathrm{e}^{Q}\mathcal{P}. \tag{9}$$

Note that $Q = -2p$ for the $\mathcal{C}$ operator in (6). Mostafazadeh has shown that the square root of the positive operator e^{Q} can be used to construct a similarity transformation that converts a non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian H to an equivalent Hermitian Hamiltonian h [13]: $h = \mathrm{e}^{-Q/2}H\,\mathrm{e}^{Q/2}$.

In all the examples studied so far the $\mathcal{C}$ operator is a combination of integer powers of x and integer numbers of derivatives multiplying the parity operator $\mathcal{P}$. Hence, the Q operator is a polynomial in the operators x and $p = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}$. The novelty of the $\mathcal{PT}$-symmetric square-well Hamiltonian (1), (2) is that $\mathcal{C}$ contains *integrals* of $\mathcal{P}$ and thus the Q operator, while it is a simple function, is *not* a polynomial in x and p and therefore cannot be found easily by the algebraic perturbative methods that were introduced in [10]. Thus, in section 2 we calculate $\mathcal{C}$ for this Hamiltonian by using the perturbative techniques that were devised in [11]. In section 3 we make some concluding remarks.

2. Perturbative calculation of the $\mathcal{C}$ operator

The procedure we use here is as follows: first, we solve the Schrödinger equation

$$-\phi_n''(x) + V(x)\phi_n(x) = E_n\phi_n(x) \qquad (n = 0, 1, 2, 3, \ldots), \tag{10}$$

subject to the boundary conditions $\phi_n(0) = \phi_n(\pi) = 0$. We obtain the eigenfunction $\phi_n(x)$ as a perturbation series to second order in powers of ϵ. The eigenfunctions are then normalized according to (4) and (5). Next, we substitute the eigenfunctions into formula (3) and evaluate the sum. The advantage of the domain of the square well being $0 < x < \pi$ is that this sum reduces to a set of Fourier sine and cosine series that can be evaluated in closed form. After evaluating the sum, it is convenient to translate the domain of the square well to the more symmetric region $-\frac{\pi}{2} < x < \frac{\pi}{2}$. On this domain the parity operator in coordinate space is $\mathcal{P}(x, y) = \delta(x + y)$. Finally, we show that the $\mathcal{C}$ operator to order ϵ^2 has the form in (9), and we evaluate the function Q to order ϵ^2. Our final result for $Q(x, y)$ on the domain $-\frac{\pi}{2} < x < \frac{\pi}{2}$ is

$$Q(x, y) = \tfrac{1}{4}\mathrm{i}\epsilon[x - y + \varepsilon(x - y)(|x + y| - \pi)] + \mathcal{O}(\epsilon^3), \tag{11}$$

where $\varepsilon(x)$ is the standard step function

$$\varepsilon(x) = \begin{cases} 1 & (x > 0), \\ 0 & (x = 0), \\ -1 & (x < 0). \end{cases} \tag{12}$$

2.1. Solution of the Schrödinger equation

We begin our analysis by solving the Schrödinger equation (10) in the right $\left(x > \frac{\pi}{2}\right)$ and left $\left(x < \frac{\pi}{2}\right)$ regions of the square well:

$$\begin{aligned}\phi_{n,\mathrm{R}}(x) = a_n\Bigg\{&\mathrm{i}^{\frac{1}{2}(1-(-1)^n)}\sin(n+1)x \\ &+ \left[\mathrm{i}^{\frac{1}{2}(1+(-1)^n)}\left(\frac{\pi}{2} - \frac{x}{2}\right)\frac{(-1)^n\cos(n+1)x}{(n+1)} - \frac{1}{2}(1-(-1)^n)\frac{\sin(n+1)x}{2(n+1)^2}\right]\epsilon \\ &+ \mathrm{i}^{\frac{1}{2}(1-(-1)^n)}\left[\frac{1}{2}(1+(-1)^n)\left(\frac{x}{4} - \frac{\pi}{4}\right)\frac{\cos(n+1)x}{(n+1)^3}\right. \\ &\left.+ \left(\frac{x^2}{8} - \frac{\pi x}{4} + \frac{\pi^2}{16}\right)\frac{\sin(n+1)x}{(n+1)^2}\right]\epsilon^2 + \mathcal{O}(\epsilon^3)\Bigg\} \qquad \left(x > \frac{\pi}{2}\right),\end{aligned} \tag{13}$$

$$\begin{aligned}\phi_{n,\mathrm{L}}(x) = a_n\Bigg\{&\mathrm{i}^{\frac{1}{2}(1-(-1)^n)}\sin(n+1)x \\ &+ \left[\mathrm{i}^{\frac{1}{2}(1+(-1)^n)}\frac{x}{2}\frac{(-1)^n\cos(n+1)x}{(n+1)} + \frac{1}{2}(1-(-1)^n)\frac{\sin(n+1)x}{2(n+1)^2}\right]\epsilon \\ &+ \mathrm{i}^{\frac{1}{2}(1-(-1)^n)}\left[\frac{1}{2}(1+(-1)^n)\frac{x}{4}\frac{\cos(n+1)x}{(n+1)^3} + \left(\frac{x^2}{8} - \frac{\pi^2}{16}\right)\frac{\sin(n+1)x}{(n+1)^2}\right]\epsilon^2 \\ &+ \mathcal{O}(\epsilon^3)\Bigg\} \qquad \left(x < \frac{\pi}{2}\right).\end{aligned} \tag{14}$$

These eigenfunctions and their first derivatives are continuous at $x = \frac{\pi}{2}$.

Having found the eigenfunction $\phi_n(x)$ to second order in ϵ, we can give the formula for the corresponding eigenvalues:

$$E_n = (n+1)^2 + \frac{(-1)^n[2-(-1)^n]}{4(n+1)^2}\epsilon^2 + \mathcal{O}(\epsilon^4).$$

However, these eigenvalues are not needed for calculating the $\mathcal{C}$ operator.

2.2. Normalization of the eigenfunctions

The normalization requirements in (4), (5) give the value of the coefficient a_n in (13), (14):

$$a_n = \sqrt{\frac{2}{\pi}}\left[1-(-1)^n\left(\frac{(2-(-1)^n)}{(6-2(-1)^n)(n+1)^4} - \frac{(-1)^n\pi^2}{16(n+1)^2}\right)\epsilon^2 + \mathcal{O}(\epsilon^4)\right]. \tag{15}$$

With this normalization, the $\mathcal{PT}$ inner product between $\phi_m(x)$ and $\phi_n(x)$ is $(-1)^n\delta_{mn}+\mathcal{O}(\epsilon^4)$.

2.3. Calculation of $\mathcal{C}(x, y)$ to leading order (zeroth order) in ϵ

The next step is to construct the operator $\mathcal{C}(x, y)$, which is given in (3) as a sum, by directly substituting the eigenfunctions $\phi_n(x)$ from (13), (14). In general, there are four different regions of x and y to consider:

(i) $x > \frac{\pi}{2}$, $y > \frac{\pi}{2}$,
(ii) $x > \frac{\pi}{2}$, $y < \frac{\pi}{2}$,
(iii) $x < \frac{\pi}{2}$, $y < \frac{\pi}{2}$,
(iv) $x < \frac{\pi}{2}$, $y > \frac{\pi}{2}$.

However, to zeroth order in ϵ, ϕ_n is common to all four regions and the calculation is easy. We find that

$$\mathcal{C}^{(0)}(x, y) = \frac{2}{\pi}\sum_{n=0}^{\infty}(-1)^n \sin(n+1)x\sin(n+1)y. \tag{16}$$

This is just the Fourier sine series for the parity operator in the range $0 < x < \pi$:

$$\mathcal{C}^{(0)}(x, y) = \delta(x+y-\pi). \tag{17}$$

On the symmetric domain $-\frac{\pi}{2} < x < \frac{\pi}{2}$ this formula becomes

$$\mathcal{C}^{(0)}(x, y) = \delta(x+y), \tag{18}$$

which is equivalent to the coordinate-space condition of completeness.

2.4. Calculation of $\mathcal{C}(x, y)$ to first order in ϵ

The calculation of $\mathcal{C}(x, y)$ to first order in ϵ requires the evaluation of Fourier sine and cosine series. These are expressed in terms of single and double integrals of delta functions. Here, we describe the calculation for the region $x > \frac{\pi}{2}$, $y > \frac{\pi}{2}$. The calculation for the other three regions is similar.

From (13) and (15) the first-order contribution to $\mathcal{C}(x, y)$ is

$$\begin{aligned}\mathcal{C}^{(1)}(x, y) = {} & \frac{1}{\pi}\sum_{n=0}^{\infty}\left[(\pi-x)\frac{\mathrm{i}(-1)^n}{n+1}\cos[(n+1)x]\sin[(n+1)y]\right] \\ & + \frac{1}{\pi}\sum_{n=0}^{\infty}\left[(\pi-y)\frac{\mathrm{i}(-1)^n}{n+1}\sin[(n+1)x]\cos[(n+1)y]\right] \\ & - \frac{1-(-1)^n}{\pi}\sum_{n=0}^{\infty}\left[\mathrm{i}^{\frac{1}{2}(1-(-1)^n)}\frac{\sin[(n+1)x]\sin[(n+1)y]}{(n+1)^2}\right].\end{aligned} \tag{19}$$

The first two terms of $\mathcal{C}^{(1)}$ can be expressed as single integrals of the parity operator, with the first having the upper limit x,

$$\int_{\frac{\pi}{2}}^{x} \mathrm{d}t\,\delta(t+y-\pi) = -\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\frac{(-1)^n}{n+1}\cos[(n+1)x]\sin[(n+1)y]\right] + \frac{1}{\pi}\sum_{n=0}^{\infty}\left[\frac{(-1)^n}{n+1}\sin[(2n+2)y]\right], \tag{20}$$

and the second having the upper limit y,

$$\int_{\frac{\pi}{2}}^{y} \mathrm{d}t\,\delta(x+t-\pi) = -\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\frac{(-1)^n}{n+1}\sin[(n+1)x]\cos[(n+1)y]\right] + \frac{1}{\pi}\sum_{n=0}^{\infty}\left[\frac{(-1)^n}{n+1}\sin[(2n+2)x]\right]. \tag{21}$$

The third term of $\mathcal{C}^{(1)}$ involves sines of even x and y. To obtain a series of sines of even x and y, we subtract the series represented by the parity operator $\delta(x+y-\pi)$ from the series represented by $\delta(x-y)$. The factor $(n+1)^2$ in the denominator implies that the third term of $\mathcal{C}^{(1)}$ may be expressed as a double integral. To maintain the symmetry, we note that a double integral with respect to x contributes half of the third term of $\mathcal{C}^{(1)}$, while a double integral with respect to y contributes the other half.

This analysis allows us to express $\mathcal{C}^{(1)}$ in the region $x > \frac{\pi}{2}, y > \frac{\pi}{2}$ in terms of single integrals of the parity operator and double integrals in x and y:

$$\mathcal{C}^{(1)}(x,y) = \mathrm{i}\left\{\left(\frac{x}{2}-\frac{\pi}{2}\right)\int_{\pi/2}^{x}\mathrm{d}t\,\delta(t+y-\pi) + \frac{1}{4}\int_{\pi/2}^{x}\mathrm{d}t\int_{\pi/2}^{t}\mathrm{d}s[\delta(s-y)-\delta(s+y-\pi)] + \frac{x}{4}-\frac{\pi}{4}+(x\leftrightarrow y)\right\}. \tag{22}$$

We simplify this result by evaluating integrals over delta functions and obtain

$$\mathcal{C}^{(1)}(x,y) = \frac{1}{4}\mathrm{i}(|x-y|+x+y-2\pi) \qquad \left(x>\frac{\pi}{2}, y>\frac{\pi}{2}\right). \tag{23}$$

The calculation of $\mathcal{C}^{(1)}(x,y)$ for the remaining three regions follows a similar procedure and we get

$$\mathcal{C}^{(1)}(x,y) = \begin{cases} \frac{1}{2}\mathrm{i}[(x-\pi)\theta(x+y-\pi)+y\theta(\pi-x-y)] & \left(x>\frac{\pi}{2}, y<\frac{\pi}{2}\right), \\ \frac{1}{4}\mathrm{i}[-|x-y|+(x+y)] & \left(x<\frac{\pi}{2}, y<\frac{\pi}{2}\right), \\ \frac{1}{2}\mathrm{i}[(y-\pi)\theta(x+y-\pi)+x\theta(\pi-x-y)] & \left(x<\frac{\pi}{2}, y>\frac{\pi}{2}\right), \end{cases} \tag{24}$$

where $\theta(x)$ is the Heaviside step function,

$$\theta(x) = \begin{cases} 1 & (x \geqslant 0), \\ 0 & (x<0). \end{cases} \tag{25}$$

Finally, we condense the four expressions for $\mathcal{C}^{(1)}(x,y)$ in the four different regions into a single expression:

$$\mathcal{C}^{(1)}(x,y) = \tfrac{1}{4}\mathrm{i}[x+y-\pi-\theta(\pi-x-y)(|x-y|-\pi)+\theta(x+y-\pi)(|x-y|-\pi)]. \tag{26}$$

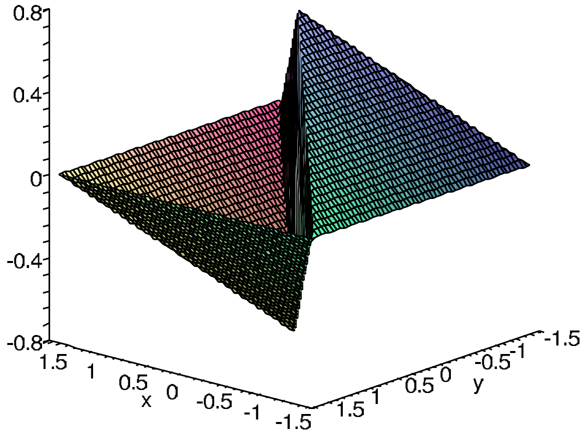

Figure 1. Three-dimensional plot of the imaginary part of $\mathcal{C}^{(1)}(x, y)$, the first-order perturbative contribution in (27) to the $\mathcal{C}$ operator in coordinate space. The plot is on the symmetric square domain $-\frac{\pi}{2} < (x, y) < \frac{\pi}{2}$. Note that $\mathcal{C}^{(1)}(x, y)$ vanishes on the boundary of this square domain because the eigenfunctions $\phi_n(x)$ in (3) are required to vanish at $x = 0$ and $x = \pi$.

On the symmetric region $-\frac{\pi}{2} < (x, y) < \frac{\pi}{2}$, this expression becomes

$$\mathcal{C}^{(1)}(x, y) = \tfrac{1}{4}\mathrm{i}[x + y + \varepsilon(x + y)(|x - y| - \pi)]. \tag{27}$$

We plot the imaginary part of $\mathcal{C}^{(1)}$ in figure 1 as a function of x and y.

2.5. Calculation of $\mathcal{C}(x, y)$ to second order in ϵ

The procedure for calculating $\mathcal{C}^{(2)}(x, y)$ is similar to that used for calculating $\mathcal{C}^{(1)}(x, y)$, albeit more tedious. We must calculate sums of products of sines and cosines, but this time the presence of factors of $(n + 1)^4$, $(n + 1)^3$ and $(n + 1)^2$ in the denominator requires the use of quadruple, triple and double integrals of delta functions to simplify the expression for $\mathcal{C}^{(2)}(x, y)$. We discuss the calculation of $\mathcal{C}^{(2)}(x, y)$ explicitly for the region $x < \frac{\pi}{2}$, $y < \frac{\pi}{2}$. The calculation of $\mathcal{C}^{(2)}(x, y)$ for the other three regions is similar.

From (13) and (15) we see that the second-order calculation of $\mathcal{C}(x, y)$ gives

$$\begin{aligned}
\mathcal{C}^{(2)}(x, y) = \frac{2}{\pi}\sum_{n=0}^{\infty}&\left[\frac{x}{4}\frac{\cos[(2n+1)x]\sin[(2n+1)y]}{(2n+1)^3}\right]\\
&+\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\frac{y}{4}\frac{\sin[(2n+1)x]\cos[(2n+1)y]}{(2n+1)^3}\right]\\
&+\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\left(\frac{x^2}{8}+\frac{y^2}{8}\right)\frac{(-1)^n\sin[(n+1)x]\sin[(n+1)y]}{(n+1)^2}\right]\\
&-\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\frac{x}{4}\frac{\cos[(2n+2)x]\sin[(2n+2)y]}{(2n+2)^3}\right]\\
&-\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\frac{y}{4}\frac{\sin[(2n+2)x]\cos[(2n+2)y]}{(2n+2)^3}\right]\\
&-\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\frac{1}{2}\frac{\sin[(2n+1)x]\sin[(2n+1)y]}{(2n+1)^4}\right]
\end{aligned}$$

$$
\begin{aligned}
&-\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\frac{1}{2}\frac{\sin[(2n+2)x]\sin[(2n+2)y]}{(2n+2)^4}\right] \\
&-\frac{2}{\pi}\sum_{n=0}^{\infty}\left[\frac{xy}{4}\frac{(-1)^n\cos[(n+1)x]\cos[(n+1)y]}{(n+1)^2}\right].
\end{aligned}
\tag{28}
$$

We have been able to evaluate each of these Fourier series exactly and to express the result as multiple integrals over delta functions:

$$
\begin{aligned}
\mathcal{C}^{(2)}(x,y) = &-\frac{1}{8}x^2\int_x^{\pi/2}\mathrm{d}t\int_t^{\pi/2}\mathrm{d}s\,\delta(s+y-\pi) \\
&-\frac{1}{4}x\int_x^{\pi/2}\mathrm{d}t\int_t^{\pi/2}\mathrm{d}s\int_s^{\pi/2}\mathrm{d}r\,\delta(r+y-\pi) \\
&-\frac{1}{4}\int_x^{\pi/2}\mathrm{d}t\int_t^{\pi/2}\mathrm{d}s\int_s^{\pi/2}\mathrm{d}r\int_r^{\pi/2}\mathrm{d}p\,\delta(p-y) \\
&-\frac{1}{8}xy\int_y^{\pi/2}\mathrm{d}t\int_x^{\pi/2}\mathrm{d}s\,\delta(s+t-\pi)+\frac{1}{8}x^2y \\
&-\frac{1}{16}xy\pi+\frac{1}{24}x^3+(x\leftrightarrow y).
\end{aligned}
\tag{29}
$$

Evaluating these integrals gives $\mathcal{C}^{(2)}(x,y)$ for the region $x<\frac{\pi}{2}$, $y<\frac{\pi}{2}$:

$$
\mathcal{C}^{(2)}(x,y)=-\tfrac{1}{24}|x-y|^3+\tfrac{1}{8}x^2y+\tfrac{1}{24}x^3-\tfrac{1}{16}x\pi y+(x\leftrightarrow y).
\tag{30}
$$

The calculation of $\mathcal{C}^{(2)}(x,y)$ for the remaining three regions follows a similar procedure. Combining the contributions from the four regions and transforming to the symmetric domain $-\frac{\pi}{2}<(x,y)<\frac{\pi}{2}$, we obtain the single expression

$$
\begin{aligned}
\mathcal{C}^{(2)}(x,y) = {} & \tfrac{1}{96}\pi^3+\tfrac{1}{8}xy\pi-\tfrac{1}{16}\pi^2(x+y)\varepsilon(x+y)+\tfrac{1}{8}\pi(x|x|+y|y|)\varepsilon(x+y) \\
&-\tfrac{1}{24}(x^3+y^3)\varepsilon(x+y)-\tfrac{1}{24}(y^3-x^3)\varepsilon(y-x) \\
&-\tfrac{1}{4}xy\{|x|[\theta(x-y)\theta(-x-y)+\theta(y-x)\theta(x+y)] \\
&+|y|[\theta(y-x)\theta(-x-y)+\theta(x-y)\theta(x+y)]\}.
\end{aligned}
\tag{31}
$$

We have plotted the function $\mathcal{C}^{(2)}(x,y)$ on the symmetric domain $-\frac{\pi}{2}<(x,y)<\frac{\pi}{2}$ in figure 2.

In summary, our final result for the $\mathcal{C}$ operator to order ϵ^2 on the symmetric domain $-\frac{\pi}{2}<(x,y)<\frac{\pi}{2}$ is given by

$$
\mathcal{C}(x,y)=\delta(x+y)+\epsilon\mathcal{C}^{(1)}(x,y)+\epsilon^2\mathcal{C}^{(2)}(x,y)+\mathcal{O}(\epsilon^3),
\tag{32}
$$

where $\mathcal{C}^{(1)}(x,y)$ is given in (27) and $\mathcal{C}^{(1)}(x,y)$ is given in (31). We have verified by explicit calculation that to order ϵ^2 this $\mathcal{C}$ operator obeys the algebraic equations (8). For example, in coordinate space the third of these equations, $\mathcal{C}^2=1$, reads

$$
\int_{-\pi/2}^{\pi/2}\mathrm{d}y\,\mathcal{C}(x,y)\mathcal{C}(y,z)=\delta(x-z)+\mathcal{O}(\epsilon^3).
\tag{33}
$$

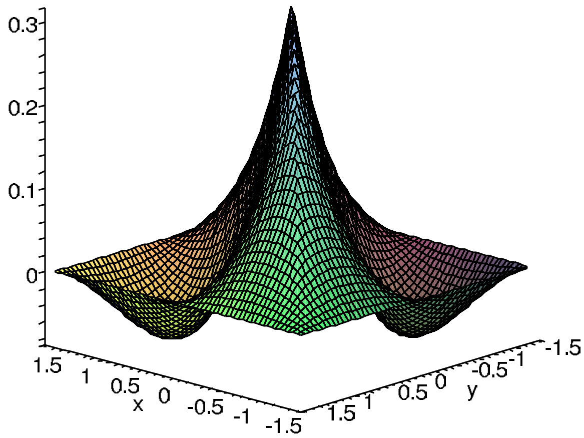

Figure 2. Three-dimensional plot of $\mathcal{C}^{(2)}(x, y)$ in (31) on the symmetric square domain $-\frac{\pi}{2} < (x, y) < \frac{\pi}{2}$. The function $\mathcal{C}^{(2)}(x, y)$ vanishes on the boundary of this square domain because the eigenfunctions $\phi_n(x)$ from which it was constructed vanish at the boundaries of the square well.

2.6. Calculation of the Q operator

The last step in the calculation is to determine the operator Q from the result in (32) by using (9). This is a long and difficult calculation: we first multiply $\mathcal{C}(x, z)$ on the right by $\delta(z + y)$, the parity operator $\mathcal{P}$ in coordinate space, and then integrate with respect to z. This gives the coordinate space representation of $\mathcal{CP} = \mathrm{e}^{Q}$. Next, we take the logarithm of the resulting expression and expand it as a series in powers of ϵ to obtain Q. We find that the coefficient of ϵ^2 in this expansion is zero, and thus we obtain the simple result in (11), which is the principal result in this paper.

3. Conclusions

In this paper we have used perturbative methods to calculate the $\mathcal{C}$ operator to second order in powers of ϵ for the complex $\mathcal{PT}$-symmetric square-well potential (2). Expressing $\mathcal{C}$ in the form $\mathrm{e}^{Q}\mathcal{P}$, we have found that the operator Q for this model has an expansion in odd powers of ϵ, just as in the case of the cubic $\mathcal{PT}$-symmetric oscillator whose Hamiltonian is given in (7). Our result (11) for Q is an elementary function. We have verified our calculation of the $\mathcal{C}$ operator by showing that it satisfies the algebraic conditions (8).

The most noteworthy property of the $\mathcal{C}$ operator is that the associated operator Q is a non-polynomial function, and this kind of structure had not been seen in previous studies of $\mathcal{C}$. At the beginning of this calculation we expected that for such a simple $\mathcal{PT}$-symmetric Hamiltonian it would be possible to calculate the $\mathcal{C}$ operator exactly and in closed form. We find it surprising that even for this elementary model the $\mathcal{C}$ operator is so non-trivial.

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