Proceedings of Institute of Mathematics of NAS of Ukraine 2004, Vol. 50, Part 2, 986–992

Calculation of $\mathcal{C}$ Operator in $\mathcal{PT}$-Symmetric Quantum Mechanics

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If a Hamiltonian H has an unbroken $\mathcal{PT}$ symmetry, then it also possesses a hidden symmetry represented by the linear operator $\mathcal{C}$. The operator $\mathcal{C}$ commutes with both H and $\mathcal{PT}$. The inner product with respect to $\mathcal{CPT}$ is associated with a positive norm and the quantum theory built on the associated Hilbert space is unitary. In this paper it is shown how to construct the operator $\mathcal{C}$ for the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + i\epsilon x^3$ using perturbative techniques. It is also shown how to construct the operator $\mathcal{C}$ for $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 - \epsilon x^4$ using nonperturbative methods [1].

1 Introduction and Background

It was observed in 1998 [2] that with properly defined boundary conditions the Sturm–Liouville differential equation eigenvalue problem associated with the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian

$$H = p^2 + x^2(ix)^\nu \qquad (\nu > 0) \tag{1}$$

exhibits a spectrum that is *real and positive*. By $\mathcal{PT}$ symmetry we mean the following: The linear parity operator $\mathcal{P}$ performs spatial reflection and thus reverses the sign of the momentum and position operators: $\mathcal{P}p\mathcal{P}^{-1} = -p$ and $\mathcal{P}x\mathcal{P}^{-1} = -x$. The antilinear time-reversal operator $\mathcal{T}$ reverses the sign of the momentum operator and performs complex conjugation: $\mathcal{T}p\mathcal{T}^{-1} = -p$, $\mathcal{T}x\mathcal{T}^{-1} = x$, and $\mathcal{T}i\mathcal{T}^{-1} = -i$. The non-Hermitian Hamiltonian H in (1) is not symmetric under $\mathcal{P}$ or $\mathcal{T}$ separately, but it *is* invariant under their combined operation; such Hamiltonians are said to possess *space-time reflection symmetry* ($\mathcal{PT}$ symmetry). We say that the $\mathcal{PT}$ symmetry of a Hamiltonian H is *not spontaneously broken* if the eigenfunctions of H are simultaneously eigenfunctions of the $\mathcal{PT}$ operator.

In a recent letter it was shown that any Hamiltonian that possesses an unbroken $\mathcal{PT}$ symmetry also has a hidden symmetry [3]. This new symmetry is represented by the linear operator $\mathcal{C}$, which commutes with both the Hamiltonian H and the $\mathcal{PT}$ operator. In terms of $\mathcal{C}$ one can construct an inner product whose associated norm is positive definite. Observables exhibit $\mathcal{CPT}$ symmetry and the dynamics is governed by unitary time evolution. Thus, $\mathcal{PT}$-symmetric Hamiltonians give rise to new classes of fully consistent complex quantum theories.

The purpose of the present paper is to present an explicit calculation of $\mathcal{C}$ for two nontrivial Hamiltonians. First, we consider the case of the $\mathcal{PT}$-symmetric Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + i\epsilon x^3, \tag{2}$$

for which we give a perturbative calculation of the operator $\mathcal{C}$ correct to *third* order in powers of ϵ. Second, we calculate $\mathcal{C}$ for the Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 - \epsilon x^4, \tag{3}$$

for which ordinary perturbative methods are ineffective and nonperturbative methods must be used. The organization of this paper is straightforward. In Section 2 we review the formal construction, first presented in Ref. [3], of the $\mathcal{C}$ operator. In Section 3 we calculate $\mathcal{C}$ for the Hamiltonian in (2) and in Section 4 we calculate $\mathcal{C}$ for the Hamiltonian in (3).

2 Formal derivation of the $\mathcal{C}$ operator

In this section we present a formal discussion of $\mathcal{PT}$-symmetric Hamiltonians and we show how to construct the $\mathcal{C}$ operator. In general, for any $\mathcal{PT}$-symmetric Hamiltonian H we must begin by solving the Sturm–Liouville differential equation eigenvalue problem associated with H:

$$H\phi_n(x) = E_n\phi_n(x) \qquad (n = 0,\, 1,\, 2,\, 3,\, \ldots). \tag{4}$$

For Hamiltonians like those in (1)–(3) the differential equation (4) must be imposed on an infinite contour in the complex-x plane. For large $|x|$ the contour lies in wedges that are placed symmetrically with respect to the imaginary-x axis. These wedges are described in Ref. [2]. The boundary conditions on the eigenfunctions are that $\phi(x) \to 0$ exponentially rapidly as $|x| \to \infty$ on the contour. For H in (2) the contour may be taken to be the real-x axis, but for H in (3) the contour lies in the two wedges $-\pi/3 < \arg x < 0$ and $-\pi < \arg x < -2\pi/3$.

For all n, the eigenfunctions $\phi_n(x)$ are simultaneously eigenstates of the $\mathcal{PT}$ operator. We can choose the phase of $\phi_n(x)$ such that the eigenvalue of $(\mathcal{PT})$ is unity:

$$\mathcal{PT}\phi_n(x) = \phi_n(x). \tag{5}$$

Next, we observe that there is an inner product, called the $\mathcal{PT}$ inner product, with respect to which the eigenfunctions $\phi_n(x)$ for two different values of n are orthogonal. For the two functions $f(x)$ and $g(x)$ the $\mathcal{PT}$ inner product (f, g) is defined by

$$(f, g) \equiv \int_{\mathrm{C}} dx\, [\mathcal{PT}f(x)]\, g(x), \tag{6}$$

where $\mathcal{PT}f(x) = [f(-x^*)]^*$ and the contour C lies in the wedges described above. For this inner product the associated norm (f, f) is independent of the overall phase of $f(x)$ and is conserved in time.

We then normalize the eigenfunctions so that $|(\phi_n, \phi_n)| = 1$ and we discover the apparent problem with using a non-Hermitian Hamiltonian. While the eigenfunctions are orthogonal, the $\mathcal{PT}$ norm is not positive definite:

$$(\phi_m, \phi_n) = (-1)^n\delta_{m,n} \qquad (m,\, n = 0,\, 1,\, 2,\, 3,\, \ldots). \tag{7}$$

Despite the fact that this norm is not positive definite, the eigenfunctions are complete. For real x and y the statement of completeness in coordinate space is[1]

$$\sum_n (-1)^n\phi_n(x)\phi_n(y) = \delta(x - y). \tag{8}$$

This is a nontrivial result that has been verified numerically to extremely high accuracy [4].

[1]It is important to remark here that the argument of the Dirac delta function in (8) must be *real* because the delta function is only defined for real argument. This may seem to be in conflict with the earlier remark in this section that the Schrödinger equation (4) must be solved along a contour that lies in wedges in the complex-x plane. To resolve this apparent conflict we specify the contour as follows. We demand that the contour lie on the real axis until it passes the points x and y. Only then may it veer off into the complex-x plane and enter the wedges. This choice of contour is allowed because the wedge conditions are *asymptotic* conditions. The positions of the wedges are determined by the boundary conditions.

We construct the linear operator $\mathcal{C}$ that expresses the hidden symmetry of the Hamiltonian H. The position-space representation of $\mathcal{C}$ is

$$\mathcal{C}(x,y)=\sum_n \phi_n(x)\phi_n(y). \tag{9}$$

The properties of the operator $\mathcal{C}$ are easy to verify using (7). First, the square of $\mathcal{C}$ is unity:

$$\int dy\,\mathcal{C}(x,y)\mathcal{C}(y,z)=\delta(x-z). \tag{10}$$

Second, the eigenfunctions $\phi_n(x)$ of the Hamiltonian H are also eigenfunctions of $\mathcal{C}$ and the corresponding eigenvalues are $(-1)^n$:

$$\int dy\,\mathcal{C}(x,y)\phi_n(y)=(-1)^n\phi_n(x). \tag{11}$$

Third, the operator $\mathcal{C}$ commutes with both the Hamiltonian H and the operator $\mathcal{PT}$. Note that while the operators $\mathcal{P}$ and $\mathcal{C}$ are unequal, both $\mathcal{P}$ and $\mathcal{C}$ are square roots of the unity operator $\delta(x-y)$. Last, the operators $\mathcal{P}$ and $\mathcal{C}$ do not commute. Indeed, $\mathcal{CP}=(\mathcal{PC})^*$.

The operator $\mathcal{C}$ does not exist as a distinct entity in conventional Hermitian quantum mechanics. Indeed, we will see that as the parameter ϵ in (2) and (3) tends to zero the operator $\mathcal{C}$ becomes identical to $\mathcal{P}$.

We can now define an inner product $\langle f|g\rangle$ whose associated norm is positive:

$$\langle f|g\rangle\equiv\int dx\,[\mathcal{CPT}f(x)]g(x). \tag{12}$$

The $\mathcal{CPT}$ norm associated with this inner product is positive because $\mathcal{C}$ contributes -1 when it acts on states with negative $\mathcal{PT}$ norm.

3 Perturbative calculation of $\mathcal{C}$ in a cubic theory

In this section we use perturbative methods to calculate the operator $\mathcal{C}(x,y)$ for the Hamiltonian $H=\frac{1}{2}p^2+\frac{1}{2}x^2+i\epsilon x^3$. We perform the calculations to third order in perturbation theory. We begin by solving the Schrödinger equation

$$-\frac{1}{2}\phi_n''(x)+\frac{1}{2}x^2\phi_n(x)+i\epsilon x^3\phi_n(x)=E_n\phi_n(x) \tag{13}$$

as a series in powers of ϵ.

The perturbative solution to this equation has the form

$$\phi_n(x)=\frac{i^n a_n}{\pi^{1/4}2^{n/2}\sqrt{n!}}e^{-\frac{1}{2}x^2}\left[H_n(x)-iP_n(x)\epsilon-Q_n(x)\epsilon^2+iR_n(x)\epsilon^3\right], \tag{14}$$

where $H_n(x)$ is the nth Hermite polynomial and $P_n(x)$, $Q_n(x)$, and $R_n(x)$ are polynomials in x of degree $n+3$, $n+6$, and $n+9$, respectively. These polynomials can be expressed as linear combinations of Hermite polynomials [1].

The energy E_n to order ϵ^3 is

$$E_n=n+\frac{1}{2}+\frac{1}{8}\left(30n^2+30n+11\right)\epsilon^2+\mathrm{O}\left(\epsilon^4\right). \tag{15}$$

The expression for $\phi_n(x)$ must be $\mathcal{PT}$-normalized according to (7) so that its square integral is $(-1)^n$:

$$\int_{-\infty}^{\infty}dx\,\left[\phi_n(x)\right]^2=(-1)^n+\mathrm{O}\left(\epsilon^4\right). \tag{16}$$

This determines the value of a_n in (14):

$$a_n = 1 + \frac{1}{144}(2n+1)\left(82n^2 + 82n + 87\right)\epsilon^2 + \mathrm{O}\left(\epsilon^4\right). \tag{17}$$

We calculate the operator $\mathcal{C}(x,y)$ by substituting the wave functions $\phi_n(x)$ in (14) into (9). We then use the completeness relation for Hermite polynomials to evaluate the sum.

To third order in ϵ the result is

$$\begin{aligned}\mathcal{C}(x,y) = \Bigg\{ & 1 - i\epsilon\left(\frac{4}{3}\frac{\partial^3}{\partial x^3} + 2xy\frac{\partial}{\partial x}\right) - \epsilon^2\left[\frac{8}{9}\frac{\partial^6}{\partial x^6} + \frac{8}{3}xy\frac{\partial^4}{\partial x^4} + \left(2x^2y^2 - 12\right)\frac{\partial^2}{\partial x^2}\right] \\ & + i\epsilon^3\left[\frac{32}{81}\frac{\partial^9}{\partial x^9} + \frac{16}{9}xy\frac{\partial^7}{\partial x^7} + \left(\frac{8}{3}x^2y^2 - \frac{176}{5}\right)\frac{\partial^5}{\partial x^5}\right. \\ & \left. + \left(\frac{4}{3}x^3y^3 - 48xy\right)\frac{\partial^3}{\partial x^3} + \left(-8x^2y^2 + 64\right)\frac{\partial}{\partial x}\right] + \mathrm{O}\left(\epsilon^4\right)\Bigg\}\,\delta(x+y).\end{aligned} \tag{18}$$

Hence, the coordinate-space representation of the operator $\mathcal{C}(x,y)$ is expressed as a derivative of a Dirac delta function. From this expression for $\mathcal{C}(x,y)$ we can verify the following properties: First, to order ϵ^3 the operator $\mathcal{C}(x,y)$ satisfies (10). That is,

$$\int_{-\infty}^{\infty} dy\, \mathcal{C}(x,y)\mathcal{C}(y,z) = \delta(x-z) + \mathrm{O}\left(\epsilon^4\right). \tag{19}$$

Second, to order ϵ^3 the operator $\mathcal{C}(x,y)$ satisfies (11); the wave functions $\phi_n(x)$ are eigenstates of $\mathcal{C}(x,y)$ with eigenvalue $(-1)^n$. That is,

$$\int_{-\infty}^{\infty} dy\, \mathcal{C}(x,y)\phi_n(y) = (-1)^n\phi_n(x) + \mathrm{O}\left(\epsilon^4\right). \tag{20}$$

Third, in the limit as $\epsilon \to 0$, the operator $\mathcal{C}(x,y)$ becomes the coordinate-space representation of the parity operator $\mathcal{P}(x,y) = \delta(x+y)$.

There is a somewhat simpler way to express the operator $\mathcal{C}(x,y)$. The derivative operator in (18) that is acting on $\delta(x+y)$ can be exponentiated so that to order ϵ^4 (and not just ϵ^3) we have

$$\mathcal{C}(x,y) = e^{-i\epsilon A - i\epsilon^3 B}\delta(x+y) + \mathrm{O}\left(\epsilon^5\right), \tag{21}$$

where the derivative operators A and B are given by

$$\begin{aligned} A &= \frac{4}{3}\frac{\partial^3}{\partial x^3} - 2x\frac{\partial}{\partial x}x, \\ B &= \frac{128}{15}\frac{\partial^5}{\partial x^5} - \frac{40}{3}x\frac{\partial^3}{\partial x^3}x + 8x^2\frac{\partial}{\partial x}x^2 - 32\frac{\partial}{\partial x}. \end{aligned} \tag{22}$$

4 Nonperturbative calculation of $\mathcal{C}$ in a quartic theory

In this section we explain briefly the nonperturbative methods that must be used to calculate the operator $\mathcal{C}(x,y)$ for the Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{2}x^2 - \epsilon x^4$. We follow the approach taken in Ref. [5], in which nonperturbative methods were used to calculate the one-point Green's function for this Hamiltonian.

4.1 Failure of perturbation theory

We begin by explaining why perturbation theory fails to produce the operator $\mathcal{C}(x,y)$. Following the approach taken in Section 3, we expand the solution to the Schrödinger equation

$$-\frac{1}{2}\phi_n''(x)+\frac{1}{2}x^2\phi_n(x)-\epsilon x^4\phi_n(x)=E_n\phi_n(x) \tag{23}$$

as a series in powers of ϵ:

$$\phi_n(x)=\frac{i^n a_n}{\pi^{1/4}2^{n/2}\sqrt{n!}}e^{-\frac{1}{2}x^2}\left[H_n(x)+P_n(x)\epsilon\right]+\mathrm{O}\left(\epsilon^2\right), \tag{24}$$

where $H_n(x)$ is the nth Hermite polynomial and $P_n(x)$ is a polynomial in x of degree $n+4$. The polynomial $P_n(x)$ is a linear combination of Hermite polynomials [1].

The energy E_n to order ϵ is

$$E_n=n+\frac{1}{2}-\frac{3}{4}\left(2n^2+2n+1\right)\epsilon+\mathrm{O}\left(\epsilon^2\right). \tag{25}$$

We must also $\mathcal{PT}$ normalize the expression for $\phi_n(x)$ according to (7) so that its square integral is $(-1)^n$:

$$\int_{-\infty}^{\infty}dx\,\left[\phi_n(x)\right]^2=(-1)^n+\mathrm{O}\left(\epsilon^2\right). \tag{26}$$

This determines the value of a_n in (24). The result is very simple; to order ϵ we have

$$a_n=1+\mathrm{O}\left(\epsilon^2\right). \tag{27}$$

Finally, we substitute $\phi_n(x)$ in (24) into (9). However, we obtain the trivial result that only the leading term (zeroth-order in powers of ϵ) survives. More generally, we can show by a parity argument that the coefficients of *all* higher powers of ϵ vanish. Thus, we get the (wrong) result that

$$\mathcal{C}(x,y)=\delta(x+y)\qquad\text{(WRONG!)}. \tag{28}$$

We know that this result is wrong because the operator $\mathcal{C}(x,y)$ is complex and the result in (28) is real. An alternative way to see this is to note (28) implies that $\mathcal{C}(x,y)$ and $\mathcal{P}(x,y)$ coincide; but in this $\mathcal{PT}$-symmetric theory, $\mathcal{C}(x,y)$ and $\mathcal{P}(x,y)$ are distinct operators. We will see that the difference between $\mathcal{C}(x,y)$ and $\mathcal{P}(x,y)$ is a nonperturbative term of order $e^{-1/(3\epsilon)}$, which is smaller than any integer power of ϵ.

4.2 Nonperturbative analysis

We will now show how to perform a nonperturbative analysis of the Schrödinger equation (23). We decompose the eigenfunction $\phi_n(x)$ into its perturbative part on the right side of (24) and a nonperturbative part:

$$\phi_n(x)=\phi_n^{\mathrm{pert}}(x)+\phi_n^{\mathrm{nonpert}}(x). \tag{29}$$

The nonperturbative part of $\phi_n(x)$ is exponentially small compared with the perturbative part, but these two contributions can be easily distinguished because for real argument x, one is real while the other is imaginary.

Following the WKB analysis in Ref. [5], we break the real-x axis into three regions: In region I, where $|x| \ll \epsilon^{-1/4}$, we have

$$\phi_n^{\rm pert}(x) \sim \frac{i^n}{\pi^{1/4}\sqrt{n!}} D_n\big(x\sqrt{2}\,\big),$$
$$\phi_n^{\rm nonpert}(x) \sim i b_n C_n\big(x\sqrt{2}\,\big), \tag{30}$$

where the coefficient of D_n is taken from (24) and the coefficient ib_n of C_n will be determined by asymptotic matching. Note that for nonnegative integer index the parabolic cylinder function D_n is expressed in terms of a Hermite polynomial H_n as

$$D_n(x\sqrt{2}) = 2^{-n/2} e^{-\frac{1}{2}x^2} H_n(x). \tag{31}$$

Also, for nonnegative integer index the functions D_n and C_n are a pair of linearly independent solutions to the parabolic cylinder equation. They can be expressed in terms of parabolic cylinder functions as follows:

$$D_n(z) \equiv \frac{n!}{\sqrt{2\pi}}\left[i^n D_{-n-1}(iz) + (-i)^n D_{-n-1}(-iz)\right],$$
$$C_n(z) \equiv \frac{i}{\sqrt{2\pi}}\left[i^n D_{-n-1}(iz) - (-i)^n D_{-n-1}(-iz)\right]. \tag{32}$$

In region II, where $1 \ll |x| \ll \epsilon^{-1/2}$, we can obtain the eigenfunction using WKB theory. We write the Schrödinger equation (23) in the form $\phi_n''(x) = \omega_n(x)\phi_n(x)$ where, to leading order in ϵ, we have $\omega_n(x) = -2\epsilon x^4 + x^2 - 2n - 1$. Then, for positive x the physical-optics WKB approximation reads

$$\phi_n^{\rm pert}(x) \sim f_n[\omega_n(x)]^{-1/4} \exp\left[-\int_{x_1}^{x} ds\,\sqrt{\omega_n(s)}\right],$$
$$\phi_n^{\rm nonpert}(x) \sim g_n[\omega_n(x)]^{-1/4} \exp\left[+\int_{x_1}^{x} ds\,\sqrt{\omega_n(s)}\right], \tag{33}$$

where the constants f_n and g_n will be determined by asymptotic matching. The lower endpoint of integration, $x_1 = \sqrt{2n+1}$, is the approximate location of the inner turning point.

In region III x is near the outer turning points at $\pm 1/\sqrt{2\epsilon}$. For positive x we define the variable r by $x = x_2\left(1 - 2^{1/3}\epsilon^{2/3} r\right)$, where $x_2 = 1/\sqrt{2\epsilon}$. The condition that x is near x_2 is that $r \ll \epsilon^{-2/3}$. In this region the Schrödinger equation becomes an Airy equation in the variable r: $\phi_n''(r) = r\phi_n(r)$. The solution in this region reads

$$\phi_n^{\rm pert}(r) \sim h_n {\rm Bi}(r),$$
$$\phi_n^{\rm nonpert}(r) \sim -i h_n {\rm Ai}(r), \tag{34}$$

where ${\rm Ai}(r)$ and ${\rm Bi}(r)$ are the exponentially decaying and growing Airy functions for large positive r. The fact that the same coefficient h_n multiplies both Bi and Ai is a nontrivial result that is established in Ref. [5].

By asymptotically matching the solutions in regions I and II and the solutions in regions II and III we obtain the formula for the coefficient of the nonperturbative part of the solution in (30):

$$b_n = -\frac{i^n \pi^{1/4}}{\sqrt{2}\,n!}\left(\frac{4}{\epsilon}\right)^{n+\frac{1}{2}} e^{-\frac{1}{3\epsilon}}. \tag{35}$$

Finally, using the wave function in region I we can construct the operator $\mathcal{C}(x,y)$ according to (9):

$$\mathcal{C}(x,y) = \sum_{n=0}^{\infty} \left[\phi_n^{\rm pert}(x)\phi_n^{\rm pert}(y) + \phi_n^{\rm pert}(x)\phi_n^{\rm nonpert}(y)\right.$$
$$\left. + \phi_n^{\rm nonpert}(x)\phi_n^{\rm pert}(y) + \phi_n^{\rm nonpert}(x)\phi_n^{\rm nonpert}(y)\right]. \qquad (36)$$

The first sum in this equation gives $\delta(x+y)$ to all orders in powers of ϵ as explained above in Subsection 4.1. The last sum is negligible compared with the second and third sums. We thus obtain

$$\mathcal{C}(x,y) = \delta(x+y)$$
$$- ie^{-\frac{1}{3\epsilon}}\sqrt{\frac{2}{\epsilon}}\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{4}{\epsilon}\right)^n \left[D_n(x\sqrt{2})C_n(y\sqrt{2}) + C_n(x\sqrt{2})D_n(y\sqrt{2})\right], \qquad (37)$$

where C_n and D_n are defined in (32). Observe that the correction to the delta function (that is, the difference between the $\mathcal{P}$ operator and the $\mathcal{C}$ operator) is nonperturbative; it is exponentially small and imaginary.

The summation in (37) can be converted to a double integral:

$$\mathcal{C}(x,y) = \delta(x+y) + i\sqrt{\frac{2}{\pi^3\epsilon}}\, e^{-\frac{1}{3\epsilon}} e^{\frac{1}{2}(x^2+y^2)} \left\{ \frac{\partial}{\partial x}\int_0^{\pi} d\theta \int_0^1 \frac{ds}{\sqrt{1+s^2}}\right.$$
$$\left. \times \exp\left[\frac{\left(2\sqrt{2s/\epsilon}\,\cos\theta - ix - isy\right)^2}{1+s^2}\right] + (x \leftrightarrow y)\right\}. \qquad (38)$$

This is the leading-order nonperturbative approximation to the coordinate-space representation of the operator $\mathcal{C}$.

Acknowledgements

This work was supported by the U.S. Department of Energy.

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