Small-ϵ behavior of the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian $H = p^2 + x^2(\mathrm{i}x)_\epsilon$

Small-ϵ behavior of the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian $H = p^2 + x^2(\mathrm{i}x)^\epsilon$

Carl M Bender[1], Karim Besseghir, Hugh F Jones and Xinghui Yin

Theoretical Physics, Blackett Laboratory, Imperial College, London SW7 2BZ, UK

E-mail: cmb@wustl.edu, karim.besseghir@epfl.ch, h.f.jones@ic.ac.uk and xinghui@gmx.de

Abstract
The energy eigenvalues of the class of non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians $H = p^2 + x^2(\mathrm{i}x)^\epsilon$ ($\epsilon \geqslant 0$) are real, positive and discrete. The behavior of these eigenvalues has been studied perturbatively for small ϵ. However, until now no other features of H have been examined perturbatively. In this paper the small-ϵ expansion of the $\mathcal{C}$ operator and the equivalent isospectral Dirac–Hermitian Hamiltonian h are derived.

PACS numbers: 11.30.Er, 12.20.−m, 02.30.Mv, 11.10.Lm

1. Introduction

For non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians it has been established that the physical requirements of spectral positivity and unitarity can be met even though the Hamiltonian is not Hermitian in the Dirac sense. (A Hamiltonian H is Hermitian in the *Dirac sense* if it satisfies $H = H^\dagger$, where the Dirac adjoint symbol $\dagger$ indicates combined complex conjugation and matrix transposition.) Many $\mathcal{PT}$-symmetric model Hamiltonians have been studied [1], but the first non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian for which spectral positivity and unitarity were verified is

$$H = p^2 + x^2(\mathrm{i}x)^\epsilon \qquad (\epsilon \geqslant 0). \tag{1}$$

It was shown in 1998 that the spectrum of the class of Hamiltonians (1) was positive and discrete [2] and it was conjectured that spectral positivity was a consequence of the invariance of H under the combination of the space-reflection operator $\mathcal{P}$ and the time-reversal operator $\mathcal{T}$. Three years later, a rigorous proof of spectral positivity was given [3]. Then, in 2002 it was demonstrated that the time-evolution operator $U = \mathrm{e}^{-\mathrm{i}Ht}$ for the Hamiltonian (1) is unitary [4]. In [4] it was shown that if the $\mathcal{PT}$ symmetry of a non-Hermitian Hamiltonian is unbroken, then it is possible to construct a new operator called $\mathcal{C}$ that commutes with the Hamiltonian H.

---

[1] Permanent address: Department of Physics, Washington University, St Louis, MO 63130, USA.

The Hilbert-space inner product with respect to the $\mathcal{CPT}$ adjoint has a positive norm. Also, the operator U is unitary with respect to the $\mathcal{CPT}$ adjoint. Thus, Dirac Hermiticity of the Hamiltonian is not a necessary requirement of a quantum theory and unbroken $\mathcal{PT}$ symmetry is sufficient to guarantee that the spectrum of H is real and positive and that the time evolution is unitary.

In subsequent papers the $\mathcal{C}$ operators for various quantum-mechanical and field-theoretic models were calculated [5–9], mostly by using conventional perturbative methods. It was shown that this operator has a natural form as the parity operator multiplied by an exponential of a Dirac Hermitian operator $\mathcal{Q}$:

$$\mathcal{C} = e^{\mathcal{Q}}\mathcal{P}, \qquad \text{where} \quad \mathcal{Q} = \mathcal{Q}^{\dagger}. \tag{2}$$

The operator $\mathcal{Q}$ vanishes in the unperturbed $\epsilon \to 0$ limit when the Hamiltonian becomes Hermitian and parity invariant. This implies that the $\mathcal{C}$ operator can be thought of as the continuation or extension of the parity operator $\mathcal{P}$ as ϵ increases from 0. It was proved by Mostafazadeh that the $\mathcal{Q}$ operator can be used to transform the non-Dirac–Hermitian Hamiltonian H to a spectrally equivalent Dirac–Hermitian Hamiltonian h [10]:

$$h = e^{\mathcal{Q}/2} H e^{-\mathcal{Q}/2}. \tag{3}$$

This similarity transformation was used by Geyer *et al* to convert Hermitian Hamiltonians to non-Hermitian Hamiltonians [11].

Originally, Bender and Boettcher introduced the Hamiltonian (1) to examine the suggestion by Bessis and Zinn-Justin [12] that the spectrum of the Hamiltonian $H = p^2 + ix^3$ might be real. Bender and Boettcher speculated that if this were true, then the reality of the spectrum might be due to the obvious symmetry of this Hamiltonian under combined $\mathcal{P}$ and $\mathcal{T}$ reflection. To study this idea Bender and Boettcher considered the Hamiltonian in (1) because (i) this Hamiltonian is $\mathcal{PT}$ symmetric for all real ϵ, and (ii) it could then be studied perturbatively for small ϵ by using the methods of the δ expansion, which had been developed much earlier by Bender *et al* [13]. (One recovers the ix^3 potential by setting $\epsilon = 1$.) The discovery that order-by-order in powers of ϵ the eigenvalues of H in (1) are *all* real led to much subsequent numerical and analytical work on this model.

Surprisingly, the methods of the δ expansion, for which the principal idea is to introduce in the *exponent* a small perturbation parameter whose effect is to quantify how nonlinear a theory is, were not used in further studies of the Hamiltonian in (1). The objective of this paper is to report a new perturbative study along these lines in which the $\mathcal{C}$ operator and the equivalent Dirac–Hermitian Hamiltonian h are calculated for small ϵ. We have determined the $\mathcal{C}$ operator to first order in powers of ϵ, and using this result we have found the equivalent Hermitian Hamiltonian h to second order in ϵ. The results can be presented compactly, but they reveal in dramatic fashion how complicated and nonlocal the isospectral Dirac–Hermitian Hamiltonian h can be.

The construction of the $\mathcal{C}$ operator in [4] was the key step in showing that time evolution for the non-Hermitian Hamiltonian (1) is unitary. However, the difficulty with the construction given in [4] is that calculating the $\mathcal{C}$ operator requires as input all of the coordinate-space eigenvectors of the Hamiltonian. This information is available in quantum mechanics but it is unwieldy. (In the case of quantum field theory this information is not available because there is no simple analog of the coordinate-space Schrödinger equation.)

Fortunately, it is possible to obtain the $\mathcal{C}$ operator by solving three simple simultaneous algebraic equations [5]:

$$\mathcal{C}^2 = 1, \tag{4}$$

$$[\mathcal{C}, \mathcal{PT}] = 0, \tag{5}$$

$$[\mathcal{C}, H] = 0. \tag{6}$$

The first two of these equations are kinematic because they are obeyed by the $\mathcal{C}$ operator for any $\mathcal{PT}$-symmetric Hamiltonian of the standard type $H = p^2 + V(x)$. If we seek a solution for $\mathcal{C}$ in the form (2), we find that these two equations imply that the operator $\mathcal{Q}(x, p)$ is an even function of the x operator and an odd function of the p operator.[2] The third equation (6) is dynamical because it makes explicit use of the Hamiltonian that defines the theory. This is the equation that we will solve perturbatively using the methods of the δ expansion.

In section 2 we calculate the $\mathcal{Q}$ operator to first order in ϵ for the $\mathcal{PT}$-symmetric Hamiltonian in (1), and in section 3 we calculate the equivalent Hermitian Hamiltonian h to second order. In section 4 we discuss the calculation of eigenvalues.

2. First-order calculation of the $\mathcal{C}$ operator

We begin our calculation of the $\mathcal{C}$ operator for H in (1) by expanding H to second order in powers of ϵ

$$H = H_0 + \epsilon H_1 + \epsilon^2 H_2 + O(\epsilon^3), \tag{7}$$

where $H_0 = p^2 + x^2$ is the Hamiltonian for the harmonic oscillator, $H_1 = x^2 \log(ix)$, and $H_2 = \frac{1}{2}[x \log(ix)]^2$. We then recall the representation of the $\mathcal{C}$ operator in (2) and expand the $\mathcal{Q}$ operator as a series in powers of ϵ:

$$\mathcal{Q} = \sum_{n=1}^{\infty} \epsilon^n \mathcal{Q}_n. \tag{8}$$

This perturbation series begins at $n = 1$ because when $\epsilon = 0$, the $\mathcal{C}$ operator reduces to the parity operator $\mathcal{P}$. We will see that even-n terms as well as odd-n terms must be included in (8). This is a significant departure from previous perturbative results for the $\mathcal{C}$ operator; for the cubic Hamiltonian $H = p^2 + x^2 + \epsilon ix^3$ [6] and the square-well Hamiltonian $H = p^2 + V(x)$, where $V(x) = \epsilon ix/|x|$ ($|x| < 1$) and $V(x) = \infty$ ($|x| > 1$) [7], there are no even-n terms.

If we then substitute the expansion for $\mathcal{C}$,

$$\mathcal{C} = \left[\mathbf{1} + \epsilon \mathcal{Q}_1 + \epsilon^2 \mathcal{Q}_2 + \tfrac{1}{2}\epsilon^2 \mathcal{Q}_1^2 + O(\epsilon^3) \right] \mathcal{P},$$

and the expansion for H in (7) into the commutator (6) and collect powers of ϵ, we obtain a sequence of equations for the coefficients of $\mathcal{Q}$. After some algebra, we find that the first-order equation simplifies to

$$[\mathcal{Q}_1, H_0] = x^2[\log(ix) - \log(-ix)] = i\pi x|x| \tag{9}$$

and that the second-order equation becomes

$$[\mathcal{Q}_2, H_0] = i\pi x|x| \log|x| - [\mathcal{Q}_1, x^2 \log|x|]. \tag{10}$$

Although we have not yet found an analytical solution to (10), it is likely from this equation that $\mathcal{Q}_2$ is nonzero, and as we stated earlier, this is an unexpected result based on previous perturbative calculations of the $\mathcal{C}$ operator. Although (9) is simple looking, it is difficult to solve. Nevertheless, we have found an exact analytical solution.

The solution of (9) relies heavily on the work of Bender and Dunne [14]. We introduce a set of Weyl-ordered operators

$$T_{m,n} \equiv \frac{1}{2^m} \sum_{k=0}^{m} \binom{m}{k} p^k x^n p^{m-k} \qquad (m, n = 0, 1, 2, \ldots). \tag{11}$$

---

[2] The operator $\mathcal{Q}$ for the Swanson model Hamiltonian $H = p^2 + x^2 + i\alpha\{x, p\}_+$ does not possess this symmetry property because H is not symmetric and consequently $\mathcal{C}$ does not satisfy equation (4).

The operator $T_{m,n}$ is a totally symmetric quantum-mechanical generalization of the classical product $p^m x^n$. Weyl-ordered operator products rely implicitly on the Heisenberg algebraic property that $[x, p] = \mathrm{i}$. We then define the generalized Weyl-ordered operator $\widetilde{T}_{m,n}$ as

$$\widetilde{T}_{m,n} \equiv \frac{1}{2^m} \sum_{k=0}^{m} \binom{m}{k} p^k |x|^n p^{m-k}. \tag{12}$$

In terms of this definition of Weyl ordering, we assert that $\mathcal{Q}_1$ can be expressed as

$$\mathcal{Q}_1 = \frac{\pi}{2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n-1)(2n+1)} \widetilde{T}_{2n+1,-2n+1}. \tag{13}$$

It is clear that $\mathcal{Q}_1$ satisfies the kinematic constraints that it be even in x and odd in p. We do not claim that (13) is the unique solution to (9). The question of nonuniqueness is addressed in [15].

To show that $\mathcal{Q}_1$ solves (9), we first demonstrate that the $n = 0$ term in the series commuted with x^2 gives $\mathrm{i}\pi x|x|$, that is,

$$-\frac{\pi}{2}[\widetilde{T}_{1,1}, x^2] = \mathrm{i}\pi x|x|. \tag{14}$$

We then show that the kth term in the series commuted with p^2 is exactly canceled by the $(k+1)$st term commuted with x^2.

To verify (14) we note that the $n = 0$ term in the series is $-\frac{\pi}{2}\widetilde{T}_{1,1} = -\frac{\pi}{4}(|x|p + p|x|)$. We then get

$$\left[-\frac{\pi}{4}(|x|p + p|x|), x^2\right] = -\frac{\pi}{4}(|x|[p, x^2] + [p, x^2]|x|) = \mathrm{i}\pi x|x|.$$

Next we show that the kth term of $\mathcal{Q}_1$ commuted with p^2 gives

$$\frac{\pi}{2}\left[\frac{(-1)^k}{(2k-1)(2k+1)} \widetilde{T}_{2k+1,-2k+1}, p^2\right]$$

$$= -\frac{\mathrm{i}\pi(-1)^k}{2^{2k+2}(2k+1)} \sum_{j=0}^{2k+2} \binom{2k+2}{j} p^j \mathrm{sgn}(x) x^{-2k} p^{2k+2-j}, \tag{15}$$

where the sign function $\mathrm{sgn}(x)$ is defined by

$$\mathrm{sgn}(x) = \begin{cases} 1 & \text{if} \quad x > 0, \\ 0 & \text{if} \quad x = 0, \\ -1 & \text{if} \quad x < 0. \end{cases}$$

The identity $\frac{\mathrm{d}}{\mathrm{d}x}|x| = \mathrm{sgn}(x)$ implies that $[|x|, p] = \mathrm{i}\mathrm{sgn}(x)$. Also, from the identity $0 = \frac{\mathrm{d}}{\mathrm{d}x}(|x|^n |x|^{-n}) = n|x|^{-1}\mathrm{sgn}(x) + |x|^n \frac{\mathrm{d}}{\mathrm{d}x}|x|^{-n}$ for all integer n, we obtain $[|x|^{-2k+1}, p] = \mathrm{i}(1 - 2k)\mathrm{sgn}(x)x^{-2k}$. It follows that

$$[\widetilde{T}_{2k+1,-2k+1}, p] = \left[\frac{1}{2^{2k+1}} \sum_{j=0}^{2k+1} \binom{2k+1}{j} p^j |x|^{-2k+1} p^{2k+1-j}, p \right]$$

$$= \frac{1}{2^{2k+1}} \sum_{j=0}^{2k+1} \binom{2k+1}{j} p^j [|x|^{-2k+1}, p] p^{2k+1-j}$$

$$= \frac{i(1-2k)}{2^{2k+1}} \sum_{j=0}^{2k+1} \binom{2k+1}{j} p^j \mathrm{sgn}(x) x^{-2k} p^{2k+1-j}.$$

Using this result, we find that

$$[\widetilde{T}_{2k+1,-2k+1}, p^2] = p[\widetilde{T}_{2k+1,-2k+1}, p] + [\widetilde{T}_{2k+1,-2k+1}, p]p$$

$$= \frac{i(1-2k)}{2^{2k+1}} \left[\sum_{r=0}^{2k+1} \binom{2k+1}{r} p^{r+1} \mathrm{sgn}(x) x^{-2k} p^{2k+1-r} \right.$$

$$\left. + \sum_{s=0}^{2k+1} \binom{2k+1}{s} p^s \mathrm{sgn}(x) x^{-2k} p^{2k+2-s} \right]$$

$$= \frac{i(1-2k)}{2^{2k+1}} \left[\sum_{r'=1}^{2k+2} \binom{2k+1}{r'-1} p^{r'} \mathrm{sgn}(x) x^{-2k} p^{2k+2-r'} \right.$$

$$\left. + \mathrm{sgn}(x) x^{-2n} p^{2n+2} + \sum_{s=1}^{2k+1} \binom{2k+1}{s} p^s \mathrm{sgn}(x) x^{-2k} p^{2k+2-s} \right]$$

$$= \frac{i(1-2k)}{2^{2k+1}} \left[\mathrm{sgn}(x) x^{-2n} p^{2n+2} + p^{2n+2} \mathrm{sgn}(x) x^{-2n} \right.$$

$$\left. + \sum_{j=1}^{2k+1} \left\{ \binom{2k+1}{j-1} + \binom{2k+1}{j} \right\} p^j \mathrm{sgn}(x) x^{-2k} p^{2k+2-j} \right].$$

We then simplify this expression by using

$$\binom{2k+1}{j-1} + \binom{2k+1}{j} = \binom{2k+2}{j},$$

which establishes the result in (15).

We now calculate the $(k+1)$st term of $\mathcal{Q}_1$ commuted with x^2. We first note that $\widetilde{T}_{m,n}$ can be rewritten as [14]

$$\widetilde{T}_{m,n} = \frac{1}{2^n} \sum_{j=0}^{n} \binom{n}{j} |x|^j p^m |x|^{n-j}.$$

Using the identity

$$[p^n, x^2] = -in(p^{n-1}x + xp^{n-1}) = -2inxp^{n-1} + n(n-1)p^{n-2}$$

$$= -2inp^{n-1}x - n(n-1)p^{n-2},$$

we obtain

$$[\widetilde{T}_{m,n}, x^2] = \frac{1}{2^n} \sum_{j=0}^{n} \binom{n}{j} |x|^j [p^m, x^2] |x|^{n-j}$$

$$= \frac{1}{2^n} \sum_{j=0}^{n} \binom{n}{j} |x|^j [-im(xp^{m-1} + p^{m-1}x)] |x|^{n-j}$$

$$= \frac{-2\mathrm{i}m}{2^n} \sum_{j=0}^{n} \binom{n}{j} |x|^j \frac{1}{2} (xp^{m-1} + p^{m-1}x)|x|^{n-j}$$

$$= \frac{-2\mathrm{i}m}{2^{m-1}} \sum_{r=0}^{m-1} \binom{m-1}{r} p^r \epsilon(x)|x|^{n+1} p^{m-1-r}.$$

Thus,

$$[\widetilde{T}_{2k+3,-2k-1}, x^2] = \frac{-2\mathrm{i}(2k+3)}{2^{2k+2}} \sum_{r=0}^{2k+2} \binom{2k+2}{r} p^r \epsilon(x) x^{-2k} p^{2k+2-r}.$$

This shows that

$$\frac{\pi}{2} \left[\frac{(-1)^k}{(2k-1)(2k+1)} \widetilde{T}_{2k+1,-2k+1}, p^2 \right] = -\frac{\mathrm{i}\pi(-1)^k}{2^{2k+2}(2k+1)} \sum_{j=0}^{2k+2} \binom{2k+2}{j} p^j \epsilon(x) x^{-2k} p^{2k+2-j}.$$

We conclude that the kth term of $\mathcal{Q}_1$ commuted with p^2 is exactly canceled by the $(k+1)$st term commuted with x^2:

$$\frac{\pi}{2} \left[\frac{(-1)^{k+1}}{(2k+1)(2k+3)} \widetilde{T}_{2k+3,-2k-1}, x^2 \right] = -\frac{\pi}{2} \left[\frac{(-1)^k}{(2k-1)(2k+1)} \widetilde{T}_{2k+1,-2k+1}, p^2 \right].$$

We have thus shown that $\mathcal{Q}_1$ in (13) solves the commutation relation (9). This argument was quite elaborate, and it is clear why we have not yet found an analytical solution to the commutation relation (10). However, having found $\mathcal{Q}_1$, we can now calculate the equivalent Hermitian Hamiltonian h to *second* order in ϵ, as we show in the next section.

3. Second-order calculation of the equivalent Hermitian Hamiltonian

In this section we use (3) to calculate the Hermitian Hamiltonian h, which is isospectral to H in (1). Expanding (3) as a perturbation series in powers of ϵ, we obtain

$$\begin{aligned}
h = \mathrm{e}^{-\frac{\mathcal{Q}}{2}} H e^{\frac{\mathcal{Q}}{2}} &= \left(1 - \frac{\mathcal{Q}}{2} + \frac{\mathcal{Q}^2}{8} + \cdots \right) H \left(1 + \frac{\mathcal{Q}}{2} + \frac{\mathcal{Q}^2}{8} + \cdots \right) \\
&= H_0 + \epsilon \left(\frac{1}{2}[H_0, \mathcal{Q}_1] + H_1 \right) \\
&\quad + \epsilon^2 \left(\frac{1}{2}[H_0, \mathcal{Q}_2] + \frac{1}{8}\{H_0, \mathcal{Q}_1^2\} + \frac{1}{2}[H_1, \mathcal{Q}_1] - \frac{\mathcal{Q}_1}{2} H_0 \frac{\mathcal{Q}_1}{2} + H_2 \right) + \mathrm{O}(\epsilon^3),
\end{aligned}$$

(16)

where curly brackets indicate anticommutation relations. We evaluate the first- and second-order terms in this equation and show that they can be reduced to compact forms.

To first order in ϵ, we use (9) to simplify (16) and get

$$h = H_0 + \epsilon \left(-\frac{\mathrm{i}\pi}{2} x|x| + x^2 \log(\mathrm{i}x) \right) = p^2 + x^2 + \epsilon x^2 \log |x|. \tag{17}$$

Thus, to first order in ϵ the potential for the equivalent Hermitian Hamiltonian h is a minor correction to the potential x^2 for the harmonic oscillator. As shown in figure 1, when ϵ is positive, the potential $x^2 + \epsilon x^2 \log |x|$ lies below x^2 for $|x| < 1$, but for $|x| > 1$ it rises faster than the parabolic potential and thus squeezes the energy levels upward.

To second order in ϵ, the equivalent Hermitian Hamiltonian takes the form

$$h = H_0 + \epsilon x^2 \log |x| + \epsilon^2 f(x, p) + \mathrm{O}(\epsilon^3),$$
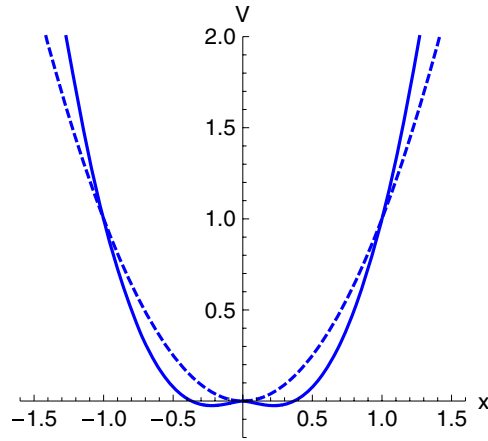
Figure 1. Two plots of the potential $V(x) = x^2 + \epsilon x^2 \log|x|$, one for the unperturbed case $\epsilon = 0$ (dashed line) and the other for $\epsilon = 1$ (solid line). Note that when $\epsilon > 0$, the potential $x^2 + \epsilon x^2 \log|x|$ lies below x^2 for $|x| < 1$, but for $|x| > 1$ it rises faster than the parabolic potential and thus squeezes the energy levels upward.

(This figure is in colour only in the electronic version)

which can be simplified by using (10):

$$
\begin{aligned}
f(x, p) &= \frac{1}{2}[H_0, \mathcal{Q}_2] + \frac{1}{8}\{H_0, \mathcal{Q}_1^2\} + \frac{1}{2}[H_1, \mathcal{Q}_1] - \frac{\mathcal{Q}_1}{2} H_0 \frac{\mathcal{Q}_1}{2} + H_2 \\
&= \frac{1}{2}\left([\mathcal{Q}_1, H_1] + \left[\frac{1}{2}\mathcal{Q}_1^2, H_0\right] - i\pi x|x|\log|x| - \mathcal{Q}_1[\mathcal{Q}_1, H_0]\right) \\
&\quad + \frac{1}{8}\{H_0, \mathcal{Q}_1^2\} + \frac{1}{2}[H_1, \mathcal{Q}_1] - \frac{1}{4}\mathcal{Q}_1 H_0 \mathcal{Q}_1 + H_2 \\
&= \frac{1}{4}[\mathcal{Q}_1^2, H_0] - \frac{1}{2}\mathcal{Q}_1[\mathcal{Q}_1, H_0] + \frac{1}{8}\{H_0, \mathcal{Q}_1^2\} - \frac{1}{4}\mathcal{Q}_1 H_0 \mathcal{Q}_1 \\
&\quad + H_2 - \frac{i\pi}{2}x|x|\log|x|.
\end{aligned}
\tag{18}
$$

The significance of this formula is that we do not need $\mathcal{Q}_2$ to calculate h to order ϵ^2.

The result in (18) may be further simplified by using

$$
H_2 - \frac{i\pi}{2}x|x|\log|x| = \frac{1}{2}x^2[\log(ix)]^2 - \frac{1}{2}i\pi x|x|\log|x| = \frac{1}{2}x^2(\log|x|)^2 - \frac{\pi^2}{8}x^2
$$

and

$$
\begin{aligned}
\tfrac{1}{4}[\mathcal{Q}_1^2, H_0] &- \tfrac{1}{2}\mathcal{Q}_1[\mathcal{Q}_1, H_0] + \tfrac{1}{8}\{H_0, \mathcal{Q}_1^2\} - \tfrac{1}{4}\mathcal{Q}_1 H_0 \mathcal{Q}_1 \\
&= \tfrac{1}{4}\mathcal{Q}_1^2 H_0 - \tfrac{1}{4}H_0\mathcal{Q}_1^2 - \tfrac{1}{2}\mathcal{Q}_1^2 H_0 + \tfrac{1}{2}\mathcal{Q}_1 H_0 \mathcal{Q}_1 + \tfrac{1}{8}H_0\mathcal{Q}_1^2 + \tfrac{1}{8}\mathcal{Q}_1^2 H_0 - \tfrac{1}{4}\mathcal{Q}_1 H_0 \mathcal{Q}_1 \\
&= -\tfrac{1}{8}\mathcal{Q}_1^2 H_0 + \tfrac{1}{4}\mathcal{Q}_1 H_0 \mathcal{Q}_1 - \tfrac{1}{8}H_0\mathcal{Q}_1^2 \\
&= \tfrac{1}{8}[[\mathcal{Q}_1, H_0], \mathcal{Q}_1].
\end{aligned}
$$

Thus, the second-order correction can be written as

$$
f(x, p) = \frac{1}{2}x^2(\log|x|)^2 - \frac{\pi^2}{8}x^2 + \frac{1}{8}[[\mathcal{Q}_1, H_0], \mathcal{Q}_1].
\tag{19}
$$

We then calculate the double commutator $[[\mathcal{Q}_1, H_0], \mathcal{Q}_1]$ as follows:

$$[[\mathcal{Q}_1, H_0], \mathcal{Q}_1] = i\pi [x|x|, \mathcal{Q}_1]$$

$$= i\pi \begin{cases} [x^2, \mathcal{Q}_1] & \text{if} \quad x > 0 \\ -[x^2, \mathcal{Q}_1] & \text{if} \quad x < 0 \end{cases}$$

$$= i\pi \begin{cases} \dfrac{\pi}{2} \displaystyle\sum_{n=0}^{\infty} \dfrac{(-1)^n}{(2n-1)(2n+1)} [x^2, T_{2n+1,-2n+1}] & \text{if} \quad x > 0 \\ \dfrac{\pi}{2} \displaystyle\sum_{n=0}^{\infty} \dfrac{(-1)^n}{(2n-1)(2n+1)} [x^2, T_{2n+1,-2n+1}] & \text{if} \quad x < 0 \end{cases}$$

$$= \frac{i\pi^2}{2} \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n-1)(2n+1)} [x^2, T_{2n+1,-2n+1}].$$

Recalling that $[x^2, T_{2n+1,-2n+1}] = 2i(2n+1)T_{2n,-2n+2}$ [14], we get

$$f(x, p) = \frac{1}{2} x^2 (\log|x|)^2 - \frac{\pi^2 x^2}{8} - \frac{\pi^2}{8} \sum_{n=0}^{\infty} \frac{(-1)^n}{2n-1} T_{2n,-2n+2}.$$

A major result of [14] is that

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} T_{2n+1,-2n-1} = \arctan\left(p\frac{1}{x}\right) - iF(x, p),$$

where

$$F(x, p) = \frac{1}{2H_0} \int_0^{\infty} ds \frac{e^s}{\cosh\left(\frac{s}{2H_0}\right)}.$$

We simply take the Dirac–Hermitian conjugate of this equation, which inverts the order of the operators p and x. The definition of the Weyl-ordered operators $T_{m,n}$ guarantees that they are Dirac Hermitian. Then, noting that $F(x, p)^{\dagger} = F(x, p)$, we deduce that

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} T_{2n+1,-2n-1} = \arctan\left(\frac{1}{x}p\right) + iF(x, p).$$

Hence,

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} T_{2n+1,-2n-1} = \frac{1}{2} \arctan\left(p\frac{1}{x}\right) + \frac{1}{2} \arctan\left(\frac{1}{x}p\right).$$

Finally, using $\{x, T_{m,n}\} = 2T_{m,n+1}$ and $\{p, T_{m,n}\} = 2T_{m+1,n}$ [14], we obtain

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{2n-1} T_{2n,-2n+1} = - \sum_{m=-1}^{\infty} \frac{(-1)^m}{2m+1} T_{2m+2,-2m}$$

$$= -x^2 - \sum_{m=0}^{\infty} \frac{(-1)^m}{2m+1} T_{2m+2,-2m}$$

$$= -x^2 - \frac{1}{4}\left\{x, \left\{p, \sum_{m=0}^{\infty} \frac{(-1)^m}{2m+1} T_{2m+1,-2m-1}\right\}\right\}$$

$$= -x^2 - \frac{1}{8}\left\{x, \left\{p, \arctan\left(p\frac{1}{x}\right) + \arctan\left(\frac{1}{x}p\right)\right\}\right\},$$

Table 1. Comparison of the exact ground-state eigenvalues for the non-Hermitian Hamiltonian in (1) and the first- and second-order perturbative calculations of the ground-state eigenvalues as given in (21–23).

ϵ	Numerical value	First order	Second order
0.1	1.003 097	1.000 912	1.003 241
0.01	1.000 114 36	1.000 091 22	1.000 114 51
0.001	1.000 009 355 38	1.000 009 122 49	1.000 009 355 22

where the curly brackets indicate anticommutators. Thus, we obtain an explicit formula for the equivalent Hermitian Hamiltonian h to second order in ϵ:

$$h = H_0 + \epsilon x^2 \log |x| + \epsilon^2 \left(\frac{1}{2} x^2 (\log |x|)^2 \right.$$

$$\left. + \frac{\pi^2}{64} \left\{ x, \left\{ p, \arctan \left(p \frac{1}{x} \right) + \arctan \left(\frac{1}{x} p \right) \right\} \right\} \right) + \mathrm{O}(\epsilon^3). \tag{20}$$

Note that h is singular and nonlocal because it contains all positive powers of p and all negative powers of x.

4. Calculation of energy eigenvalues

If we expand (1) as a series in powers of ϵ, we obtain

$$H = p^2 + \epsilon x^2 \log(\mathrm{i}x) + \tfrac{1}{2} \epsilon^2 [\log(\mathrm{i}x)]^2 + \cdots,$$

where $\log(\mathrm{i}x) = \log(|x|) + \tfrac{1}{2} \mathrm{i}\pi \, \mathrm{sgn}(x)$. We can then use conventional perturbation techniques to calculate the ground-state energy as a series in powers of ϵ:

$$E_{\text{ground state}} = 1 + a\epsilon + b\epsilon^2 + \mathrm{O}(\epsilon^3). \tag{21}$$

In first-order perturbation theory the coefficient a is the expectation value of the perturbing potential $\epsilon x^2 \log(\mathrm{i}x)$ in the unperturbed harmonic-oscillator ground state, whose wavefunction is $\exp(-x^2/2)$. We find that

$$a = \frac{1}{4} \psi \left(\frac{3}{2} \right) = \frac{1}{2} - \frac{\gamma}{4} - \frac{1}{2} \log 2 = 0.009\,122\,49 \ldots. \tag{22}$$

The same result for a is obtained by truncating the equivalent Hermitian Hamiltonian h in (20) after the first-order term.

We calculate the coefficient b in (21) by using second-order perturbation theory applied to H. The calculation is lengthy, and we do not discuss it here except to give the result:

$$b = \tfrac{1}{128} [8 + 2\pi^2 \log 2 + 4(\gamma - 2 + 2 \log 2)(\gamma + 2 \log 2) + 7\zeta(3)] = 0.232\,89 \ldots, \tag{23}$$

where $\gamma = 0.5772 \ldots$ is Euler's constant.

Note that the ground-state energy of the non-Hermitian Hamiltonian $H = p^2 + x^2(\mathrm{i}x)^\epsilon$ is slightly higher than the ground-state energy of the harmonic oscillator. This is consistent with previous numerical calculations in [2] and agrees with a precise numerical calculation of the ground-state energy for the non-Hermitian Hamiltonian (1) when ϵ is small, as is shown in table 1.

Because the second-order equivalent Dirac–Hermitian Hamiltonian h in (20) is nonlocal, it is not clear how to use h to calculate the energy eigenvalues beyond first order. If we try to do so by using standard Rayleigh–Schrödinger methods, we are faced with the problem

of calculating the expectation value of the arctangent functions in (20). This is a singular and ill-defined calculation that requires the introduction of a regulator. The singular nature of this calculation can be seen from the identity $\frac{1}{x}p|0\rangle = i|0\rangle$. This identity gives the formal result $\arctan\left(\frac{1}{x}p\right)|0\rangle = \arctan(i)|0\rangle$, which is infinite in the absence of a regulator. In fact, the singularity is even more severe than this observation suggests. If we attempt to evaluate the expectation value of the arctangent functions without a regulator and use the Taylor expansion

$$\arctan(s) = \sum_{k=0}^{\infty}(-1)^k s^{2k+1}/(2k+1),$$

we can only recover the value of b in (23) if we can interpret the sum of the divergent series $0 + 1 + 0 + 1 + 0 + 1 + 0 + \cdots$ as $\frac{1}{2}\log(2)$.

We conclude that, while the equivalent isospectral Hamiltonian h is formally Dirac Hermitian, using h to calculate the energies presents serious difficulties. We have encountered here the same kind of difficulties that were discovered in [17], namely, that the Dirac–Hermitian Hamiltonian h suffers from nonlocality and consequently is hard to use in a calculation. In [17] dimensional regulation was used to eliminate divergences in Feynman diagrams. We defer to a future paper the search for a suitable regulator for the present problem.

Acknowledgments

References

[1] Levai G and Znojil M 2000 *J. Phys. A: Math. Gen.* **33** 7165
[2] Bender C M and Boettcher S 1998 *Phys. Rev. Lett.* **80** 5243
[3] Dorey P, Dunning C and Tateo R 2001 *J. Phys. A: Math. Gen.* **34** L391
    Dorey P, Dunning C and Tateo R 2001 *J. Phys. A: Math. Gen.* **34** 5679
[4] Bender C M, Brody D C and Jones H F 2002 *Phys. Rev. Lett.* **89** 270401
    Bender C M, Brody D C and Jones H F 2003 *Am. J. Phys.* **71** 1095
[5] Bender C M, Brody D C and Jones H F 2004 *Phys. Rev. Lett.* **93** 251601
    Bender C M, Brody D C and Jones H F 2004 *Phys. Rev.* D **70** 025001
[6] Bender C M, Meisinger P N and Wang Q 2003 *J. Phys. A: Math. Gen.* **36** 1973
[7] Bender C M and Tan B 2006 *J. Phys. A: Math. Gen.* **39** 1945
[8] Milton K A 2004 *Czech. J. Phys.* **54** 85
    Bender C M, Cavero-Pelaez I, Milton K A and Shajesh K V 2005 *Phys. Lett.* B **613** 97
[9] Bender C M and Jones H F 2004 *Phys. Lett.* A **328** 102
    Bender C M, Brod J, Refig A and Reuter M E 2004 *J. Phys. A: Math. Gen.* **37** 10139
    Bender C M, Brandt S F, Chen J-H and Wang Q 2005 *Phys. Rev.* D **71** 025014
    Bender C M, Jones H F and Rivers R J 2005 *Phys. Lett.* B **625** 333
    Bender C M, Brandt S F, Chen J-H and Wang Q 2005 *Phys. Rev.* D **71** 065010
[10] Mostafazadeh A 2002 *J. Math. Phys.* **43** 205
    Mostafazadeh A 2003 *J. Phys. A: Math. Gen.* **36** 7081
[11] Scholtz F, Geyer H and Hahne F 1992 *Ann. Phys.* **213** 74
[12] Bessis D 1993 Private conversation with C M Bender, C E N Saclay
[13] Bender C M, Milton K A, Moshe M, Pinsky S S and Simmons L M Jr 1988 *Phys. Rev.* D **37** 1472
    Bender C M, Milton K A, Pinsky S S and Simmons L M Jr 1989 *J. Math. Phys.* **30** 1447
[14] Bender C M and Dunne G V 1989 *Phys. Rev.* D **40** 10
[15] Bender C M and Klevansky S P 2009 *Phys. Lett.* A **273** 2670
[16] Bender C M, Milton K A, Moshe M, Pinsky S S and Simmons L M Jr 1988 *Phys. Rev.* D **37** 1472
[17] Bender C M, Chen J-H and Milton K A 2006 *J. Phys. A: Math. Gen.* **39** 1657