An Equivalent Hermitian Hamiltonian for the non-Hermitian $-x^4$ Potential

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Abstract

The potential $V(x) = -x^4$, which is unbounded below on the real line, can give rise to a well-posed bound state problem when $x$ is taken on a contour in the lower-half complex plane. It is then $PT$-symmetric rather than Hermitian. Nonetheless it has been shown numerically to have a real spectrum, and a proof of reality, involving the correspondence between ordinary differential equations and integrable systems, was subsequently constructed for the general class of potentials $-(ix)^N$. For such Hamiltonians the natural $PT$ metric is not positive definite, but a dynamically-defined positive-definite metric can be defined, depending on an operator $Q$. Further, with the help of this operator an equivalent Hermitian Hamiltonian $h$ can be constructed. This programme has been carried out exactly for a few soluble models, and the first few terms of a perturbative expansion have been found for the potential $m^2x^2 + igx^3$. However, until now, the $-x^4$ potential has proved intractable. In the present paper we give explicit, closed-form expressions for $Q$ and $h$, which are made possible by a particular parametrization of the contour in the complex plane on which the problem is defined. This constitutes an explicit proof of the reality of the spectrum. The resulting equivalent Hamiltonian has a potential with a positive quartic term together with a linear term.

1 Introduction

There has been a great deal of interest in non-Hermitian Hamiltonians since the numerical observation by Bender and Boettcher [1] that Hamiltonians of
the form

\[ H = p^2 - g(ix)^N \]  

have a real positive spectrum for \( N \geq 2 \). As illustrated in Fig. 1 (from Ref. [1], where \( g = 1 \)), their spectra constitute a smooth extrapolation from the simple harmonic oscillator, for which \( N = 2 \). The reality of their spectra is understood as being due to their unbroken \( PT \) symmetry, but there is no simple way of telling in advance whether or not this symmetry is broken, as indeed it is for \( N < 2 \), where the spectra are partly complex. Eventually a rather intricate proof of the reality of the spectrum, involving the correspondence between the differential equations for such potentials and integrable models, was constructed by Dorey et al. [2].

A potential problem with such Hamiltonians is their physical interpretation, since the natural \( PT \) norm on the Hilbert space, \( \int dx \psi^*(x)\psi(-x) \), is not positive definite, in contrast to the usual norm \( \int dx \psi^*(x)\psi(x) \). However, it turns out to be possible to construct an alternative norm, the \( CPT \) norm [3], which is indeed positive definite. This norm is different from the usual norm, in that it is dynamically determined by the Hamiltonian itself, and needs to be calculated in each individual case.

![Figure 1: Energy levels of Eq. (1) for \( N = 4 \) with \( g = 1 \), from Ref. [1]](image-url)
Such calculations were encompassed by Mostafazadeh [4] in the more general framework of pseudo-Hermiticity, whereby

\[ H^\dagger = \eta H \eta^{-1} \]  

Here the operator \( \eta \) is Hermitian and positive definite, and may usefully be written as \( \eta = e^{-Q} \), in order to connect with the notation of Ref. [5], where, for \( PT \)-symmetric Hamiltonians, \( \eta = PC \) and \( Q \) was defined by \( C = e^{Q}P \).

For calculational purposes it is much easier to deal with \( Q \) rather than \( \eta \) directly. Mostafazadeh showed further that

\[ h \equiv e^{-\frac{1}{2}Q}He^{\frac{1}{2}Q} \]  

is an equivalent Hermitian Hamiltonian, obtained from \( H \) by a similarity (Darboux) transformation.

In general it is difficult to solve Eqs. (2), (3) exactly; instead one uses perturbation theory in a small parameter \( \varepsilon \). If \( H \) is of the form \( H = H_0 + \varepsilon H_1 \), where \( H_0 \) is Hermitian and \( H_1 \) anti-Hermitian, then \( Q \) can be taken as \( Q = \sum r \text{odd} Q_r \varepsilon^r \), which then gives \( h = \sum r \text{even} h_r \varepsilon^r \). In this case the first few equations for the \( Q_r \), arising from the expansion of Eq. (2), read:

\[
\begin{align*}
[Q_1, H_0] & = 2H_1 \\
[Q_3, H_0] & = \frac{1}{6}[Q_1, [Q_1, H_1]] \\
[Q_5, H_0] & = \frac{1}{6}([Q_3, [Q_1, H_1]] + [Q_1, [Q_3, H_1]]) - \frac{1}{360}[Q_1, [Q_1, [Q_1, H_1]]]
\end{align*}
\]

and so on. Using these, the first few equations for the \( h_r \), arising from the expansion of Eq. (3), can be cast in the form

\[
\begin{align*}
h_0 & = H_0 \\
h_2 & = -\frac{1}{4}[Q_1, H_1] \\
h_4 & = \frac{1}{192}[Q_1, [Q_1, [Q_1, H_1]]] - \frac{1}{4}[Q_3, H_1].
\end{align*}
\]

The smooth continuation from the harmonic oscillator, and the ODE-IM correspondence of Ref. [2], rest on the fact that the Schrödinger differential equation has several different sectors, defined by wedges in the complex \( x \)-plane. Along the centre of the wedges the wave-function decays exponentially at infinity, while along the edges the wave-function is purely oscillatory. Figure 2, taken from Ref. [1], shows the particular wedge that connects smoothly with that for the harmonic oscillator.

The critical case, where the upper edge of the wedge coincides with the real axis is the case \( N = 4 \), i.e. the potential \(-x^4\). For \( N < 4 \), it is possible to stay on the real axis, where the wave function decays exponentially, albeit with an oscillatory modulation, but for \( N \geq 4 \) we have no option but to formulate the problem on a contour in the lower half \( x \) plane.

\[ ^1 \text{The equations of even order are satisfied identically by } Q_{2n} = 0. \]
Figure 2: Wedges in the complex plane in which the Schrödinger equation for Eq. (1) is posed.

This is the fundamental reason why the $-gx^4$ potential has proved so intractable. At first sight it appears Hermitian: it is only because of the contour on which it must be defined that it is non-Hermitian. The problem is inherently non-perturbative, so any expansion to be attempted can not be in the coupling constant $g$. A previous attempt [6] used WKB methods, and was able to calculate $Q$ to leading non-perturbative order.

2 Choice of Contour

Our present approach starts with the idea of Mostafazadeh [7], to map the problem back onto the real axis using a real parametrization of a suitable contour. A wide variety of contours are possible, as long as they go off to infinity at an angle within the wedges. Taking $N = 4$ and writing the original $x$ variable of Eq. (1) as $z$ to reflect its complex character, so that

$$H = -\frac{d^2}{dz^2} - g \, z^4,$$

the parametrization used in Ref. [7] was

$$z = x \cos \theta - i|x| \sin \theta,$$

corresponding to straight-line contours, with an infinitesimal rounding off near the origin. Here $\theta$ was taken as $\pi/6$, the optimal angle for $N = 4$. The resulting Hamiltonian was

$$H = e^{i\text{sgn}(x)\pi/3} \left( -\frac{d^2}{dx^2} + g|x|^4 \right).$$
Because of rounding, there are non-trivial boundary conditions at \( x = 0 \), namely (i) \( \psi \) is real and continuous, (ii) \( \psi'(0^-) = e^{4i\theta} \psi'(0^+) \). Consequently, in calculating \( H^\dagger \) there is an additional term \( \delta H \) beyond the obvious one.

A calculation of \( Q \) with this Hamiltonian is very difficult because of the boundary conditions at \( x = 0 \) and the lack of an obvious expansion parameter. In Ref. [8] we attempted to make an expansion in \( \theta \), freeing it from its optimal value for \( N = 4 \), noting that any positive value for \( \theta \) would suffice to make the wave function vanish with an exponential component. In addition we smoothed out the curve chosen in Ref. [7], taking the hyperbola

\[
z = x \cos \theta - i \sin \theta \sqrt{(1 + x^2)},
\]

in order to remove the boundary conditions at \( x = 0 \). Unfortunately this calculation did not produce a very useful \( h \), but rather one which still had a \(-x^4\) term, so that the asymptotic behaviour of the wave function was oscillatory, with only a power suppression.

In the present paper we adopt a different approach. First we choose a new parametrization, whose asymptotes are not in fact in the centre of the wedges, but rather are inclined at \( \pi/4 \) to the real axis, and then we introduce an artificial parameter \( \varepsilon \) multiplying \( H_1 \), the non-Hermitian part of \( H(x) \).

The contour that turns out to give particularly simple results is of the form

\[
z = -2i \sqrt{(1 + ix)}. \tag{10}
\]

Notice that with this choice, the \( PT \)-symmetry of the original Hamiltonian, which is a real function of \( iz \), will be respected by the new Hamiltonian, written in terms of \( x \). This new Hamiltonian is in fact

\[
H = \frac{1}{2} \{(1 + ix), p^2\} - \frac{1}{2} p - \alpha (1 + ix)^2,
\]

where \( \{.,.\} \) denotes the anticommutator, \( p \equiv d/dx \), and for convenience we have introduced \( \alpha \equiv 16g \). Separating \( H \) into its Hermitian and anti-Hermitian parts, and multiplying the latter by the artificial parameter \( \varepsilon \), which at the end will be set equal to one, we write

\[
H = H_0 + \varepsilon H_1, \tag{12}
\]

where

\[
H_0 = p^2 - \frac{1}{2}p + \alpha (x^2 - 1) \\
H_1 = \frac{1}{2} i \{x, p^2\} - 2i\alpha x
\]
3 Calculation of $Q$ and $h$

First we calculate $Q_1$ from the first of Eqs. (4), namely $[Q_1, H_0] = 2H_1$. As a general, systematic procedure for such problems we would write the Hermitian operator $Q_1$ as a sum of anticommutators of the form $Q_1 = \sum n \text{odd} \{f_n(x), p^n\}$, where $f_n(x)$ is a real function of $x$, and gradually increase the order $n$. However, in this case $H_0$ and $H_1$ are so simple that the solution can essentially be found by inspection. Thus a $p^3$ term in $Q_1$ will produce the desired structure $i \{x, p^2\}$ when commuted with the $x^2$ term of $H_0$, while a term in $p$ will produce the $x$ term of $H_1$. By equating coefficients we find that

$$Q_1 = -\frac{p^3}{3\alpha} + 2p.$$  \hspace{1cm} (14)

In order to calculate $Q_3$ from the second of Eqs. (4) we need the double commutator $[Q_1, [Q_1, H_1]]$. First let us calculate the inner commutator $[Q_1, H_1]$, which will also be needed for the computation of $h$:

$$[Q_1, H_1] = -\frac{p^4}{\alpha} + 4p^2 - 4\alpha.$$  \hspace{1cm} (15)

The crucial point is that this is a function of $p$ only, and therefore commutes with $Q_1$. Thus $[Q_1, [Q_1, H_1]] = 0$, which means that $Q_3 = 0$. Then the third of Eqs. (4) shows that $Q_5 = 0$ and so on. Thus we have an exact solution for $Q$, after setting $\varepsilon = 1$, namely

$$Q = -\frac{p^3}{3\alpha} + 2p.$$  \hspace{1cm} (16)

Having obtained the metric operator $Q$ we are in a position to calculate the equivalent Hermitian Hamiltonian $h$ of Eq. (3). Because the expansion for $Q$ has truncated, so does that for $h$, namely $h = H_0 + h_2$. The commutator required for the evaluation of $h_2$ has already been calculated in Eq. (15), so it is straightforward to evaluate $h$, with the remarkably simple result that

$$h = \frac{p^4}{4\alpha} - \frac{1}{2}p + \alpha x^2.$$  \hspace{1cm} (17)

We emphasize that this Hermitian Hamiltonian, defined on the real line, has the same energy spectrum as that of the original $H$ of Eq. (5) defined on a complex contour. The only unusual feature of $h$ is that it does not have the standard form of a quadratic kinetic term plus a potential. However, just such a Hamiltonian results if we take the Fourier transform. In terms of the
transformed variable $y$, and after a rescaling $y \rightarrow y\sqrt{\alpha}$, we have

$$\tilde{h} = p_y^2 + \frac{1}{4} \alpha y^4 - \frac{1}{2} \sqrt{\alpha} y$$

(18)

4 Discussion

Equations (16) and (18) constitute our main results. The latter exhibits a standard Hermitian Hamiltonian, with a positive quartic potential plus a linear term, shown in Fig. 3, whose spectrum is the same as that of the original problem, with a $-z^4$ potential posed on a contour in the complex plane. It constitutes the first direct, constructive proof of the reality of the spectrum of Eq. (6). In accordance with our introductory remarks, we note that $\tilde{h}$ is completely non-perturbative, since, without a harmonic term $m^2 x^2$ term in the potential, $g$ can rescaled to 1.

![Figure 3: The potential of Eq. (18), with $\alpha = 16$ ($g = 1$).](image)

We have performed a numerical calculation of the energy eigenvalues of Eq. (18), using both Runge-Kutta integration and the variational truncated
matrix method of Ref. [9]. Both methods give eigenvalues that are indistinguishable from those cited by Bender and Boettcher (calculated by Runge-Kutta integration along a complex contour) in their original paper [1].

A simple extension of the above result can be obtained when an additional harmonic term $m^2 z^2$ is introduced into Eq. (6). The only change in Eq. (17) is that $h$ becomes

$$h = \frac{(p^2 - 4m^2)^2}{4\alpha} - \frac{1}{2}p + \alpha x^2$$

with corresponding scaled Fourier transform

$$\tilde{h} = p_y^2 + \frac{1}{4\alpha}(\alpha y^2 - 4m^2)^2 - \frac{1}{2}\sqrt{\alpha} y$$

After completion of this work we were made aware of an earlier paper by Buslaev and Grecchi [10], which showed the spectral equivalence of the massive version of the $-x^4$ theory (their $H_\varepsilon(ig, j)$, with $j = 1$), formulated on the line $z = x - i\eta$, with a Hermitian Hamiltonian that can be identified with Eq. (20) on setting $\alpha = 4g^2$, $m = 1/2$. Their method made use of the perturbation series for the energy eigenvalues of the two Hamiltonians, which only exists for $m \neq 0$. However, they were subsequently able to go the massless limit by rescaling and taking $g$ to $\infty$. In this way they obtained the spectral equivalence between Eq. (6) and Eq. (17) (see their Theorem 6, with $j = 1$, $\alpha = 0$ after a simple rescaling).

The present paper approaches the problem from a completely different perspective and offers a simple, explicit and transparent derivation of these spectral equivalences, together with the operator $Q$ required to define the positive-definite metric, and the observables [4], of the non-Hermitian Hamiltonians.

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