Generating converging eigenenergy bounds for the discrete states of the -ix^3 non-Hermitian potential

2001 J. Phys. A: Math. Gen. 34 L271

(http://iopscience.iop.org/0305-4470/34/19/102)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) L271–L277 www.iop.org/Journals/ja PII: S0305-4470(01)22235-5

LETTER TO THE EDITOR

Generating converging eigenenergy bounds for the discrete states of the $-ix^3$ non-Hermitian potential

C R Handy

Department of Physics and Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia 30314, USA

Received 21 February 2001

Abstract

Recent investigations by Bender and Boettcher and by Mezincescu have argued that the discrete spectrum of the non-Hermitian potential $V(x) = -ix^3$ should be real. We give further evidence for this through a novel formulation which transforms the general one-dimensional Schrodinger equation (with complex potential) into a fourth-order linear differential equation for $|\Psi(x)|^2$. This permits the application of the eigenvalue moment method, developed by Handy, Bessis and coworkers, yielding rapidly converging lower and upper bounds to the low-lying discrete state energies. We adapt this formalism to the pure imaginary cubic potential, generating tight bounds for the first five discrete state energy levels.

PACS number: 0365

1. Introduction

In the recent work by Bender and Boettcher (1998) they conjectured that certain $\mathcal{PT}$ invariant systems should have real discrete spectra. Various examples were presented, including the $-ix^3$ potential. The interest in such systems has increased, as documented in the recent work of Mezincescu (2000). We present a radically new way of attacking such problems. Although the results presented here combine rigorous mathematical theorems and their numerical implementation, it should also be possible to develop them purely within an algebraic context, and confirm that the $-ix^3$ potential can only have real discrete spectra. This particular approach is under investigation, and the results will be presented elsewhere.

Our starting point is the observation that the one-dimensional Schrodinger equation (on the real line),

$$-\partial_x^2\Psi(x) + V(x)\Psi(x) = E\Psi(x) \tag{1}$$

for complex potentials, $V = V_R + \mathrm{i}V_I$, can be transformed into a fourth-order, linear differential equation for $S(x) = |\Psi(x)|^2$:

$$-\frac{1}{V_I}S^{(4)} - \left(\frac{1}{V_I}\right)' S^{(3)} + 4\left(\frac{V_R - E}{V_I}\right) S^{(2)} + \left(4\left(\frac{V_R}{V_I}\right)' + 2\left(\frac{V_R{}'}{V_I}\right) - 4E\left(\frac{1}{V_I}\right)'\right) S^{(1)}$$
$$+ \left(4V_I + 2\left(\frac{V_R{}'}{V_I}\right)'\right) S = 0 \qquad (2)$$

where $S^{(i)} \equiv \partial_x^i S$. This equation assumes that the eigenenergy, E, is real. We derive it in the next section.

We could also assume that E is complex and incorporate its imaginary part into V_I. Since our objective is to show, numerically, that the conjecture that E is real is a viable one, we restrict our considerations to this case only, here. The method presented in this work is so powerful (both theoretically and numerically) that if the discrete state is not purely real, then it will be detected, at some sufficiently high calculation order.

The above fourth-order differential equation can be generalized to include any complex contour in the complex plane. However, for the particular problem considered here, we have only focused on the simplest representation for $S(x)$, as given by equation (2).

If the potential is real, $V_I = 0$, then Handy *et al* (1987a, b, 1988c) have shown that $S(x)$ satisfies a third-order differential equation. This is easy to see from the above by simply taking $V_I \to 0$, and recognizing that equation (2) becomes the total derivative of the third-order equation

$$-\tfrac{1}{2}S^{(3)}(x) + 2V(x)S^{(1)}(x) + V'(x)S(x) = 2ES^{(1)}(x). \qquad (3)$$

The importance of converting the discrete state problem into the non-negative $S(x)$ representation is that for rational fraction complex potentials, one can then exploit the eigenvalue moment method (EMM) of Handy, Bessis and coworkers (1985, 1988a, b), enabling the generation of converging lower and upper bounds for the low-lying discrete eigenenergies.

For rational fraction potentials, equation (2) can be transformed into a moment equation (ME) involving the Hamburger moments

$$\mu_p \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p S(x) \qquad p \geqslant 0. \qquad (4)$$

The ME takes on the form

$$\mu_p = \sum_{\ell=0}^{m_s} M_{p,\ell}(E)\mu_\ell \qquad p \geqslant 0 \qquad (5)$$

where the energy-dependent coefficients are easily obtained, and satisfy (i.e. 'initialization conditions'): $M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_{1,2} \leqslant m_s$. The *missing moments*, $\{\mu_\ell | 0 \leqslant \ell \leqslant m_s\}$, are to be considered as independent variables. The missing moment order, m_s, is problem dependent.

The homogeneous nature of the Schrodinger equation requires the imposition of an appropriate normalization condition. Although this requires some care, usually, a convenient choice is to take

$$\sum_{\ell=0}^{m_s} \mu_\ell = 1. \qquad (6)$$

Solving for μ_0, and substituting into the ME relation, gives

$$\mu_p = \sum_{\ell=0}^{m_s} \hat{M}_{p,\ell}(E)\hat{\mu}_\ell \qquad (7)$$

where

$$\hat{\mu}_\ell = \begin{cases} 1 & \ell = 0 \\ \mu_\ell & 1 \leqslant \ell \leqslant m_s \end{cases} \tag{8}$$

and

$$\hat{M}_{p,\ell}(E) = \begin{cases} M_{p,0}(E) & \ell = 0 \\ M_{p,\ell}(E) - M_{p,0}(E) & 1 \leqslant \ell \leqslant m_s. \end{cases} \tag{9}$$

From the Hankel–Hadamard (HH) positivity theorems (Shohat and Tamarkin 1963) the Hamburger moments must satisfy the conditions $\int_{-\infty}^{+\infty} \mathrm{d}x \left(\sum_{j=0}^{J} C_j x^j \right)^2 S(x) > 0$, for all C and $J \geqslant 0$. These become the quadratic form expressions

$$\sum_{j_{1,2}=0}^{J} C_{j_1} \mu_{j_1+j_2} C_{j_2} > 0. \tag{10}$$

In terms of the (unconstrained) normalized μ this becomes

$$\sum_{\ell=0}^{m_s} \hat{\mu}_\ell \left(\sum_{j_{1,2}=0}^{J} C_{j_1} \hat{M}_{j_1+j_2,\ell}(E) C_{j_2} \right) > 0 \tag{11}$$

which defines the linear programming equations (Chvatal 1983):

$$\sum_{\ell=1}^{m_s} \mathcal{A}_\ell(C, E) \mu_\ell < \mathcal{B}(C, E) \tag{12}$$

for all possible C (except those identically zero), where

$$\mathcal{A}_\ell(C, E) = -\left(\sum_{j_{1,2}=0}^{J} C_{j_1} \hat{M}_{j_1+j_2,\ell}(E) C_{j_2} \right) \tag{13}$$

and

$$\mathcal{B}(C, E) = \left(\sum_{j_{1,2}=0}^{J} C_{j_1} \hat{M}_{j_1+j_2,0}(E) C_{j_2} \right). \tag{14}$$

If at a given order, J, and arbitrary energy value, E, there exists a solution set to all of the above inequalities, $\mathcal{U}_E^{(J)}$, then it must be convex. Through a linear programming based *cutting* procedure (Handy *et al* 1988a, b) one can find optimal C which (in a finite number of steps) establish the existence or nonexistence of $\mathcal{U}_E^{(J)}$. The energy values for which missing moment solution sets exist, define energy intervals,

$$E \in \bigcup_{n=0}^{N(J)} \left[E_{L;n}^{(J)}, E_{U;n}^{(J)} \right] \qquad \text{if} \quad \mathcal{U}_E^{(J)} \neq \emptyset \tag{15}$$

which become smaller as J increases, converging to the corresponding discrete state energy (which must always lie within the respective interval):

$$E_{L;n}^{(J)} \leqslant E_{L;n}^{(J+1)} \leqslant \cdots \leqslant E_{\text{physical};n} \leqslant \cdots \leqslant E_{U;n}^{(J+1)} \leqslant E_{U;n}^{(J)}. \tag{16}$$

Through the EMM approach, we can easily generate the converging lower and upper bounds to the desired discrete state energy.

We note that although the traditional moment problem theorems are concerned with uniqueness questions (i.e. is there a unique function with the moments μ_p satisfying the HH positivity conditions?) within the context of physical systems such issues are usually inconsequential. This is because the very nature of the ME relation will guarantee uniqueness. That is, our moments are associated with an underlying differential equation with unique physical solutions.

2. Deriving the positivity equation for $S(x)$

We derive equation (2) as follows. First, multiply the Schrodinger equation by Ψ^*:

$$-\Psi^*(x)\Psi''(x) + V(x)S(x) = ES(x). \tag{17}$$

The complex conjugate becomes

$$-\Psi(x)\Psi^{*\prime\prime}(x) + V^*(x)S(x) = ES(x). \tag{18}$$

Adding both expressions, and using $\Psi^*\Psi'' = (\Psi^*\Psi')' - |\Psi'|^2$, yields

$$-[S'' - 2|\Psi'|^2] + 2V_R S = 2ES. \tag{19}$$

This in turn becomes (upon differentiating)

$$-S''' + 2\big(|\Psi'|^2\big)' + 2\big(V_R S\big)' = 2ES'. \tag{20}$$

If we subtract equation (18) from (17), then

$$\partial_x\big(\Psi^*\Psi' - \Psi\Psi^{*\prime}\big) = 2\mathrm{i}V_I S. \tag{21}$$

Returning to the Schrodinger equation, we multiply both sides by $\Psi^{*\prime}$:

$$-\Psi^{*\prime}\Psi'' + V\Psi\Psi^{*\prime} = E\Psi\Psi^{*\prime}. \tag{22}$$

The complex conjugate is

$$-\Psi'\Psi^{*\prime\prime} + V^*\Psi^*\Psi' = E\Psi^*\Psi'. \tag{23}$$

Substituting $V = V_R + \mathrm{i}V_I$, we add both expressions (and divide by $\mathrm{i}V_I$):

$$-\frac{\big(|\Psi'|^2\big)'}{\mathrm{i}V_I} + \frac{V_R S'}{\mathrm{i}V_I} + [\Psi\Psi^{*\prime} - \Psi^*\Psi'] = E\frac{S'}{\mathrm{i}V_I}. \tag{24}$$

Differentiating with respect to x, and substituting equation (21) yields

$$-\left(\frac{\big(|\Psi'|^2\big)'}{\mathrm{i}V_I}\right)' + \left(\frac{V_R S'}{\mathrm{i}V_I}\right)' - 2\mathrm{i}V_I S = E\left(\frac{S'}{\mathrm{i}V_I}\right)'. \tag{25}$$

Upon dividing equation (19) by $\mathrm{i}V_I$, and differentiating, we obtain

$$-\left(\frac{S'''}{\mathrm{i}V_I}\right)' + 2\left(\frac{\big(|\Psi'|^2\big)'}{\mathrm{i}V_I}\right)' + 2\left(\frac{\big(V_R S\big)'}{\mathrm{i}V_I}\right)' = 2E\left(\frac{S'}{\mathrm{i}V_I}\right)'. \tag{26}$$

Finally, we substitute equation (25) for the second term in equation (26), obtaining a fourth-order linear differential equation for S:

$$-\left(\frac{S'''}{\mathrm{i}V_I}\right)' + 2\left(\left(\frac{V_R S'}{\mathrm{i}V_I}\right)' - 2\mathrm{i}V_I S - E\left(\frac{S'}{\mathrm{i}V_I}\right)'\right) + 2\left(\frac{\big(V_R S\big)'}{\mathrm{i}V_I}\right)' = 2E\left(\frac{S'}{\mathrm{i}V_I}\right)' \tag{27}$$

or

$$-\left(\frac{S'''}{V_I}\right)' + 4\left(\left(\frac{V_R S'}{V_I}\right)' + V_I S\right) + 2\left(\frac{V_R' S}{V_I}\right)' = 4E\left(\frac{S'}{V_I}\right)' \tag{28}$$

which becomes equation (2).

The positivity differential representation in equation (2) is a fourth-order linear differential equation, with four independent solutions, for any E. Within the EMM formalism, it is important to prove that the physical solution is the only one which is both non-negative ($S(x) \geqslant 0$) and bounded, with finite moments (i.e. $S(x)$ is in L^2). We can prove this for equation (2).

For any real energy variable value, $E \in \mathbb{R}$, let $\Psi_1(x)$ and $\Psi_2(x)$ denote the two independent solutions to the Schrodinger equation. The expression $S(x) = |\alpha\Psi_1(x) + \beta\Psi_2(x)|^2 = |\alpha|^2 \times |\Psi_1(x)|^2 + |\beta|^2 \times |\Psi_2(x)|^2 + \alpha\beta^*\Psi_1(x)\Psi_2^*(x) + \alpha^*\beta\Psi_1^*(x)\Psi_2(x)$, then becomes a solution to equation (2). So too are $|\Psi_1(x)|^2$ and $|\Psi_2(x)|^2$. Accordingly, since α and β are arbitrary, and $\Psi_1(x)$ and $\Psi_2(x)$ are complex, the configurations $\Psi_1(x)\Psi_2^*(x)$ and $\Psi_1^*(x)\Psi_2(x)$ are independent (complex) solutions to equation (2) as well.

From low-order JWKB asymptotic analysis (Bender and Orszag 1978) in either asymptotic direction ($x \to \pm\infty$), one of the semiclassical modes will be exponentially increasing, while the other is exponentially decreasing. Therefore it becomes clear that the only possible non-negative and bounded $S(x)$ configuration is that corresponding to the physical solutions.

3. The $-\mathrm{i}x^3$ potential

The positivity differential equation for the $V(x) = -\mathrm{i}x^3$ potential is (i.e. $V_R = 0$, $V_I = -x^3$)

$$x^{-3}S^{(4)}(x) - 3x^{-4}S^{(3)}(x) + 4Ex^{-3}S^{(2)}(x) - 12Ex^{-4}S^{(1)}(x) - 4x^3S(x) = 0. \tag{29}$$

Multiplying both sides by x^{p+4}, and integrating over $\mathbb{R}$, produces the ME relation

$$4\mu_{p+7} = (p+4)p(p-1)(p-2)\mu_{p-3} + 4Ep(p+4)\mu_{p-1} \tag{30}$$

for $p \geqslant 0$.

The ME separates into two relations, one for the odd moments, the other for the even moments. Assuming that the discrete states are nondegenerate and have real eigenenergies, we have

$$\Psi^*(-x) = \Psi(x) \tag{31}$$

and

$$S(-x) = \Psi^*(-x)\Psi(-x) = \Psi(x)\Psi^*(x) = S(x). \tag{32}$$

Thus, the physical $S(x)$ are symmetric, and the odd-order moments are zero.

The even-order Hamburger moments

$$\mu_{2\rho} \equiv u_\rho \tag{33}$$

correspond to the Stieltjes moments,

$$u_\rho \equiv \int_0^\infty \mathrm{d}y\, y^\rho \Upsilon(y) \tag{34}$$

of the function

$$\Upsilon(y) \equiv \frac{S(\sqrt{y})}{\sqrt{y}}. \tag{35}$$

The corresponding Stieltjes ME for the $-\mathrm{i}x^3$ potential becomes (i.e. substitute $p = 2\rho + 1$ in equation (30))

$$4u_{\rho+4} = (2\rho+5)(2\rho+1)(2\rho)(2\rho-1)u_{\rho-1} + 4E(2\rho+1)(2\rho+5)u_\rho \tag{36}$$

for $\rho \geqslant 0$. This is an $m_s = 3$ order problem. One can convert this into the form in equation (5) (i.e. $u_\rho = \sum_{\rho=0}^{m_s} M_{\rho,\ell}(E)u_\ell$), where the M coefficients satisfy equation (36), with respect to the first index (ρ), as well as the initial conditions previously identified.

One convenient feature about the Stieltjes representation is that the normalization condition

$$\sum_{\ell=0}^{3} u_\ell = 1 \tag{37}$$

involves non-negative moments.

Table 1. Bounds for the ground state energy of the $-ix^3$ potential.

P_{max}	$E_{L;0}$	$E_{U;0}$
10	0.825	1.405
20	1.156 19	1.156 45
30	1.156 266 9	1.156 267 2
40	1.156 267 071 8	1.156 267 072 1
50	1.156 267 071 988 016	1.156 267 071 988 161
60	1.156 267 071 988 113 24	1.156 267 071 988 113 35

Table 2. Bounds for the first excited state energy of the $-ix^3$ potential.

P_{max}	$E_{L;1}$	$E_{U;1}$
20	4.105 6	4.116 8
30	4.109 225	4.109 236
40	4.109 228 750 9	4.109 228 757 8
50	4.109 228 752 806	4.109 228 752 812

Table 3. Bounds for the second excited state energy of the $-ix^3$ potential.

P_{max}	$E_{L;2}$	$E_{U;2}$
20	7.420	7.594
30	7.562 13	7.562 42
40	7.562 273 794	7.562 273 999
50	7.562 273 8549	7.562 273 8551

From the Stieltjes moment problem (Shohat and Tamarkin 1963) we know that the counterpart to equation (10) is

$$\sum_{j_{1,2}=0}^{J} C_{j_1} u_{\sigma+j_1+j_2} C_{j_2} > 0 \tag{38}$$

for $\sigma = 0, 1$. Accordingly, the necessary linear programming equations to consider are

$$\sum_{\ell=1}^{m_s} \mathcal{A}_\ell(C, E; \sigma) < \mathcal{B}(C, E; \sigma) \tag{39}$$

where

$$\mathcal{A}_\ell(C, E; \sigma) = -\left(\sum_{j_{1,2}=0}^{J} C_{j_1} \hat{M}_{\sigma+j_1+j_2,\ell}(E) C_{j_2}\right) \tag{40}$$

and

$$\mathcal{B}(C, E; \sigma) = \left(\sum_{j_{1,2}=0}^{J} C_{j_1} \hat{M}_{\sigma+j_1+j_2,0}(E) C_{j_2}\right). \tag{41}$$

The numerical implementation of the EMM procedure yields the excellent results quoted in tables 1–5. Our results are in agreement with those of Bender and Boettcher (1998), as well as those of Handy *et al* (2001). We indicate the maximum moment order generated, P_{max}, through the ME relation.

Since our results are based on equations that explicitly assume E is real, and the EMM procedure is very stable and highly accurate (as evidenced through the tightness of its bounds),

Table 4. Bounds for the third excited state energy of the $-ix^3$ potential.

P_{max}	$E_{L;3}$	$E_{U;3}$
30	11.311 5	11.315 9
40	11.314 418	11.314 425
50	11.314 421 818	11.314 421 824

Table 5. Bounds for the fourth excited state energy of the $-ix^3$ potential.

P_{max}	$E_{L;4}$	$E_{U;4}$
30	15.20	15.80
40	15.291 45	15.291 60
50	15.291 553 66	15.291 553 80
60	15.291 553 750 37	15.291 553 750 41

any imaginary part to the discrete state energy would reveal itself through some anomalous behaviour in the generated bounds. That is, at some order P_{max}, no feasible energy interval would survive (i.e. $\mathcal{U}_E^{(J)} = \oslash$, for all E). This is never observed, to the order indicated. As such, our analysis strongly supports the reality of the (low-lying) discrete state spectrum for the $-ix^3$ potential.

The application of EMM to the complex-E generalization of equation (2) has been successfully implemented with respect to the $ix^3 + iax$ potential of Delabaere and Trinh (2000), generating converging bounds to the complex energy ($\mathcal{PT}$ symmetry breaking) discrete states (Handy 2001, Handy *et al* 2001).

This work was supported in part by a grant from the National Science Foundation (HRD 9632844) through the Center for Theoretical Studies of Physical Systems (CTSPS). The author is appreciative of stimulating discussions with Dr Alfred Z Msezane, Dr G Andrei Mezincescu, and Dr Daniel Bessis which stimulated this work.

References

Bender C and Boettcher S 1998 *Phys. Rev. Lett.* **80** 5243
Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)
Chvatal V 1983 *Linear Programming* (New York: Freeman)
Delabaere E and Trinh D T 2000 *J. Phys. A: Math. Gen.* **33** 8771
Handy C R 1987a *Phys. Rev.* A **36** 4411
——1987b *Phys. Lett.* A **124** 308
Handy C R 2001 Clark Atlanta University *Preprint* LANL math-ph/0104036 (*J. Phys. A: Math. Gen.* submitted)
Handy C R and Bessis D 1985 *Phys. Rev. Lett.* **55** 931
Handy C R, Bessis D and Morley T D 1988a *Phys. Rev.* A **37** 4557
Handy C R, Bessis D, Sigismondi G and Morley T D 1988b *Phys. Rev. Lett.* **60** 253
Handy C R, Khan D and Wang Xian-Qiao 2001 Clark Atlanta University *Preprint* LANL math-ph/0104037 (*J. Phys. A: Math. Gen.* submitted)
Handy C R, Luo L, Mantica G and Msezane A 1988c *Phys. Rev.* A **38** 490
Mezincescu G A 2000 *J. Phys. A: Math. Gen.* **33** 4911
Shohat J A and Tamarkin J D 1963 *The Problem of Moments* (Providence, RI: American Mathematical Society)