Generating Converging Eigenenergy Bounds for the Discrete States of the $-ix^3$ Non-Hermitian Potential

C. R. Handy

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

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Abstract

Recent investigations by Bender and Boettcher (Phys. Rev. Lett 80, 5243 (1998)) and Mezincescu (J. Phys. A. 33, 4911 (2000)) 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 Schrödinger 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 (Phys. Rev. Lett. 55, 931 (1985); 60, 253 (1988a,b)), 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.
I. 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, particularly through the more recent work of Bender et al (1999), Bender et al (2000), Bender and Wang (2001), Caliceti (2000), Delabaere and Pham (1999), Delabaere and Trinh (2000), Levai and Znojil (2000), Mezincescu (2000, 2001), Shin (2000), and Znojil (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. However, we have been able to implement the procedure discussed below, numerically, for the case of complex energies, $E$, and find no evidence for such discrete states (for moderate energy values). The details of this will be communicated in a forthcoming work focusing on the $ix^3 + i\alpha x$ potential studied by Delabaere and Trinh (2000). Our principal objective in this communication is to emphasize the importance of positivity as a quantization condition, within the appropriate (moment based) representation.

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

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

for complex potentials, $V = V_R + iV_I$, and real energies, $ImE = 0$, can be transformed into a fourth order, linear differential equation for $S(x) = |\Psi(x)|^2$ :

$$- \frac{1}{V_I}S^{(4)} - \left(\frac{1}{V_I}\right)'S^{(3)} + 4\left(\frac{V_R - E}{V_I}\right)S^{(2)} + \left(4\frac{V_R'}{V_I} + 2\left(\frac{V_R}{V_I}\right)' - 4E\left(\frac{1}{V_I}\right)'\right)S^{(1)} + \left(4V_I + 2\left(\frac{V_R'}{V_I}\right)\right)S = 0,$$  \hspace{1cm} (2)
where \( S^{(i)} = \partial x^i S \). 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 Eq.(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 Eq.(2) becomes the total derivative of the third order equation

\[
-\frac{1}{2} S^{(3)}(x) + 2 V(x) S^{(1)}(x) + V'(x) S(x) = 2 E S^{(1)}(x).
\]

The importance of converting the discrete state problem into the nonnegative \( S(x) \) 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 states.

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

\[
\mu_p \equiv \int_{-\infty}^{+\infty} dx \, x^p S(x),
\]

\( p \geq 0 \). The Moment Equation (ME) takes on the form

\[
\mu_p = \sum_{\ell=0}^{m_s} M_{p,\ell}(E) \mu_\ell,
\]

\( p \geq 0 \), 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 \( 0 \leq \ell_{1,2} \leq m_s \). The missing moments,
\{\mu_\ell|0 \leq \ell \leq 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

\[
\sum_{\ell=0}^{m_s} \mu_p = 1. \tag{6}
\]

Solving for \(\mu_0\), and substituting into the ME relation, gives

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

where

\[
\hat{\mu}_\ell = \begin{cases} 
1, & \ell = 0 \\
\mu_\ell, & 1 \leq \ell \leq m_s
\end{cases} \tag{8}
\]

and

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

From the Hankel-Hadamard (HH) positivity theorems (Shohat and Tamarkin (1963)), the Hamburger moments must satisfy the conditions

\[
\int_{-\infty}^{+\infty} dx \left( \sum_{j=0}^{J} C_j x^j \right)^2 S(x) > 0, \text{ for all } C's \text{ and } J \geq 0. \tag{10}
\]

These become the quadratic form expressions

\[
\sum_{j_1,j_2=0}^{J} C_{j_1} \mu_{j_1+j_2} C_{j_2} > 0. \tag{11}
\]

In terms of the (unconstrained) normalized \(\mu\)'s this becomes

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

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 \(C\)'s (except those identically zero), where
\[ A_\ell(C, E) = -\left( \sum_{j_1, j_2=0}^J C_{j_1} \hat{M}_{j_1+j_2, \ell}(E) C_{j_2} \right), \]  

(13)

and

\[ B(C, E) = \left( \sum_{j_1, j_2=0}^J C_{j_1} \hat{M}_{j_1+j_2, 0}(E) C_{j_2} \right). \]  

(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 \( C \)'s 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,

\[ E \in \bigcup_{n=0}^{N(J)} [E_{L;n}^{(J)}, E_{U;n}^{(J)}], \text{ if } \mathcal{U}_E^{(J)} \neq \emptyset, \]

(15)

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

\[ E_{L;n}^{(J)} \leq E_{L;n}^{(J+1)} \leq \ldots \leq E_{\text{physical}};n \leq \ldots \leq E_{U;n}^{(J+1)} \leq E_{U;n}^{(J)}. \]  

(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 \( \mu_p \) 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.
II. DERIVING THE POSITIVITY EQUATION FOR $S(X)$

We derive Eq.(2) as follows. First, multiply the Schrodinger equation ($E$ real) by $\Psi^*$:

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

The complex conjugate becomes

$$-\Psi(x)\Psi''(x) + V^*(x)S(x) = ES(x). \quad (18)$$

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

$$-\left[S'' - 2|\Psi'|^2\right] + 2V_RS = 2ES. \quad (19)$$

This in turn becomes (upon differentiating)

$$-S''' + 2\left(|\Psi'|^2\right)' + 2\left(V_RS\right)' = 2ES'. \quad (20)$$

If we subtract Eq.(18) from Eq.(17), then

$$\partial_x \left(\Psi^*\Psi' - \Psi\Psi''\right) = 2iV_IS. \quad (21)$$

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

$$-\Psi''\Psi' + V\Psi\Psi' = ES. \quad (22)$$

The complex conjugate is

$$-\Psi'\Psi'' + V^*\Psi\Psi' = E\Psi^*\Psi'. \quad (23)$$

Substituting $V = V_R + iV_I$, we add both expressions (and divide by $iV_I$):

$$-\left(|\Psi'|^2\right)' + \frac{V_RS'}{iV_I} + \left[\Psi\Psi' - \Psi^*\Psi'\right] = ES'. \quad (24)$$

Differentiating with respect to $x$, and substituting Eq.(21) yields

$$-\left(|\Psi'|^2\right)' + \left(V_RS\right)' - 2iV_IS = E\left(S'/iV_I\right)' \quad (25)$$
Upon dividing Eq.(19) by $iV_I$, and differentiating, we obtain

$$-\left(\frac{S'''}{iV_I}\right)' + 2\left(\left(\frac{|\Psi|^2\right)'\right) + 2\left(\frac{(V_R S)'}{iV_I}\right)' = 2E\left(\frac{S'}{iV_I}\right)'.$$  \hspace{1cm} (26)

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

$$-\left(\frac{S'''}{V_I}\right)' + 2 \times \left(\left(\frac{V_RS'}{V_I}-2iV_I S - E\left(\frac{S'}{V_I}\right)\right)' + 2\left(\frac{(V_R S)'}{V_I}\right)' = 2E\left(\frac{S'}{V_I}\right)'$$, \hspace{1cm} (27)

or

$$-\left(\frac{S'''}{V_I}\right)' + 4 \times \left(\left(\frac{V_RS'}{V_I}\right)' + V_I S\right) + 2\left(\frac{(V_R S)'}{V_I}\right)' = 4E\left(\frac{S'}{V_I}\right)'$$, \hspace{1cm} (28)

which becomes Eq.(2).

The positivity differential representation in Eq.(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 nonnegative ($S(x) \geq 0$) and bounded, with finite moments (i.e. $S(x)$ is in $L^2$). We can prove this for Eq.(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 Eq.(2). So too are $|\Psi_1(x)|^2$ and $|\Psi_2(x)|^2$. Accordingly, since $\alpha$ and $\beta$ 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 Eq.(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 nonnegative and bounded $S(x)$ configuration is that corresponding to the physical solutions.
III. THE $-IX^3$ POTENTIAL

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

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

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

$$4\mu_{p+7} = (p + 4)p(p - 1)(p - 2)\mu_{p-3} + 4E_p(p + 4)\mu_{p-1},$$ \hspace{1cm} (30)

for $p \geq 0$.

The moment equation 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:

$$\Psi^*(-x) = \Psi(x),$$ \hspace{1cm} (31)

and

$$S(-x) = \Psi^*(-x)\Psi(-x) = \Psi(x)\Psi^*(x) = S(x).$$ \hspace{1cm} (32)

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

The even order Hamburger moments

$$\mu_{2p} \equiv u_p,$$ \hspace{1cm} (33)

correspond to the Stieltjes moments,

$$u_p \equiv \int_0^\infty dy \, y^p \Upsilon(y),$$ \hspace{1cm} (34)

of the function

$$\Upsilon(y) \equiv \frac{S(\sqrt{y})}{\sqrt{y}}.$$ \hspace{1cm} (35)
The corresponding Stieltjes moment equation for the $-ix^3$ potential becomes (i.e. substitute $p = 2\rho + 1$ in Eq.(30))

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

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

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

$$\sum_{\ell=0}^{3} u_\ell = 1, \quad (37)$$

involves nonnegative moments.

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

$$\sum_{j_1, j_2 = 0}^{J} C_{j_1} u_{\sigma+j_1+j_2} C_{j_2} > 0, \quad (38)$$

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

$$\sum_{\ell=1}^{m_s} A_\ell(C, E; \sigma) < B(C, E; \sigma), \quad (39)$$

where

$$A_\ell(C, E; \sigma) = -\left( \sum_{j_1, j_2 = 0}^{J} C_{j_1} M_{\sigma+j_1+j_2, \ell}(E)C_{j_2} \right), \quad (40)$$

and

$$B(C, E; \sigma) = \left( \sum_{j_1, j_2 = 0}^{J} C_{j_1} M_{\sigma+j_1+j_2, 0}(E)C_{j_2} \right). \quad (41)$$

The numerical implementation of the EMM procedure yields the excellent results quoted in Tables I - V. Our results are in agreement with those of Bender and Boettcher (1998), as well as those of Handy, Khan, and Wang (2000). We indicate the maximum moment order generated, $P_{\text{max}}$, 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), any imaginary part to the discrete state energy would reveal itself through some anomalous behavior in the generated bounds. That is, at some order $P_{max}$, no feasible energy interval would survive (i.e. $\mathcal{U}_E^{(j)} = \emptyset$, 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.
TABLES

TABLE I. Bounds for the Ground State Energy of the $-ix^3$ Potential

| $P_{\text{max}}$ | $E_{L;0}$   | $E_{U;0}$   |
|------------------|-------------|-------------|
| 10               | .825        | 1.405       |
| 20               | 1.15619     | 1.15645     |
| 30               | 1.1562669   | 1.1562672   |
| 40               | 1.1562670718| 1.1562670721|
| 50               | 1.156267071988016| 1.156267071988161|
| 60               | 1.15626707198811324| 1.15626707198811335|

TABLE II. Bounds for the First Excited State Energy of the $-ix^3$ Potential

| $P_{\text{max}}$ | $E_{L;1}$   | $E_{U;1}$   |
|------------------|-------------|-------------|
| 20               | 4.1056      | 4.1168      |
| 30               | 4.109225    | 4.109236    |
| 40               | 4.1092287509| 4.1092287578|
| 50               | 4.109228752806| 4.109228752812|
### TABLE III. Bounds for the Second Excited State Energy of the $-ix^3$ Potential

| $P_{\text{max}}$ | $E_{L;2}$     | $E_{U;2}$     |
|------------------|---------------|---------------|
| 20               | 7.420         | 7.594         |
| 30               | 7.56213       | 7.56242       |
| 40               | 7.56223794    | 7.562273999   |
| 50               | 7.5622738549  | 7.5622738551  |

### TABLE IV. Bounds for the Third Excited State Energy of the $-ix^3$ Potential

| $P_{\text{max}}$ | $E_{L;3}$     | $E_{U;3}$     |
|------------------|---------------|---------------|
| 30               | 11.3115       | 11.3159       |
| 40               | 11.314418     | 11.314425     |
| 50               | 11.314421818  | 11.314421824  |

### TABLE V. Bounds for the Fourth Excited State Energy of the $-ix^3$ Potential

| $P_{\text{max}}$ | $E_{L;4}$     | $E_{U;4}$     |
|------------------|---------------|---------------|
| 30               | 15.20         | 15.80         |
| 40               | 15.29145      | 15.29160      |
| 50               | 15.29155366   | 15.29155380   |
| 60               | 15.29155375037| 15.29155375041|
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