Extension of a spectral bounding method to complex rotated Hamiltonians, with application to $p^2 - ix^3$

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Abstract
We show that a recently developed method for generating bounds for the
discrete energy states of the non-Hermitian $-ix^3$ potential (Handy C R 2001
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the Hamiltonian. This has important implications for extension of the method
in the analysis of resonant states, Regge poles, and general bound states in the
complex plane (Bender and Boettcher 1998 *Phys. Rev. Lett.* **80** 5243).

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1. Introduction

In a recent work, Handy (2001a) presented a novel quantization formalism for generating
converging bounds to the (complex) discrete spectra of non-Hermitian, one-dimensional,
potentials. The first part of this analysis makes use of the fact that the modulus squared
of the wavefunction, $S(x) \equiv |\Psi(x)|^2$, for $x \in \Re$, and any (complex) potential function, $V(x)$,
satisfies a fourth-order, linear differential equation:

$$-\frac{1}{V_I - E_I} S^{(4)} - \left(\frac{1}{V_I - E_I}\right)' S^{(3)} + 4\left(\frac{V_R - E_R}{V_I - E_I}\right) S^{(2)} + \left(4\left(\frac{V_R}{V_I - E_I}\right)' + 2\left(\frac{V_R'}{V_I - E_I}\right)\right)$$

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

where $S^{(n)}(x) \equiv \partial_x^n S(x)$, and $E = E_R + iE_I$, etc.

The bounded (L^2) and nonnegative solutions of this differential equation uniquely
correspond to the physical states. For the case of rational fraction potentials, there is an
associated (recursive) moment equation, whose solutions are parameterized by the energy,
E. Constraining these through the appropriate moment problem conditions for nonnegative
functions (Shohat and Tamarkin 196), generates rapidly converging bounds on the discrete
state energies. This entire procedure is referred to as the eigenvalue moment method (EMM)
and was originally developed by Handy and Bessis (1985) and Handy *et al* (1988a, 1988b). An

important theoretical and algorithmic component is the use of linear programming (Chvatal 1983).

The EMM procedure is not solely a numerical implementation of some very important mathematical theorems. It is possible to implement it algebraically, deriving bounding formulas for the eigenenergies (Handy and Bessis 1985). Furthermore, it does not depend on the Hermitian or non-Hermitian structure of the Hamiltonian. What is important is that the desired solutions be the unique nonnegative and bounded solutions of the differential system being investigated. In this sense, it provides an important example of how positivity can be used as a quantization procedure.

Many important problems can be analyzed through the application of EMM on equation (1), and its generalization as outlined in section 2. This includes generating bounds to Regge poles (which first motivated Handy's formalism), as presented in a companion work (Handy and Msezane 2001). Other problems include the calculation of resonant states as well as bound states in the complex plane as discussed by Bender and Boettcher (1998), and elaborated upon by others cited in the more recent work of Mezincescu (2001).

However, the realization of these depends on understanding the complex rotation extension of Handy's original formulation. Indeed, such concerns introduce a new class of EMM problems not encountered before, and thereby motivate the present work.

Our basic objective is to extend the $S(x)$-EMM formulation to complex rotated transformations of the Hamiltonian $p^2 - \mathrm{i}x^3$. We are particularly interested in the effectiveness of such an analysis. Indeed, once the correct moment equation is developed, one finds that the EMM approach works very well in this case, and yields the anticipated result, as detailed in section 3.

In the following sections we present a more general derivation of the $S(x)$ equation, and apply the resulting formalism to the rotated $-\mathrm{i}x^3$ Hamiltonian.

2. Generalized S-equation

Consider the (normalized) Schrödinger equation

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

for complex energy, E, and complex potential, $\mathcal{V}(x)$. Assume that the (complex) bound state, $\Psi(x)$, lies within the complex-x plane, along some infinite contour, $\mathcal{C}$. Let $x(\xi)$ define a differentiable map from a subset of the real axis to the entire complex contour:

$$x(\xi) : \xi \in \Re \to \mathcal{C}. \tag{3}$$

The transformed Schrödinger equation is

$$-\left(D(\xi)\partial_\xi\right)^2 \Psi(\xi) + V(\xi)\Psi(\xi) = E\Psi(\xi) \tag{4}$$

where $D(\xi) \equiv (\partial_\xi x)^{-1}$, and $V(\xi) \equiv \mathcal{V}(x(\xi))$. Alternatively, we may rewrite the above as

$$H_\xi \Psi(\xi) \equiv A(\xi)\partial_\xi^2 \Psi(\xi) + B(\xi)\partial_\xi \Psi(\xi) + C(\xi)\Psi(\xi) = 0 \tag{5}$$

where $A(\xi) \equiv -(D(\xi))^2$, $B(\xi) = -\frac{1}{2}\partial_\xi (D(\xi))^2$ and $C(\xi) = V(\xi) - E$. The previous work (Handy 2001a) showed how such an expression, without the $\partial_\xi \Psi$ term, leads to a fourth-order equation for $S(\xi) = |\Psi(\xi)|^2$. We broaden this derivation to include the above general case.

Define the following four functions:

$$\Sigma_1(\xi) \equiv \Psi^*(\xi)H_\xi\Psi(\xi) + \text{c.c.} = 0 \tag{6}$$

$$\Sigma_2(\xi) \equiv \Psi'^*(\xi)H_\xi\Psi(\xi) + \text{c.c.} = 0 \tag{7}$$

$$\Delta_1(\xi) \equiv \Psi^*(\xi) H_\xi \Psi(\xi) - \text{c.c.} = 0 \tag{8}$$

and

$$\Delta_2(\xi) \equiv \Psi'^*(\xi) H_\xi \Psi(\xi) - \text{c.c.} = 0 \tag{9}$$

where 'c.c.' denotes the complex conjugate.

Define

$$S(\xi) = \Psi^*(\xi)\Psi(\xi) \tag{10}$$

$$P(\xi) = \Psi'^*(\xi)\Psi'(\xi) \tag{11}$$

$$J(\xi) = \frac{\Psi(\xi)\partial_\xi\Psi^*(\xi) - \Psi^*(\xi)\partial_\xi\Psi(\xi)}{2\mathrm{i}} \tag{12}$$

and

$$T(\xi) = \frac{\partial_\xi\Psi(\xi)\partial_\xi^2\Psi^*(\xi) - \partial_\xi\Psi^*(\xi)\partial_\xi^2\Psi(\xi)}{2\mathrm{i}}. \tag{13}$$

These correspond to important physical quantities. The first two are nonnegative functions corresponding to the probability density and the 'momentum density', while $J(\xi)$ is the probability flux.

We then have (i.e. $A = A_R + \mathrm{i}A_I$, etc):

$$\Sigma_1(\xi) = (S''(\xi) - 2P(\xi))A_R(\xi) + S'(\xi)B_R(\xi) + 2S(\xi)C_R(\xi) + 2(B_I(\xi) + A_I(\xi)\partial_\xi)J(\xi)$$
$$= 0 \tag{14}$$

$$\frac{\Delta_1(\xi)}{\mathrm{i}} = \left(S''(\xi) - 2P(\xi)\right)A_I(\xi) + S'(\xi)B_I(\xi) + 2S(\xi)C_I(\xi) - 2(B_R(\xi) + A_R(\xi)\partial_\xi))J(\xi)$$
$$= 0 \tag{15}$$

$$\Sigma_2(\xi) = P'(\xi)A_R(\xi) + 2T(\xi)A_I(\xi) + 2P(\xi)B_R(\xi) + S'(\xi)C_R(\xi) - 2J(\xi)C_I(\xi) = 0 \tag{16}$$

and

$$\frac{\Delta_2(\xi)}{\mathrm{i}} = P'(\xi)A_I(\xi) - 2T(\xi)A_R(\xi) + 2P(\xi)B_I(\xi) + S'(\xi)C_I(\xi) + 2J(\xi)C_R(\xi) = 0. \tag{17}$$

For the case of the ordinary (real potential) Schrödinger equation where $x = \xi$, and $A_I = 0$, $B = 0$ and $C_I = 0$, we can combine equation (14) (divided by A_R) and equation (16) to generate a third-order differential equation for S (Handy 1987a, 1987b, Handy *et al* 1988c).

If $A_I = 0$ and $B = 0$, the case considered by Handy (2001a), then equation (14) (divided by A_R) yields an equation for P. Differentiating this relation, and inserting equation (16) defines a third-order equation in S, which also depends on J. We can eliminate J by differentiating (after dividing out C_I/A_R) one more time, and substituting equation (15). The resulting expression corresponds to that in equation (1), assuming $A_R = 1$.

If $A_I = 0$ and $C_I \neq 0$, or $A_R = 0$ and $C_I \neq 0$, we can determine J from equation (16) or equation (17), respectively, and procede with the analysis discussed below.

If both $A_{R,I} \neq 0$, multiplying equation (16) and equation (17) by $A_R(\xi)$ and $A_I(\xi)$, respectively, and adding, yields an equation for J:

$$J(\xi) = \frac{P'(\xi)|A(\xi)|^2 + 2P(\xi)\text{Re}(A(\xi)B^*(\xi)) + S'(\xi)\text{Re}(A(\xi)C^*(\xi))}{-2\text{Im}(A(\xi)C^*(\xi))}. \tag{18}$$

We can now substitute this expression, $J(\xi; P, P', S')$, into equation (14) and equation (15) yielding two coupled differential equations for P and S. Instead of the formalism presented by Handy (2001a), we can work with these two coupled equations, since they involve two nonnegative configurations (for the physical solutions). However, depending on the nature of

the function coefficients (i.e. $A(\xi)$, $B(\xi)$, $C(\xi)$) it may be expedient to reduce these to one fourth-order linear differential equation for S. This is particularly the case corresponding to that discussed by Handy (2001a).

For completeness, we note that the analytic extension of $S(\xi)$ onto the complex-ξ plane (which is of no immediate concern to us) corresponds to

$$S(\xi) = \Psi^*(\xi^*)\Psi(\xi). \tag{19}$$

That is, if we assume that $\Psi(\xi)$ is analytic at the origin (for simplicity), then $\Psi(\xi) = \sum_{j=0}^{\infty} c_j \xi^j$ and $\Psi^*(\xi^*) = \sum_{j=0}^{\infty} c_j^* \xi^j$ are convergent power series, defining an analytic product which is nonnegative along the real ξ-axis.

3. The complex rotated $p^2 - \mathrm{i}x^3$ Hamiltonian

Consider the non-Hermitian potential problem

$$-\Psi''(x) - \mathrm{i}x^3\Psi(x) = E\Psi(x) \tag{20}$$

first considered in the work by Bender and Boettcher (1998). From their analysis, it is known that bound states exist along the real axis. They satisfy

$$E = \frac{\int \mathrm{d}x\, P(x) - \mathrm{i}\int \mathrm{d}x\, x^3 S(x)}{\int \mathrm{d}x\, S(x)}. \tag{21}$$

If the physical solution conforms with the $\mathcal{PT}$ invariant nature of the Hamiltonian,

$$\Psi^*(-x) = \Psi(x) \tag{22}$$

then $S(-x) = S(x)$, and the discrete state energy is real. Exhaustive investigations by many individuals support this. These include the works by (in addition to those cited previously) Bender *et al* (1999a, 1999b, 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). The analysis of Handy (2001a) has also been extended to the case of complex E, also supporting that the discrete states of the $-\mathrm{i}x^3$ potential do not violate $\mathcal{PT}$ symmetry (Handy 2001b). In accordance with all of this, we procede assuming that the discrete spectrum is real.

Let $x \equiv \mathrm{e}^{\mathrm{i}\theta}|x|$. Adopting Bender and Boettcher's notation, it is known that the bound states decrease exponentially fast in any asymptotic direction within the 'wedges' defined by

$$|\theta - \theta_{\mathrm{L,R}}| < \frac{\pi}{5} \tag{23}$$

where $\theta_{\mathrm{L}} = -\pi + \frac{\pi}{10}$, and $\theta_{\mathrm{R}} = -\frac{\pi}{10}$. The anti-Stokes lines (along which the asymptotic decrease is fastest) is centered at $\theta_{\mathrm{L,R}}$.

We first considered the general transformation

$$x(\xi) = \mathrm{e}^{\mathrm{i}\theta}\xi - \frac{\mathrm{e}^{-\mathrm{i}\theta}}{\xi} \tag{24}$$

for $0 < \xi < \infty$, and θ lying within the boundedness wedge(s). Such transformations would be relevant not only for the $-\mathrm{i}x^3$ potential, but all the other non-Hermitian potentials considered by Bender and Boettcher. However, the generation of a moment equation, following the formalism in section 2, made this approach inefficient, due to the large order of the associated moment equation relation.

Instead of this approach, the $-\mathrm{i}x^3$ problem affords a particularly simpler formulation, since the wedges intersect the entire real axis. This is not the case for all the other potentials

(i.e. $(-ix)^n$, $n \geqslant 4$) considered by Bender and Boettcher. The generalization of the present approach can be made to these cases as well; however, we defer this to another communication, since it requires a completely different linear programming formalism.

Consistent with the formalism in section 2, if we take

$$x = e^{i\theta}\xi \tag{25}$$

where $\xi \in (-\infty, +\infty)$, then the bound state solution $\Psi(e^{i\theta}\xi)$ will be asymptotically zero (i.e. at $\xi = \pm\infty$) for

$$-\frac{\pi}{10} < \theta < \frac{\pi}{10}. \tag{26}$$

Clearly, this includes the real axis. However, for fixed $\theta \neq 0$, the closer $e^{i\theta}\xi$ is to the anti-Stokes line along the positive real-ξ axis (i.e. $\theta \to \theta_R$) the farther is $e^{i\theta}\xi$ from its respective anti-Stokes line, for $\xi < 0$ (and conversely). Only along the real axis ($\theta = 0$), will the exponential decay be equally balanced between both the positive and negative real axis.

The work by Handy(2001a) introduces a very accurate bounding technique which was used to generate the first five low-lying states. Our immediate interest is in testing the same EMM formalism with respect to complex rotations of the system.

3.1. Moment equation for the complex rotated $-ix^3$ potential

As noted, we will be solving the Schrödinger equation along the complex-x infinite contour defined by $x = e^{i\theta}\xi$, for $-\infty < \xi < +\infty$. The resulting differential equation is

$$-\partial_\xi^2 \Psi(\xi) - ie^{i5\theta}\xi^3 \Psi(\xi) = Ee^{i2\theta}\Psi(\xi). \tag{27}$$

We will assume E to be real. The resulting fourth-order differential equation for $S(\xi)$ is then

$$\frac{1}{\Lambda(\xi)}S^{(4)}(\xi) - \frac{3c_5\xi^2}{\Lambda(\xi)^2}S^{(3)}(\xi) + \frac{4c_2E - 4\xi^3 s_5}{\Lambda(\xi)}S^{(2)}(\xi)$$

$$- \frac{6\xi^2(2c_2c_5E + c_5s_5\xi^3 + 3Es_2s_5)}{\Lambda(\xi)^2}S^{(1)}(\xi)$$

$$- \frac{4c_5^3\xi^9 + 12c_5^2s_2E\xi^6 + 12c_5s_2^2E^2\xi^3 + 4E^3s_2^3 - 6c_5s_5\xi^4 + 12Es_2s_5\xi}{\Lambda(\xi)^2}S^{(0)}(\xi)$$

$$= 0 \tag{28}$$

where

$$\Lambda(\xi) = c_5\xi^3 + Es_2 \tag{29}$$

and $c_n \equiv \cos(n\theta)$, $s_n \equiv \sin(n\theta)$ and $S^{(n)}(\xi) \equiv \partial_\xi^n S(\xi)$.

We know that all of the solutions to this equation are regular in the entire complex-ξ plane, despite the singular function coefficients. This follows from the argument presented in the context of equation (19). That is, all of the solutions to equation (27) are analytic in ξ; therefore, the product $\Psi^*(\xi^*)\Psi(\xi) = S(\xi)$ represents an analytic extension onto the entire complex-ξ plane.

There is a real singularity at $\xi = b$, defined by

$$b = -\left(\frac{Es_2}{c_5}\right)^{1/3} \in \Re. \tag{30}$$

In terms of the implicit θ dependence, $\lim_{\theta\to 0} b(\theta) = 0$.

In all of the previous applications of the EMM approach, we have never considered problems with function coefficients singular within the physical domain. The types of singularities encountered have either been close to the physical domain, or at the boundaries.

Despite the fact that the singularities in question do not affect the regular nature of the solutions, they are of concern within the EMM formalism, as discussed in the recent work by Handy *et al* (2001b). Intuitively, let us represent the above fourth-order equation by $\mathcal{O}_\xi S(\xi)$. If one is to generate a moment equation by multiplying both sides of this differential equation by $\Lambda(\xi)^2$, one must make sure that the resulting moment equation does not admit solutions to the more general problem of $\mathcal{O}_\xi S(\xi) = \mathcal{D}(\xi - b)$, where $\mathcal{D}(\xi - b)$ is a distribution-like expression supported at b. Such expressions disappear when multiplied by $\Lambda(\xi)$ (with a zero at b). If one is not careful, the naive moment equation may not correspond to the desired problem, $\mathcal{D} = 0$. That is, an inappropriate specification of the moment equation would not produce any converging bounds. Such concerns are generally inconsequential, within the EMM framework, if it is known that the desired solution also has a zero at b (Handy *et al* 2001). For the present problem, this is not the case, and a suitable modification of the standard EMM formalism is required.

In order to address this problem, one should first perform a translation change of variables:

$$\chi = \xi - b. \tag{31}$$

The ensuing fourth-order differential equation will then involve function coefficients whose singularity is no more singular than $1/\chi^2$. Specifically, let $\Lambda(\chi) = \chi \Upsilon(\chi)$, where $\Upsilon(\chi) = c_5(3b^2 + 3b\chi + \chi^2) \neq 0$. Upon multiplying both sides of the translated fourth-order equation ($\mathcal{O}_\chi S(\chi) = 0$) by $\Upsilon(\chi)$, one obtains an expression of the form

$$\frac{C_4(\chi)}{\chi} S^{(4)}(\chi) + \frac{C_3(\chi)}{\chi^2} S^{(3)}(\chi) + \frac{C_2(\chi)}{\chi} S^{(2)}(\chi) + \frac{C_1(\chi)}{\chi^2} S^{(1)}(\chi) + \frac{C_0(\chi)}{\chi^2} S(\chi) = 0 \tag{32}$$

where all the $C_n(\chi)$ are polynomials in χ.

Let us now multiply by χ^ρ, where $\rho \geqslant 0$. Upon doing so, through the operational procedure corresponding to 'integration by parts', we can rewrite the expression

$$\chi^\rho \Upsilon(\chi) \mathcal{O}_\chi S(\chi) = \left(\sum_{j=0}^{4} U_j(\chi^{\rho+9}, \ldots, \chi^{\rho-2}; \rho) \right) S(\chi) + \partial_\chi \left(T(\chi; S(\chi), \ldots, S^{(4)}(\chi)) \right)$$
$$= 0 \tag{33}$$

involving the total derivative expression noted, and functions of the power expressions, χ^q, where the exponent may be negative.

Since the physical solution must decay exponentially, along the asymptotic directions ($\chi \to \pm\infty$), we can now integrate along a contour that sits on top of the real axis, except near the origin where it deviates around it. Denote this contour by $\mathcal{C}$. Define the moments

$$\mu_\rho \equiv \int_{\mathcal{C}} \mathrm{d}\chi \, \chi^\rho S(\chi). \tag{34}$$

If $\rho \geqslant 0$, because of the analyticity of the solution, these moments correspond to the Hamburger moments taken along the real axis: $\mu_\rho = \int_{-\infty}^{+\infty} \mathrm{d}\chi \, \chi^\rho \Psi(\chi)$, for $\rho \geqslant 0$.

The moments will satisfy the moment equation (i.e. $p = \rho - 2 \geqslant -2$)

$$\mu_{p-3}\left[-\frac{3Es_2}{b} p(4 - 4p - p^2 + p^3) \right] + \mu_{p-2}\left[-\frac{3Es_2}{b^2} p(-4 - p + 4p^2 + p^3) \right]$$
$$+ \mu_{p-1}\left[-\frac{Es_2}{b^3} p(p+2)(6 + 12b^2 c_2 E + 7p + p^2 - 12b^5 s_5) \right]$$
$$+ \mu_p\left[\frac{6Es_2}{b^2}(-2c_2 E(4 + 5p + p^2) + s_5 b^3(14 + 25p + 8p^2)) \right]$$
$$+ \mu_{p+1}\left[\frac{2Es_2}{b^3}(-2c_2 E(12 + 8p + p^2) + b^3 s_5(168 + 169p + 38p^2)) \right]$$

$$+ \mu_{p+2}\left[\frac{12Es_2s_5}{b}(42 + 30p + 5p^2)\right]$$

$$+ \mu_{p+3}\left[\frac{6Es_2}{b^3}(18E^2s_2^2 + bs_5(56 + 31p + 4p^2))\right]$$

$$+ \mu_{p+4}\left[\frac{2Es_2}{b^4}(162E^2s_2^2 + bs_5(42 + 19p + 2p^2))\right] + \mu_{p+5}\left[\frac{432E^3s_2^3}{b^5}\right]$$

$$+ \mu_{p+6}\left[\frac{324E^3s_2^3}{b^6}\right] + \mu_{p+7}\left[\frac{144E^3s_2^3}{b^7}\right] + \mu_{p+8}\left[\frac{36E^3s_2^3}{b^8}\right]$$

$$+ \mu_{p+9}\left[\frac{4E^3s_2^3}{b^9}\right] = 0 \tag{35}$$

where $p \geqslant -2$.

We note that for $p \geqslant 0$, the first nine Hamburger moments, $\{\mu_0, \ldots, \mu_8\}$, generate all of the other moments (μ_p, $p \geqslant 9$) through the linear relation

$$\mu_p = \sum_{\ell=0}^{8} \tilde{M}_{p,\ell}(E)\mu_\ell \tag{36}$$

where the energy-dependent coefficients $\tilde{M}_{p,\ell}(E)$ satisfy the moment equation (equation (35), for $p \geqslant 0$) with respect to the p-index. In addition, they satisfy the initialization conditions $\tilde{M}_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_{1,2} \leqslant 8$.

If the moment equation is restricted to $p \geqslant 0$, then the associated differential equation would be of the form $\mathcal{O}_\chi S(\chi) = \mathcal{D}(\chi)$, with $\mathcal{D}$ an unknown distribution supported at the origin (as discussed before). By also including $p = -1, -2$, we are imposing $\mathcal{D} = 0$.

For these two values of the p index, the moment equation becomes, for $p = -1$,

$$\mu_0\left[\frac{2Es_2}{b^3}(-10c_2E + 37b^3s_5)\right] + \mu_1\left[\frac{204Es_2s_5}{b}\right] + \mu_2\left[\frac{6Es_2}{b^3}(18E^2s_2^2 + 29bs_5)\right]$$

$$+ \mu_3\left[\frac{2Es_2}{b^4}(162E^2s_2^2 + 25bs_5)\right] + \mu_4\left[\frac{432E^3s_2^3}{b^5}\right] + \mu_5\left[\frac{324E^3s_2^3}{b^6}\right]$$

$$+ \mu_6\left[\frac{144E^3s_2^3}{b^7}\right] + \mu_7\left[\frac{36E^3s_2^3}{b^8}\right] + \mu_8\left[\frac{4E^3s_2^3}{b^9}\right] = \Sigma(\mu_{-1}, \mu_{-2}, \mu_{-4}) \tag{37}$$

where

$$\Sigma(\mu_{-1}, \mu_{-2}, \mu_{-4}) = \left(18bEs_2s_5\mu_{-1} - \frac{Es_2}{b^3}(12b^2c_2E - 12b^5s_5)\mu_{-2} - \frac{18Es_2}{b}\mu_{-4}\right) \tag{38}$$

and, for $p = -2$,

$$\mu_0\left[\frac{24Es_2s_5}{b}\right] + \mu_1\left[\frac{6Es_2}{b^3}(18E^2s_2^2 + 10bs_5)\right] + \mu_2\left[\frac{2Es_2}{b^4}(162E^2s_2^2 + 12bs_5)\right]$$

$$+ \mu_3\left[\frac{432E^3s_2^3}{b^5}\right] + \mu_4\left[\frac{324E^3s_2^3}{b^6}\right] + \mu_5\left[\frac{144E^3s_2^3}{b^7}\right] + \mu_6\left[\frac{36E^3s_2^3}{b^8}\right]$$

$$+ \mu_7\left[\frac{4E^3s_2^3}{b^9}\right] = \frac{2}{b}\Sigma(\mu_{-1}, \mu_{-2}, \mu_{-4}). \tag{39}$$

Therefore, we can use both relations to constrain the μ_8 moment in terms of the moments $\{\mu_0, \mu_1, \ldots, \mu_7\}$. These in turn can be used with the moment equation (equation (35)), for $p \geqslant 0$, to generate all of the other Hamburger moments. Thus, we have

$$\mu_8 = \sum_{\ell=0}^{7} \tilde{M}_{8,\ell}(E)\mu_\ell \tag{40}$$

defined by subtracting equation (39) from equation (37) (after dividing the former by $2/b$).

Incorporating this within the expression in equation (36) (dependencies on E are implicitly assumed),

$$\mu_p = \sum_{\ell=0}^{7} \tilde{M}_{p,\ell} \mu_\ell + \tilde{M}_{p,8} \sum_{\ell=0}^{7} \tilde{M}_{8,\ell} \mu_\ell \tag{41}$$

yields

$$\mu_p = \sum_{\ell=0}^{7} M_{p,\ell} \mu_\ell \tag{42}$$

where

$$M_{p,\ell} = \begin{cases} \tilde{M}_{8,\ell} & p = 8 \\ \tilde{M}_{p,\ell} + \tilde{M}_{p,8} \tilde{M}_{8,\ell} & p \geqslant 9 \end{cases} \tag{43}$$

and $M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_1, \ell_2 \leqslant 7$. This is the moment generating relation required in implementing EMM.

An additional important point is specifying the choice of normalization. Since we are only dealing with Hamburger moments, some of the odd-order moments may be negative. However, the even-order moments are positive, and by working with the first eight of them

$$u_\ell \equiv \mu_{2\ell} \tag{44}$$

we can impose the normalization

$$\sum_{\ell=0}^{7} u_\ell = 1. \tag{45}$$

Working with the positive quantities, u_ℓ, makes the implementation of the linear programming algorithm more efficient (since one is working within a bounded polytope corresponding to the unit hypercube, $[0, 1]^7$).

Thus, we take

$$u_\ell = \mu_{2\ell} = \sum_{\ell_v}^{7} M_{2\ell,\ell_v} \mu_{\ell_v} \tag{46}$$

for $0 \leqslant \ell \leqslant 7$. The inverse of this relation is denoted by

$$\mu_\ell = \sum_{\ell_v=0}^{7} N_{\ell,\ell_v} u_{\ell_v} \tag{47}$$

and substituted in equation (42) producing

$$\mu_p = \sum_{\ell,\ell_v=0}^{7} M_{p,\ell} N_{\ell,\ell_v} u_{\ell_v} \tag{48}$$

or

$$\mu_p = \sum_{\ell=0}^{7} \mathcal{M}_{p,\ell} u_\ell \tag{49}$$

for $p \geqslant 0$, where $\mathcal{M}_{p,\ell} = \sum_{\ell_v=0}^{7} M_{p,\ell_v} N_{\ell_v,\ell}$.

Finally, the normalization condition is incorporated ($u_0 = 1 - \sum_{\ell=1}^{7} u_\ell$), producing

$$\mu_p = \sum_{\ell=0}^{7} \hat{\mathcal{M}}_{p,\ell}(E) \hat{u}_\ell \tag{50}$$

where

$$\hat{\mathcal{M}}_{p,\ell}(E) = \begin{cases} \mathcal{M}_{0,\ell}(E) & p = 0 \\ \mathcal{M}_{p,\ell}(E) - \mathcal{M}_{0,\ell}(E) & p \geqslant 1 \end{cases} \tag{51}$$

and

$$\hat{u}_\ell = \begin{cases} 1 & \ell = 0 \\ u_\ell & 1 \leqslant \ell \leqslant 7. \end{cases} \tag{52}$$

3.2. Numerical results

Although the computational algorithmic structure of the EMM formulation has been presented in many of the works cited previously, for completeness, we repeat the essentials of its structure here.

The physical solution, $S(\xi)$, must be nonnegative and integrable (i.e. L^1, since Ψ must be L^2); therefore, it must satisfy

$$\int_{-\infty}^{+\infty} d\xi \left(\sum_{j=0}^{J} C_j \, \xi^j \right)^2 S(\xi) > 0 \tag{53}$$

for arbitrary C_j's and $J < \infty$. This leads to the quadratic form inequalities

$$\sum_{j_1, j_2=0}^{J} C_{j_1} \mu_{j_1+j_2} C_{j_2} > 0. \tag{54}$$

From the linear dependence of the Hamburger moments on the positive variables $\{u_\ell \equiv \mu_{2\ell} | 1 \leqslant \ell \leqslant 7\}$, as given by equation (50), the above inequalities become

$$\sum_{\ell=1}^{7} A[C; \ell] \, u_\ell < B[C] \tag{55}$$

where

$$A[C; \ell] = - \sum_{j_1, j_2=0}^{J} C_{j_1} \hat{\mathcal{M}}_{j_1+j_2, \ell}(E) \, C_{j_2} \tag{56}$$

and

$$B[C] = \sum_{j_1, j_2=0}^{J} C_{j_1} \hat{\mathcal{M}}_{j_1+j_2, 0}(E) \, C_{j_2}. \tag{57}$$

In addition, from equation (45), and the positivity of the u_ℓ's, we know that

$$0 < u_\ell < 1. \tag{58}$$

The above constraints must be satisfied by the physical solution. Conversely, because one is working with the moments of a physical system, with a unique physical solution, these constraints are sufficient to uniquely single out the physical solution(s).

At a given dimension, $J + 1$, for an arbitrary energy value, E, if there is a $\{u_\ell\}$ solution set to equation (55), it must be convex. Denote this set by $\mathcal{U}(J, E)$. The EMM algorithm generates

a finite number of optimal C-vectors that tell us whether $\mathcal{U}(J, E)$ exists or not. Generally, the E values admitting such solution sets define intervals, $E \in (E_{\min}(J, n), E_{\max}(J, n))$, whose endpoints converge to the corresponding physical energy from below and above:

$$E_{\min}(J, n) \leqslant E_{\min}(J + 1, n) \leqslant \cdots < E_{\text{phys}}^{(n)} < \cdots \leqslant E_{\max}(J + 1, n) \leqslant E_{\max}(J, n). \tag{59}$$

The numerical implementation of the EMM procedure is given in table 1. We only investigate the lowest energy state, $E_{\text{phys}}^{(0)}$. The parameter $P_{\max}$ denotes the maximum moment order generated, $\{\mu_p | 0 \leqslant p \leqslant P_{\max}\}$ (i.e. $j_1 + j_2 \leqslant P_{\max}$).

We see that as the rotation angle increases, the tightness of the bounds decreases, as expected. Furthermore, for $\theta > \frac{\pi}{10}$, no EMM solution is generated, consistent with the fact that the bound state becomes exponentially unbounded, in the corresponding direction in the complex-x plane.

Table 1. Bounds for the ground state energy of the $-\mathrm{i}x^3$ potential ($P_{\max} = 40$).

θ	$E_{\mathrm{L};0}$	$E_{\mathrm{U};0}$
0 [a]	1.15619	1.15645
0.01	1.15617	1.15652
0.05	1.15510	1.15761
0.10	1.14201	1.17298
0.15	1.0	1.3
0.20	0.5	8.0

[a] Using Stieltjes EMM formulation by Handy(2001a).

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