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Spectral bounds for the PT-breaking Hamiltonian $p^2 + x^4 + iax$

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Abstract

The non-Hermitian Hamiltonian $p^2 + x^4 + iax$, which spontaneously breaks PT-symmetry, and the subject of a recent study by Bender *et al* (2001 *J. Phys. A: Math. Gen.* **34** L31), is amenable to a positivity representation, facilitating the generation of converging bounds to the complex-eigenenergies of the PT-breaking states. This system is much easier (i.e. fewer variational parameters) than the previously studied case of the Hamiltonian $p^2 + ix^3 + iax$ (2001 Handy *J. Phys. A: Math. Gen.* **34** 5065, Handy *et al* 2001 *J. Phys. A: Math. Gen.* **34** 5593), as first proposed by Delabaere and Trinh (2000 *J. Phys. A: Math. Gen.* **33** 8771), enabling the generation of low order algebraic spectral bounds (i.e. $\mathrm{Re}(E) > \frac{81}{4}(\frac{\mathrm{Im}(E)}{a})^4 + O(a^2)$), in addition to high order, numerically generated, converging bounds to the discrete states. We examine both approaches here.

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1. General overview

1.1. New results

In two recent works by Bender *et al* (2001) and Delabaere and Pham (1998), various WKB-related methods (*complex WKB* and *exact WKB*, respectively) were developed for the PT-symmetry breaking Hamiltonian

$$-\Psi''(x) + (x^4 + iax)\Psi(x) = E\Psi(x). \qquad (1)$$

This established that discrete states exist, on the real axis, for arbitrary values of the parameter $a > 0$; and some of these exhibit PT-symmetry breaking, yielding complex eigenenergies, $E = (E_R, E_I)$.

Although a detailed analysis was presented for the onset of symmetry breaking, no numerical values were provided for the complex eigenenergies associated with the symmetry breaking solutions. It appears that these quantities cannot be readily generated through their approach, because of numerical difficulties.

In contrast, the eigenvalue moment method (EMM) analysis presented here is exceptionally numerically stable, and easily generates the low-lying eigenenergies both for the PT-invariant and PT-breaking states. This is demonstrated in this work, with respect to the first four discrete states.

The EMM algorithm determines the (complex) eigenenergies through the generation of converging lower and upper bounds to the (real and imaginary parts of the) discrete state energies. An important feature of the EMM approach is that it is not dependent on the existence of a Hilbert space structure in order to quantize the system, distinguishing it from other bounding methods, such as Lowdin's inner projection theory, or the Kato (1949) approach.

The capabilities of the EMM approach have already been demonstrated on other non-Hermitian potentials (Handy 2001a, 2001b, Handy *et al* 2001, Handy and Wang 2001), including the PT-symmetry breaking potential, $(\mathrm{i}x)^3 + \mathrm{i}ax$, first studied (analytically but not numerically) by Delabaere and Trinh (2000). In all these cases, the EMM approach generates very accurate numerical values for the low-lying eigenenergies (complex or real), through the generation of converging lower and upper bounds to $E = (E_R, E_I)$.

The EMM analysis is inherently algebraic; however, for most problems, understanding the algebraic consequences of the EMM relations is very difficult, and as yet, non-intuitive. For this reason, the implementation of EMM has, for the most part, focused only on the numerical consequences of these relations (i.e. the spectral bounds).

What makes the $x^4 + \mathrm{i}ax$ potential particularly interesting, from the EMM approach, is that whereas the $(\mathrm{i}x)^3 + \mathrm{i}ax$ potential involves five linear variational parameters (i.e. *missing moments*), the quartic non-Hermitian problem only involves one such parameter. This means that we can also extract, low order, algebraic formulae that define a lower bound on E_R, for the discrete state spectrum.

We demonstrate both approaches here. That is, we use EMM to generate high precision (tight) numerical bounds on the first four discrete state energy levels, for various values of the parameter a, including regions of symmetry breaking. We also analyse the complicated structure of the EMM positivity relations (in terms of their nonlinear equivalents) in order to extract algebraic bounds. Even for this problem, this is not easy, and some of our results, although given in closed form, provide no intiutive understanding, beyond their explicit algebraic structure, of what is taking place.

We can easily show that $E_R > 0$, regardless of the PT-invariant or PT-breaking nature of the solutions. This is done in section 2.1. However, the precise (low order) form of these spectral positivity properties (i.e. specific lower bounds for E_R) requires the moment analysis developed here (refer to equations (45), (74) and (81)). For very small values of the parameter a, these rigorous constraints result in the lower bound $\mathrm{Re}(E) > \frac{81}{4}\left(\frac{\mathrm{Im}(E)}{a}\right)^4 + O(a^2)$.

Such relations do not appear to be obtainable through conventional means, and provide one additional, algebraic, advantage the EMM analysis can provide, for amenable systems.

1.2. Moment problem quantization: Hankel–Hadamard analysis and the eigenvalue moment method

In order for the methods used here to work, it is important that the solutions of interest be associated with nonnegative configurations which are uniquely bounded, in the sense of having finite power moments. If this is not satisfied, one cannot generate converging bounds. Given both of these conditions, preferably for linear systems, we can then impose well-known positivity, moment constraints, arising from the classic *moment problem* in mathematics (Shohat and Tamarkin 1963). Until the work by Handy and Bessis (1985), researchers had not anticipated the utility of moment problem theorems in quantizing physical systems. We refer to this general philosophy as *moment problem quantization* (MPQ).

There are various versions of MPQ. Three of these will be used in this work in order to generate both numerical and algebraic bounds to the complex discrete state energies of interest.

The first of these involves the Hankel–Hadamard (HH) determinantal moment constraints (Shohat and Tamarkin 1963), which are intrinsically nonlinear in the moments.

The second involves an equivalent, linear reformulation, which exploits the use of linear programming (Chvatal 1983). It was made possible by Handy's development of the *cutting algorithm*, which allowed the MPQ methodology to be applied to the ground state binding energy of the quadratic Zeeman effect, for hydrogenic atoms in superstrong magnetic fields (Handy *et al* 1988a, 1988b). This approach is referred to as the eigenvalue moment method (EMM).

The third approach exploits limited convexity properties enjoyed by successive ratios of HH determinants (Handy *et al* 1996).

Given the complex-analytical nature of the non-Hermitian system(s) in question, it is remarkable that a nonnegative differential representation is possible, consistent with the stipulated requirements for applicability of MPQ–HH/EMM.

In several previous communications by Handy (2001a, 2001b) and Handy and Wang (2001), it was established that for the one-dimensional Schrödinger equation, with arbitrary (complex) potential (i.e. $V(x) = V_R(x) + \mathrm{i}V_I(x)$), the configuration $S(\chi) = |\Psi(x(\chi))|^2$ (involving the discrete state wavefunction, Ψ, along an appropriate complex contour, $x(\chi) : \Re \to \mathcal{C}$) satisfies a fourth-order, linear differential equation.

For systems with discrete states along the real axis, this relation becomes

$$\partial_x \left[-\frac{\partial_x^3 S(x)}{V_I(x) - E_I} + 4\left(\frac{V_R(x) - E_R}{V_I(x) - E_I}\right)\partial_x S(x) + 2\left(\frac{\partial_x V_R(x)}{V_I(x) - E_I}\right) S(x)\right] + 4(V_I(x) - E_I)S(x) = 0. \tag{2}$$

It is easy to argue, for problems on the entire real axis, that the physical solutions uniquely correspond to those configurations that are nonnegative, and bounded, having finite Hamburger power moments:

$$\mu_p = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p S(x) < \infty. \tag{3}$$

The above fourth-order equation can be transformed into a moment equation, by multiplying both sides by x^p and integrating by parts. The moments generated from this recursive relation, involving the complex energy as a parameter, $E = E_R + \mathrm{i}E_I$, are then constrained by the HH determinantal positivity theorems. These, in turn, constrain the energy, and produce converging lower and upper bounds to the discrete state values for E_R and E_I, as more moments are used.

The above type of analysis is useful for extracting algebraic relations, provided the order of the finite difference moment equation, referred to as the *missing moment* order, m_s, is small, as it is for the problem in question ($m_s = 1$).

More generally, for problems with a large missing moment order (particularly multidimensional problems), the previous HH analysis in numerically inefficient, and one must use the eigenvalue moment method.

We will use the latter approach to generate numerical values for the four low-lying discrete states, for various a parameter values, including regions of PT-symmetry breaking.

We will use the HH approach, combined with the additional (restricted) convexity relations for successive ratios of HH determinants, in order to generate low order, algebraic, spectral bounds.

For completeness, we note that the impetus for deriving equation (2), stems from several prior studies on HH/EMM as applied to real potentials, $V_I = 0$, wherein $S(x)$ satisfies a third-order differential equation (discernable from equation (2)):

$$-\partial_x^3 S(x) + 4(V(x) - E)\partial_x S(x) + 2(\partial_x V(x))S(x) = 0. \tag{4}$$

This was first published by Handy (1987a, 1987b), and subsequently published, independently, by Namias (1987); although several other researchers had known of this relation (i.e. F Cooper, E Power). The emphasis on $|\Psi(x)|^2$, as opposed to just $\Psi^2(x)$, was to enable extension of the HH/EMM analysis to scattering problems (Handy *et al* 1988c). The recent interest in these positivity, differential formulations, by Milward and Wilkin (2000, 2001), albeit from the perspective of perturbation theory, is incomplete in its review of the published literature. Specifically, as cited in the works by Handy, quantum chemists already knew of the moment equation structure associated with the above third-order differential equation, and used it for similar perturbative analysis, although they had no compelling interest in uncovering the associated differential structure.

In contrast to the lack of interest by quantum chemists in the existence of the above third-order equation, this is indispensable within the HH/EMM framework, precisely because it is the means by which one can confirm that converging bounds can be derived (i.e. the physical solutions are uniquely nonnegative and bounded).

2. Moment equation representation for $|\Psi(X)|^2$

It turns out that the required moment equation relation, derived solely from equation (2), is incomplete, for PT-breaking systems. For such cases, one must also consider a broader set of coupled differential equations involving $S(x) = |\Psi(x)|^2$, the probability current, $J(x) = \mathrm{Im}(\Psi^*(x)\Psi'(x))$ and the 'kinetic energy density', $P(x) = |\Psi'(x)|^2$. This was first described in the works by Handy (2001b) and Handy and Wang (2001), and used to show the numerical stability of the MPQ/EMM analysis, for non-Hermitian problems undergoing analytic continuation into the complex plane. This also served to guide the extension of MPQ/EMM to the PT-invariant states of the $-(\mathrm{i}x)^N$ potential (Yan and Handy 2001).

In the next two subsections, after specifying the form of the nonnegative differential representation, we generate the relevant moment equations for both the PT-breaking case involving a Hamburger power moment representation, and then the PT-invariant solutions, where $S(x) = S(-x)$, and $E_I = 0$, requiring a Stieltjes moment representation.

2.1. Nonnegative differential representation (proof $E_R > 0$)

It can readily be shown that the three configurations, $\{S(x), J(x), P(x)\}$, satisfy the following coupled set of differential equations (Handy 2001b, Handy and Wang 2001)

$$P(x) - \tfrac{1}{2}S''(x) + (V_R(x) - E_R)S(x) = 0 \tag{5}$$

$$-P'(x) + (V_R(x) - E_R)S'(x) + 2(V_I(x) - E_I)J(x) = 0 \tag{6}$$

$$(V_I(x) - E_I)S(x) - \partial_x J(x) = 0. \tag{7}$$

These can be combined to yield equation (2).

From equation (5), we see that since $S(x) > 0$ and $P(x) > 0$, in addition to their boundedness properties, it then follows that

$$E_R = \frac{\langle S|P\rangle + \frac{1}{2}\langle S'|S'\rangle + \langle S|V_R|S\rangle}{\langle S|S\rangle} > 0 \tag{8}$$

having assumed that $V_R(x) > 0$, which is true for the present case, $V_R(x) = x^4$.

We should point out that the above relation is more complicated than required, in order to conclude $E_R > 0$; although the form of the relation, as given, is highly suggestive of the usual relation for Hermitian operators. One can reach the same conclusion by simply integrating both sides of equation (5) and using the explicit form of $V_R(x)$. This was noted in the earlier work by Handy (2001b).

In addition to the Hamburger moments for $S(x)$, we also need to consider the Hamburger moments for the other two configurations: $\nu_p \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p P(x)$ and $\omega_p \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p J(x)$.

2.1.1. Hamburger moment representation. We can now transform the coupled differential relations, for the case $V_R(x) = x^4$ and $V_I(x) = ax$, into the coupled moment equations:

$$\frac{p(p-1)}{2}\mu_{p-2} + E_R\mu_p - \mu_{p+4} - \nu_p = 0 \tag{9}$$

$$E_R p\mu_{p-1} - (p+4)\mu_{p+3} + p\nu_{p-1} - 2(-E_I\omega_p + a\omega_{p+1}) = 0 \tag{10}$$

$$-E_I\mu_p + a\mu_{p+1} - p\omega_{p-1} = 0 \tag{11}$$

for $p \geqslant 0$.

From equation (11), we obtain two relations, the first for $p = 0$, the second for $p > 0$ (or $p \to p+1$):

$$\mu_1 = \frac{E_I}{a}\mu_0 \tag{12}$$

$$\omega_p = \frac{a\mu_{p+2} - E_I\mu_{p+1}}{p+1} \tag{13}$$

for $p \geqslant 0$. In particular, when $a = 0$, from equation (12), we see that since $\mu_0 < \infty$ then $E_I = 0$ is required!

Using equation (9) to solve for ν_p and equation (13) for ω_p, we make the corresponding substitutions in equation (10), generating the moment equation

$$\mu_{p+3} = \frac{\frac{p(p-1)(p-2)}{2}\mu_{p-3} + 2E_R p\mu_{p-1} - \frac{2E_I^2}{p+1}\mu_{p+1} + 2aE_I\left(\frac{1}{p+1} + \frac{1}{p+2}\right)\mu_{p+2}}{4 + 2p + \frac{2a^2}{p+2}} \tag{14}$$

for $p \geqslant 0$, in addition to equation (12).

The last moment equation corresponds to a finite difference equation of (effective) order 3, since specification of the initialization (*missing*) moments, $\{\mu_0, \mu_1, \mu_2\}$, in addition to the energy parameter(s), $E = (E_R, E_I)$, generate all of the other moments. We can express this in terms of the relation

$$\mu_p = \sum_{\ell=0}^{2} M_{p,\ell}(E, a)\mu_\ell \tag{15}$$

where $M_{p,\ell}(E, a)$ satisfies the same moment equation, with respect to the p-index, provided the initialization conditions are satisfied

$$M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2} \tag{16}$$

for $0 \leqslant \ell_{1,2} \leqslant 2$. We can now make use of equation (12) to solve for μ_1 in terms of μ_0:

$$\mu_p = \sum_{\ell=0}^{1} N_{p,\ell}(E,a)\chi_\ell \tag{17}$$

where $\chi_0 = \mu_0$, $\chi_1 = \mu_2$ and

$$N_{p,\ell}(E,a) = \begin{cases} M_{p,0}(E,a) + \frac{E_I}{a} M_{p,1}(E,a) & \ell = 0 \\ M_{p,2}(E,a) & \ell = 1. \end{cases} \tag{18}$$

Since both $\chi_{0,1}$ must be positive (for the physical solutions), they become the natural variables within the EMM framework. We can now also impose the normalization

$$\chi_0 + \chi_1 = 1 \tag{19}$$

solving for the first variable, $\chi_0 = 1 - \chi_1$, and restricting both to $0 < \chi_{0,1} < 1$. Incorporating this within the above relation, we finally obtain

$$\mu_p = \hat{N}_{p,0}(E,a) + \hat{N}_{p,1}(E,a)\chi_1 \tag{20}$$

where

$$\hat{N}_{p,\ell}(E,a) = \begin{cases} N_{p,0}(E,a) & \ell = 0 \\ N_{p,1}(E,a) - N_{p,0}(E,a) & \ell = 1. \end{cases} \tag{21}$$

2.1.2. Stieltjes moment representation. For the case of PT-symmetric states, where $S(-x) = S(x)$, and $E_I = 0$, the previous Hamburger moment formulation simplifies. This is because the odd order moments of $S(x)$ are necessarily zero, $\mu_{\mathrm{odd}} = 0$. It turns out that the even order Hamburger moments become ordinary Stieltjes moments, of a suitably defined function, restricted to the nonnegative real axis:

$$\Phi(y) \equiv \frac{S(\sqrt{y})}{\sqrt{y}}. \tag{22}$$

Thus,

$$\mu_{2p} = u_p \equiv \int_0^\infty \mathrm{d}y\, y^p \Phi(y) \tag{23}$$

which can easily be shown through the change of variables $y \equiv x^2$.

For this case, from equation (12), it follows that if $\mu_1 = 0$, then $E_I = 0$, since $0 < \mu_0 < \infty$. The Stieltjes moment equation follows from equation (14), upon taking $p \to 2p+1$:

$$u_{p+2} = \frac{p(4p^2-1)u_{p-1} + 2E_R(2p+1)u_p}{6 + 4p + \frac{2a^2}{2p+3}} \tag{24}$$

for $p \geqslant 0$. This is also an $m_s = 1$ Stieltjes missing moment relation, after imposing the same normalization condition as before (i.e. $u_0 + u_1 = 1, u_{0,1} = \chi_{0,1}$). In particular, before imposing the normalization, we can express the moment-missing moment Stieltjes relation by

$$u_p = \sum_{\ell=0}^{1} M_{p,\ell}(E_R)u_\ell \tag{25}$$

where $M_{p,\ell}(E_R)$ satisfies the Stieltjes moment equation with respect to the p-index, in addition to the initialization (self-consistency) conditions, $M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}$.

After imposing the normalization, $u_0 = 1 - u_1$, and substituting, we obtain the unconstrained (normalized) missing moment relation

$$u_p = \hat{M}_{p,0}(E_R) + \hat{M}_{p,1}(E_R)u_1 \tag{26}$$

where $\hat{M}_{p,0}(E_R) = M_{p,0}(E_R)$ and $\hat{M}_{p,1}(E_R) = M_{p,1}(E_R) - M_{p,0}(E_R)$.

3. Hankel–Hadamard and eigenvalue moment method positivity constraints

3.1. Hamburger moment problem

From the moment problem theorems, given a nonnegative function, $S(x) > 0$, on the entire real axis, the corresponding Hamburger power moments must satisfy the integral constraints

$$\int_{-\infty}^{+\infty} \mathrm{d}x \left(\sum_{j=0}^{J} C_j x^j \right)^2 S(x) > 0 \tag{27}$$

for arbitrary C (not all identically zero) and $J \geqslant 0$. These become the quadratic form inequalities, involving the Hamburger power moments:

$$\sum_{j_1=0}^{J} \sum_{j_2=0}^{J} C_{j_1} \mu_{j_1+j_2} C_{j_2} > 0. \tag{28}$$

The indicated, Hankel moment matrix, $\mathcal{M}_{j_1,j_2} \equiv \mu_{j_1+j_2}$, is real and symmetric. Therefore, the requirement that it be a positive matrix, means that all of its eigenvalues must be positive, or alternatively, the Hankel–Hadamard determinants must be positive:

$$\Delta_{0,J}(\mu) \equiv \mathrm{Det} \begin{pmatrix} \mu_0, \ldots, \mu_J \\ \mu_1, \ldots, \mu_{J+1} \\ \cdots \\ \mu_J, \ldots, \mu_{2J} \end{pmatrix} > 0 \tag{29}$$

for $J \geqslant 0$. The zero subscript in $\Delta_{0,J}(\mu)$ is retained in order to distinguish this case from the Stieltjes moment representation formulation.

For the present problem, upon substituting the moment-missing moment relation in equation (20), relating the μ_p to μ_2 (including the energy dependence), the HH determinantal inequalities become implicit constraints on μ_2, E_R, and E_I:

$$\Delta_{0,J}(E_R, E_I, \mu_2) > 0 \tag{30}$$

for $J \geqslant 0$.

In the following analysis, we will consider all HH determinants that can be formed from the first $1 + 2J$ Hamburger moments ($\{\mu_0, \ldots, \mu_{2J}\}$). This will be referred to as 'to order J'.

The objective of the MPQ approach is to establish, for arbitrary energy, the existence/non-existence of the missing moment solution set, $\mathcal{U}_{2J}(E)$, to order J, for equation (30). If such a solution set exists, it must be convex.

It follows from the definition of the solution sets, $\mathcal{U}_{2J}(E)$, that they must be nested, assuming they exist (i.e. are not null):

$$(0, 1) \supset \mathcal{U}_2(E) \supset \cdots \supset \mathcal{U}_{2J}(E). \tag{31}$$

The $E = (E_R, E_I)$ regions for which $\mathcal{U}_{2J}(E) \neq \oslash$, define the energy feasibility regions, to order J. The boundaries of these regions then become the lower and upper bounds to the particular discrete state energy in question.

We will make use of these HH positivity relations in deriving algebraic bounds. We will also make use of the following theorem (Handy *et al* 1996) concerning successive ratios of HH moment determinants (the E dependence is implicitly understood).

Define the ratios

$$D_{(0,n)}(\chi) \equiv \frac{\Delta_{0,n}(\chi)}{\Delta_{0,n-1}(\chi)}. \tag{32}$$

At a given E, assume that the (convex) missing moment sets, $\mathcal{U}_{2n}(E_R, E_I)$, exist for $0 \leqslant n \leqslant N$, then

$$D_{0,N+1}(\chi) = \text{Convex function for } \chi \in \mathcal{U}_{2N}(E_R, E_I). \tag{33}$$

We emphasize that although this function is convex on the $\mathcal{U}_{2N}$, it can be completely negative as well, in which case, $\mathcal{U}_{2(N+1)}(E_R, E_I)$ does not exist, indicating that the associated E is not physically possible.

This convexity property allows for some simplification in the algebraic analysis of the HH relations.

3.2. *Stieltjes moment problem*

For the case of PT-invariant solutions, the underlying moment representation is Stieltjes, as previously noted. In this case, the relevant HH theorems ensue from the integral inequalities:

$$\int_0^{+\infty} \mathrm{d}y\, y^\sigma \left(\sum_{n=0}^{N} C_n y^n\right)^2 \Phi(y) > 0 \tag{34}$$

or

$$\sum_{n_1=0}^{N} \sum_{n_2=0}^{N} C_{n_1} u_{\sigma+n_1+n_2} C_{n_2} > 0 \tag{35}$$

for arbitrary C_n (so long as they are not all identically zero), $N \geqslant 0$, and $\sigma = 0, 1$.

The positivity of the quadratic forms means that the underlying Hankel moment (symmetric) matrices must be positive, having real eigenvalues. These eigenvalues must interlace, for fixed σ, and varying N. Accordingly, the determinants must be positive:

$$\Delta_{\sigma,N}(u) \equiv \mathrm{Det}\begin{pmatrix} u_\sigma, u_{\sigma+1}, \ldots, u_{\sigma+N} \\ u_{\sigma+1}, u_{\sigma+2}, \ldots, u_{\sigma+N+1} \\ \ldots \\ u_{\sigma+N}, u_{\sigma+N+1}, \ldots, u_{\sigma+2N} \end{pmatrix} > 0 \tag{36}$$

for $\sigma = 0, 1$ and $N \geqslant 0$.

Again, upon making use of the Stieltjes moment-missing moment relation in equation (26), the relevant HH relations become

$$\Delta_{\sigma,N}(E_R, u_1) > 0 \tag{37}$$

for $\sigma = 0, 1$.

As before, the feasible (physically possible) energy values, to order P, are those that satisfy the above HH inequalities for all HH determinant matrices that can be formed from the first $1 + P$ Stieltjes moments (i.e. $\sigma + 2N \leqslant P$). We denote this by $\mathcal{U}_P(E_R)$. The energy values admitting missing moment solutions to these positivity constraints, define feasibility intervals whose endpoints become the lower and upper bounds to the corresponding (real) discrete state energy.

The Stieltjes counterpart to equation (32) also holds, for each fixed σ value. Denote by $\mathcal{S}_{\sigma,N}(E_R)$ the missing moment solution set to the Stieltjes HH inequalities, $\Delta_{\sigma,n}(E_R, u_1) > 0$, for $0 \leqslant n \leqslant N$, and fixed σ. Each $\mathcal{S}_{\sigma,N}(E_R)$ is convex (i.e. an interval, in this case). By definition

$$\mathcal{S}_{\sigma,0}(E_R) \supset \mathcal{S}_{\sigma,1}(E_R) \supset \cdots \supset \mathcal{S}_{\sigma,N}(E_R). \tag{38}$$

Note that $\mathcal{S}_{0,0}(E_R) = (0, 1)$, and $\mathcal{S}_{1,0}(E_R) = (0, 1)$; although the restricted convexity property can extend to regions outside of the normalization interval.

Define the successive Stieltjes determinant ratios:

$$\tilde{D}_{\sigma,n}(E_R, u_1) = \frac{\Delta_{\sigma,n}(E_R, u_1)}{\Delta_{\sigma,n-1}(E_R, u_1)}. \tag{39}$$

If the successive missing moment solution sets exist, $\mathcal{S}_{\sigma,0}(E_R) \supset \cdots \supset \mathcal{S}_{\sigma,N}(E_R)$, then $\tilde{D}_{\sigma,N+1}(E_R, u_1)$ is a convex function over the set $\mathcal{S}_{\sigma,N}(E_R)$.

3.3. The eigenvalue moment method

As noted, in order to generate spectral bounds, to a given moment expansion order, we must determine the existence or nonexistence of the missing moment solution sets. For problems with a large missing moment order (particularly for multidimensional problems), to do so with respect to the nonlinear HH inequalities becomes numerically expensive or impossible. In most references, it is these nonlinear relations which are emphasized. However, from the quadratic form relations in equations (28) and (35), an equivalent, linear (in the moments), infinite set of moment constraints becomes a useful alternative. That is, we can either work with a finite number of nonlinear constraints, whose missing moment solution set is convex (if it exists); or, we can work with an infinite number of linear constraints, with the same solution set.

With respect to the quadratic forms in equation (28) or (35), the eigenvalue moment method (EMM) optimally selects a finite number of C-vectors, to be designated as $\vec{C}_\kappa$, $1 \leqslant \kappa \leqslant K$, which generate corresponding linear inequalities in the missing moment solution space, $\vec{\mathcal{A}}(\vec{C}_\kappa) \cdot \vec{\chi} < \mathcal{B}(\vec{C}_\kappa)$. The solution set, to these K linear inequalities, define a polytope, $\mathcal{P}(E)$ (a convex set formed by intersecting hyperplanes, although in the present problem the polytope is an interval), which bounds the missing moment solution set: $\mathcal{U}_P(E) \subset \mathcal{P}(E)$.

Each linear inequality *cuts* the starting, normalization, polytope, $(0, 1)^{m_s}$. The EMMs cutting algorithm (Handy *et al* 1988a, 1988b), through the generation of these K *cutting vectors*, will result in one of two possibilities:

(a) The K linear inequalities have no solution set, resulting in $\mathcal{P}(E) = \oslash$, which tells us that $\mathcal{U}_P(E) = \oslash$, and the E value in question is not a possible physical value.
(b) The K linear inequalities have a solution set, and by construction, the centre, $\vec{\chi}_c$, of the largest inscribed hypersphere (or interval, in the present case) within $\mathcal{P}(E)$ must satisfy the HH inequalities, to the order of the moment expansion being considered. Thus, $\mathcal{U}_P(E)$ must exist, since it contains at least one point, $\vec{\chi}_c$.

We make the above more explicit, by way of the problem being considered. We limit this discussion to the Hamburger case, for simplicity.

Let us substitute the moment/missing moment relation in equation (20), into the quadratic form relations in equation (28). We obtain

$$\mathcal{A}(E_R, E_I, J; C)\chi_1 < \mathcal{B}(E_R, E_I, J; C) \tag{40}$$

where

$$\begin{pmatrix} \mathcal{A}(E_R, E_I, J; C) \\ \mathcal{B}(E_R, E_I, J; C) \end{pmatrix} = \begin{pmatrix} -\sum_{j_1=0}^{J} \sum_{j_2=0}^{J} C_{j_1} \hat{N}_{j_1+j_2,1}(E_R, E_I) C_{j_2} \\ \sum_{j_1=0}^{J} \sum_{j_2=0}^{J} C_{j_1} \hat{N}_{j_1+j_2,0}(E_R, E_I) C_{j_2} \end{pmatrix}. \tag{41}$$

We are always working within the normalization domain, $\chi_1 \in (0, 1)$, which is our starting polytope.

The EMM procedure is inductive. Given a polytope, $\mathcal{P}'$, one determines the centre of the largest inscribed interval (or more generally, hypersphere), χ_c. Surprisingly, this is a linear programming problem. At χ_c, which is referred to as a deep interior point (DIP), we define the corresponding Hankel matrix: $\mathcal{M}_{j_1,j_2}(E_R, E_I; \chi_c) = \hat{\mathcal{N}}_0 + \hat{\mathcal{N}}_1 \chi_c$. If this is a positive matrix, then χ_c satisfies the HH inequalities, and $\mathcal{U}_{2J}(E_R, E_I)$ exists (hence the energy $E = (E_R, E_I)$ is physically possible, to order J).

If the Hankel matrix at the DIP point is not positive, it must have at least one nonpositive eigenvector. Any one of these becomes the new $\vec{C}_\kappa$. Clearly, the DIP point violates the HH conditions, since it satisfies $\langle \vec{C}_\kappa | \hat{\mathcal{N}}_0 + \hat{\mathcal{N}}_1 \chi_c | \vec{C}_\kappa \rangle \leqslant 0$. Therefore, if $\mathcal{U}_{2J}(E_R, E_I)$ exists (i.e. the HH missing moment solution set), it must lie within $\mathcal{P}'$, but on the other side of the linear-inequality defined by the DIP point.

We can now update the polytope, and replace it by a new one,

$$\mathcal{P}'' = \mathcal{P}' \bigcap \{\chi_1 | \langle \vec{C}_\kappa | \hat{\mathcal{N}}_0 + \hat{\mathcal{N}}_1 \chi_1 | \vec{C}_\kappa \rangle > 0\}. \tag{42}$$

The entire procedure is repeated, with respect to the updated polytope, $\mathcal{P}''$, until either a null polytope is obtained (i.e. the starting, normalization, polytope has been completely cut up), or a positive Hankel matrix is obtained at some DIP point.

This is the essence of the EMM procedure, which allows us to solve arbitrary, multidimensional, systems.

4. Numerical implementation of EMM

In this section, we numerically implement the previous formalism by applying the EMM formulation to the linearized positivity moment constraints, both in the Stieltjes case, for *PT* invariant solutions ($E_I = 0$) and for *PT* breaking solutions ($E_I \neq 0$). In the following section, we investigate the algebraic structure of both formulation, to very low moment order.

In the following tables, the notation $\mathcal{P}_{\max}$ refers to the maximum moment order used (i.e. $\mu_0, \ldots, \mu_{\mathcal{P}_{\max}}$, in the Hamburger case; $u_0, \ldots, u_{\mathcal{P}_{\max}}$, in the Stieltjes case).

4.1. Energy bounds for PT-invariant solutions ($E_I = 0$)

The Stieltjes formulation presented in the previous section was implemented. Assuming that $E_I = 0$, we generate bounds on the low-lying discrete state energies, for varying a parameter values. This is given in table 1.

The numerical results in table 1 are consistent with the numerical analysis provided by Bender *et al* (2001) which show that at critical a-parameter values, various real eigenvalue curves intersect (i.e. the first two discrete states at $a \approx 3.169\,035$, the next two at $a \approx 7.625\,95$), marking the onset of complex-E discrete state formation.

4.2. Energy bounds for PT-breaking solutions ($E_I \neq 0$)

For PT-breaking solutions, the linear (EMM) Hamburger moment positivity constraints allow us to bound the real and imaginary parts of the energy. In this case, for each discrete energy level, E, the complex conjugate is also a discrete energy level, E^*. In table 2 we only quote the discrete states with $\mathrm{Im}(E) > 0$. We note that for Hamburger moments, $\mathcal{P}_{\max} \approx O(60)$ corresponds to the Stieltjes moment order expansion of $O(30)$. Hence, the results in table 2 are consistent with those of table 1 (in those cases where $\mathcal{P}_{\max} \approx O(60)$ results are provided).

Table 1. EMM analysis of PT-invariant, low-lying bound states, $E_R^{(n)}$, for $V(x) = x^4 + \mathrm{i}ax$.

a	Energy bounds	$\mathcal{P}_{\max}$
0	$1.060\,362\,090\,481\,86 < E_R^{(0)} < 1.060\,362\,090\,491\,33$	30
0	$3.799\,673\,029\,698\,10 < E_R^{(1)} < 3.799\,673\,030\,099\,43$	30
0	$7.455\,697\,936\,462\,36 < E_R^{(2)} < 7.455\,697\,944\,507\,62$	30
0	$11.644\,745\,412\,4944 < E_R^{(3)} < 11.644\,745\,591\,6097$	30
0.5	$1.093\,466\,139\,185\,68 < E_R^{(0)} < 1.093\,466\,139\,196\,01$	30
0.5	$3.803\,502\,880\,280\,26 < E_R^{(1)} < 3.803\,502\,880\,674\,61$	30
0.5	$7.460\,854\,269\,224\,25 < E_R^{(2)} < 7.460\,854\,277\,171\,00$	30
0.5	$11.648\,836\,105\,3757 < E_R^{(3)} < 11.648\,836\,284\,4910$	30
1	$1.194\,489\,941\,696\,22 < E_R^{(0)} < 1.194\,489\,941\,710\,63$	30
1	$3.813\,357\,264\,785\,37 < E_R^{(1)} < 3.813\,357\,265\,215\,82$	30
1	$7.476\,329\,558\,857\,12 < E_R^{(2)} < 7.476\,329\,566\,592\,95$	30
1	$11.661\,074\,380\,6709 < E_R^{(3)} < 11.661\,074\,584\,1871$	30
2	$1.630\,730\,794\,288\,93 < E_R^{(0)} < 1.630\,730\,794\,319\,49$	30
2	$3.821\,467\,528\,136\,36 < E_R^{(1)} < 3.821\,467\,528\,719\,07$	30
2	$7.538\,646\,459\,915\,53 < E_R^{(2)} < 7.538\,646\,470\,408\,70$	30
2	$11.709\,505\,909\,3736 < E_R^{(3)} < 11.709\,506\,231\,6998$	30
3	$2.622\,699\,057\,103\,35 < E_R^{(0)} < 2.622\,699\,057\,278\,84$	30
3	$3.570\,160\,017\,892\,98 < E_R^{(1)} < 3.570\,160\,018\,843\,70$	30
3	$7.647\,030\,402\,008\,32 < E_R^{(2)} < 7.647\,030\,414\,846\,59$	30
3	$11.788\,210\,364\,1407 < E_R^{(3)} < 11.788\,210\,866\,2897$	30
3.1	$2.834\,732\,127\,106\,82 < E_R^{(0)} < 2.834\,732\,127\,402\,29$	30
3.1	$3.448\,205\,084\,363\,44 < E_R^{(1)} < 3.448\,205\,085\,386\,80$	30
3.1	$7.660\,945\,180\,039\,06 < E_R^{(2)} < 7.660\,945\,192\,235\,50$	30
3.1	$11.797\,621\,761\,6381 < E_R^{(3)} < 11.797\,622\,316\,8970$	30
3.15	$3.002\,388\,021\,945\,82 < E_R^{(0)} < 3.002\,388\,022\,697\,77$	30
3.15	$3.326\,652\,891\,277\,98 < E_R^{(1)} < 3.326\,652\,892\,692\,36$	30
3.169 035	$3.172\,130\,272\,514\,38 < E_R^{(0)} < 3.172\,130\,285\,129\,14$	33
3.169 035	$3.174\,647\,781\,263\,65 < E_R^{(1)} < 3.174\,647\,794\,153\,44$	33
4	$7.822\,593\,260\,984\,11 < E_R^{(3)}(*) < 7.822\,593\,282\,240\,12$	30
4	$11.893\,210\,346\,8105 < E_R^{(4)}(*) < 11.893\,211\,245\,7331$	30
7.5	$10.683\,399\,185\,8115 < E_R^{(3)} < 10.683\,403\,717\,9701$	30
7.5	$11.796\,828\,861\,1545 < E_R^{(4)} < 11.796\,842\,150\,4399$	30
7.625 95	$11.322\,538\,125\,0000 < E_R^{(3)} < 11.322\,588\,750\,0000$	32
7.625 95	$11.332\,624\,125\,0000 < E_R^{(4)} < 11.332\,681\,500\,0000$	32

* These are actually the two lowest, real energy, states.

In those cases in table 2 where $\mathcal{P}_{\max} = 30$ results are quoted, we could have worked to higher order, but chose not to, for expediency, since we were more interested in determining the behaviour of the energies near the a-critical points.

Table 2. EMM analysis of PT-breaking, low-lying bound states, for $V(x) = x^4 + \mathrm{i}ax$.

a	Energy bounds	$\mathcal{P}_{\max}$
3.17	$3.173\,839\,992 < E_R^{(0,1)} < 3.173\,839\,997$, $0.036\,578\,872 < \vert E_I^{(0,1)}\vert(*) < 0.036\,578\,881$	60
4.0	$3.608\,235\,46 < E_R^{(0,1)} < 3.608\,235\,51$, $1.201\,260\,46 < \vert E_I^{(0,1)}\vert < 1.201\,260\,58$	50
4.5	$3.905 < E_R^{(0,1)} < 3.913$, $1.628 < \vert E_I^{(0,1)}\vert < 1.632$	30
5.0	$4.234 < E_R^{(0,1)} < 4.239$, $2.051 < \vert E_I^{(0,1)}\vert < 2.056$	30
5.5	$4.576 < E_R^{(0,1)} < 4.583$, $2.486 < \vert E_I^{(0,1)}\vert < 2.490$	30
6.0	$4.929 < E_R^{(0,1)} < 4.937$, $2.937 < \vert E_I^{(0,1)}\vert < 2.942$	30
6.5	$5.284 < E_R^{(0,1)} < 5.298$, $3.405 < \vert E_I^{(0,1)}\vert < 3.412$	30
7.0	$5.654 < E_R^{(0,1)} < 5.664$, $3.890 < \vert E_I^{(0,1)}\vert < 3.896$	30
7.5	$6.016 < E_R^{(0,1)} < 6.032$, $4.389 < \vert E_I^{(0,1)}\vert < 4.396$	30
7.63	$6.113 < E_R^{(0,1)} < 6.128$, $4.520 < \vert E_I^{(0,1)}\vert < 4.529$	30
7.63	$11.330\,45 < E_R^{(2,3)} < 11.330\,48$, $0.100\,9904 < \vert E_I^{(2,3)}\vert < 0.101\,0948$	60

* If $E_I \neq 0$, the discrete energy levels come in conjugate pairs.

5. Algebraic implementation of EMM

In light of the low missing moment order (i.e. $m_s = 1$) for the complex quartic potential under consideration, we are interested in an algebraic analysis of the previous positivity constraints, to very low moment order, so as to extract algebraic relations for the energy and missing moment.

In both cases, PT-invariant (Stieltjes moments) and PT-breaking (Hamburger moments), we will first make use of the low dimension HH, nonlinear inequality constraints. Direct use of the EMM procedure does not appear to facilitate this type of analysis, although one would think that a better understanding of the optimal $\vec{C}_\kappa$, within the EMMs *cutting algorithm* procedure, would assist in any algebraic analysis. Instead, it is the restricted convexity properties of successive HH determinant ratios (equations (32) and (39)) that help us to improve upon the initial algebraic results.

5.1. Algebraic analysis of HH determinants: PT-invariant solutions, $E_I = 0$

For simplicity, we first investigate the (low order) HH determinantal inequality constraints for the Stieltjes problem corresponding to (assumed) real eigenenergies, $E_I = 0$, for which the nonnegative configuration, $S(x)$, is symmetric. The corresponding HH determinants are given in equation (36). Upon substituting the moment/missing moment relation in equation (26), the $\Delta_{\sigma,n}$ determinant becomes a polynomial in $\chi \equiv u_0$, of degree $n+1$:

$$\Delta_{\sigma,n}(u(E,\chi)) \equiv \mathcal{P}_E^{(\sigma,n)}(\chi) = \sum_{\eta=0}^{n+1} \Omega_\eta^{(\sigma,n)}(E)\chi^\eta. \tag{43}$$

Note that contrary to the EMM formalism previously presented, we will regard the zeroth-order moment as the unconstrained variable, after imposing the normalization condition $u_0 + u_1 = 1$. That is, $u_0 \equiv \chi$ and $u_1 = 1 - \chi$.

In principle, for given $E = (E_R, 0)$, we want to determine the zeros of these HH polynomials, defined through the notation:

$$\mathcal{P}_E^{(\sigma,n)}\big(\chi_{o;\eta}^{(\sigma,n)}\big) \equiv 0. \tag{44}$$

We recall that energy bounds are generated by determining those E admitting (convex) missing moment solution sets, $\mathcal{U}_N(E)$, to all HH inequalities generated from the first $N+1$ Stieltjes moments.

5.1.1. Lower bound for E_R, if $E_I = 0$. The positivity of E_R, for PT-invariant solutions, follows from the structure of the HH (Stieltjes) constraints for $\Delta_{0,0} = u_0 = \chi > 0$ and $\Delta_{0,1} = u_0 u_2 - u_1^2 > 0$ (i.e. $u_2 > \frac{u_1^2}{u_0}$). Specifically, from equation (24) for $p = 0$, it follows that $u_2 = \frac{3E_R u_0}{9+a^2}$. Utilizing the previous two HH inequalities we obtain (i.e. $0 < \chi < 1$):

$$E_R > \left(\frac{9+a^2}{3}\right)\left(\frac{1}{\chi} - 1\right)^2 > 0 \qquad \text{if} \quad E_I = 0. \tag{45}$$

2×2 *HH constraints.* The one-dimensional HH constraints are trivially nonnegative within the unit interval, normalization domain for the (effective) missing moment, $0 < \chi < 1$. That is $\mathcal{P}^{(0,0)}(\chi) = \chi > 0$ and $\mathcal{P}^{(1,0)}(\chi) = 1 - \chi > 0$.

The next two higher degree polynomials are the quadratic expressions $\mathcal{P}^{(0,1)}(\chi)$ and $\mathcal{P}^{(1,1)}(\chi)$. The corresponding Ω polynomial coefficients (equation (43)) are readily identified from the following relations:

$$\mathcal{P}^{(0,1)}(\chi) = -1 + 2\chi + \left(\frac{3E_R}{9+a^2} - 1\right)\chi^2 \tag{46}$$

and

$$\mathcal{P}^{(1,1)}(\chi) = \frac{15E_R}{25+a^2} + \left(\frac{\frac{15}{2} - 30E_R}{25+a^2}\right)\chi + \left(\frac{15E_R - \frac{15}{2}}{25+a^2} - \frac{9E_R^2}{(9+a^2)^2}\right)\chi^2. \tag{47}$$

We remind the reader that the objective is to determine those positive E_R values for which the above polynomials in χ become positive on a common subinterval of the χ-unit interval. To this end, we note that the roots take on the form

$$\chi_{o;\eta}^{(0,1)} = \frac{\pm 1}{\sqrt{\frac{3E_R}{9+a^2}} \pm 1} \qquad \text{for} \quad \eta = \pm \tag{48}$$

(note, here the root notation does not imply smaller/larger relation),

$$\chi_{o;\eta}^{(1,1)} = \frac{E_R - \frac{1}{4} \pm \sqrt{\frac{1}{16} + \frac{3}{5}E_R^3 \frac{25+a^2}{(9+a^2)^2}}}{E_R - \frac{1}{2} - \frac{3}{5}E_R^2 \frac{25+a^2}{(9+a^2)^2}} \qquad \text{for} \quad \eta = \pm \tag{49}$$

where, again, $\eta = \pm$ does not imply an algebraic ordering of the roots.

Regardless of the magnitude of the positive ratio $\frac{3E_R}{9+a^2}$, only the $\chi_{o;+}^{(0,1)}$ root in equation (48) will lie within the unit interval. The other root, $\chi_{o;-}^{(0,1)}$, will either be negative, or greater than unity.

Consider the following simple identities for the two quadratic, χ-polynomials:

$$\begin{aligned} \mathcal{P}^{(0,1)}(0) &= -1 \qquad & \mathcal{P}^{(0,1)}(1) &= \frac{3E_R}{9+a^2} \\ \mathcal{P}^{(1,1)}(0) &= \frac{15E_R}{25+a^2} \qquad & \mathcal{P}^{(1,1)}(1) &= -\frac{9E_R^2}{(9+a^2)^2}. \end{aligned} \tag{50}$$

For the physical case $E_R > 0$, it is the $\chi_{o;+}^{(0,1)}$ which satisfies the first two relations for the $\mathcal{P}^{(0,1)}$ polynomial.

Similarly, only one root can satisfy the last two inequalities in equation (50), of differing signature (implicitly assuming $E_R > 0$), for the quadratic polynomial, $\mathcal{P}^{(1,1)}$.

In particular, if $\Omega_2^{(1,1)}(E_R) > 0$ (and the parabola is concaved), then the root in question must be the algebraically smaller one. If $\Omega_2^{(1,1)}(E_R) < 0$ (convexed parabola), then the algebraically larger root lies within the unit interval. It turns out that the root denoted by $\chi_{o;-}^{(1,1)}$, in equation (49), satisfies both cases, as explained below.

The denominator in equation (49) is, up to a positive factor, the $\Omega_2^{(1,1)}(E_R)$ function. When it is positive, the algebraic ordering of the roots corresponds to the $\pm$ notation given in equation (49). When it is negative, then the '$-$' root in equation (49) is actually the larger root, algebraically. Hence, $\chi_{o;-}^{(1,1)}(E_R)$ is always the root lying within the unit interval, for $\mathcal{P}^{(1,1)}(\chi)$, regardless of $\Omega_2^{(1,1)}(E_R)$ signature.

From the previous discussion, only one root contributes to each of the set of relations in equation (50). In order for E_R to be feasible, then the root of $\mathcal{P}^{(0,1)}(\chi)$ defines the left boundary point of the feasible interval $\mathcal{U}_3(E_R) \subset (0, 1)$ (i.e. the HH solution set corresponding to the first four Stieltjese moments, $u_0, \ldots, u_3$); whereas the root of the $\mathcal{P}^{(1,1)}(\chi)$ polynomial defines the right boundary point.

In other words, for E_R to be feasible we must have

$$\chi_{o;-}^{(1,1)}(E_R) - \chi_{o;+}^{(0,1)}(E_R) \geqslant 0. \tag{51}$$

It turns out that this condition holds for all $E_R > 0$; therefore, it does not define any constraints on the real part of the energy (although it does constrain the $u_0 = \chi$ moment). The following analysis pertains to proving that equation (51) holds for all E_R.

The coefficient function $\Omega_2^{(1,1)}(E_R)$ is quadratic with respect to its E_R dependence. Its roots are $E_{R;o,\pm} = \frac{1\pm\sqrt{1-\frac{6}{5}T}}{\frac{6}{5}T}$, where $T = \frac{25+a^2}{(9+a^2)^2}$, and $0 \leqslant T \leqslant \left(\frac{5}{9}\right)^2$. Between these two roots, $\Omega_2^{(1,1)}(E_R)$ is positive.

So long as $E_R > 0$, the root $\chi_{o;-}^{(1,1)}(E_R)$ must always lie within the unit interval. However, the denominator in equation (49) has roots, for positive energy values; consequently, the numerator expression in equation (49) must also have these same roots, otherwise $\chi_{o;-}^{(1,1)}(E_R)$ would become unbounded and violate the relation in equation (51). Indeed, it is easy to check this. Specifically, the zeros of the numerator in equation (49) satisfy $\left(E_R - \frac{1}{4}\right)^2 = \frac{1}{16} + \frac{3}{5}E_R^3 T$, yielding $\left(E_R - \frac{1}{2}\right) = \frac{3}{5}E_R^2 T$, which is the root relation for the zeros of the denominator in equation (49). Furthermore, a simple algebraic analysis reveals that the '$-$' numerator in equation (49) shares both roots, $E_{R;o,\pm}$.

It is for this reason also that equation (51) is satisfied for all $E_R \geqslant 0$. That is, equation (51) explicitly becomes

$$\frac{E_R - \frac{1}{4} - \sqrt{\frac{1}{16} + \frac{3}{5}E_R^3 \frac{25+a^2}{(9+a^2)^2}}}{E_R - \frac{1}{2} - \frac{3}{5}E_R^2 \frac{25+a^2}{(9+a^2)^2}} - \frac{1}{\sqrt{\frac{3E_R}{9+a^2}} + 1} \geqslant 0 \tag{52}$$

and is valid for arbitrary, real a, and $E_R \geqslant 0$. To see this, simply note that if we rewrite the first term (i.e. $\chi_{o;-}^{(1,1)}$) as $\frac{N(E_R)}{D(E_R)}$, this ratio becomes $\frac{D(E_R)+S(E_R)}{D(E_R)} = 1 + \frac{S(E_R)}{D(E_R)}$, where $S(E_R) \equiv N(E_R) - D(E_R)$. However, $S(E_R)$ must also have the same roots as $D(E_R)$ (i.e. for $E_R \geqslant 0$, since $N(E_R)$ has the same roots as the denominator), and $\lim_{E_R\to+\infty} \frac{S(E_R)}{D(E_R)} = 0^+$; hence the ratio $\frac{S(E_R)}{D(E_R)} \geqslant 0$, for $E_R \geqslant 0$. Since $1 - \chi_{o:+}^{(1,0)}(E_R) \geqslant 0$, we confirm equation (52).

For completeness, even though equation (52) does not serve to define any bounds on $E_R > 0$, it does define bounds on the Stieltjes zeroth-order moment ($\chi = u_0 \equiv \mu_0$), which in turn are essential in implementing EMM at the next higher Stieltjes moment order:

Bounds on u_0 stieltjes moment

$$\chi_{o;+}^{(0,1)}(E_R) < u_0 < \chi_{o;-}^{(1,1)}(E_R) \qquad \text{for} \quad E_I = 0 \tag{53}$$

or

$$\mathcal{U}_3(E_R) \equiv \left(\chi_{o;+}^{(0,1)}(E_R), \chi_{o;-}^{(1,1)}(E_R)\right) \tag{54}$$

where the bounds become zero both at $E_R = 0$ and $E_R = +\infty$. Thus, the allowed range for χ, for given E_R, becomes severely restricted both near the origin, and as E_R goes to positive infinity.

3×3 *HH constraints.* The analysis in the previous subsection was not simple, despite the low dimension nature of the underlying Hankel matrices. At the next level of difficulty, we should consider the 3×3 Stieltjes Hankel matrices, utilizing the results derived for the 2×2 case. We find that a direct HH determinantal analysis is extremely difficult, even for this 1-missing moment problem.

One simplification is to exploit the restricted convexity properties of successive HH determinant ratios, as defined in equation (39). In the present Stieltjes case, we must consider two families of missing moment feasibility domains. That is, the determinants $\{\Delta_{0,0}(E_R, \chi), \Delta_{0,1}(E_R, \chi), \Delta_{0,2}(E_R, \chi)\}$ and $\{\Delta_{1,0}(E_R, \chi), \Delta_{1,1}(E_R, \chi), \Delta_{1,2}(E_R, \chi)\}$, formed from the first six Stieltjes moments $\{\chi = u_0, u_1 = 1 - \chi, u_2, \ldots, u_5\}$, must be considered separately.

Thus, the HH-ratio function $\tilde{D}_{0,1}(E_R, \chi)$ is convex on the interval $\mathcal{S}_{0,0} = (0, 1)$ (i.e. due to the positivity of $\Delta_{0,0}(\chi) = \chi > 0$), for any E_R. Since we know that $\Delta_{0,1}(E_R, \chi) > 0$ on the interval $\mathcal{S}_{0,1}(E_R) = \left(\chi_{o;+}^{(0,1)}(E_R), 1\right)$, the function $\tilde{D}_{0,2}(E_R, \chi)$ must be convex on this interval as well. Again, as previously stated, convexity does not preclude $\tilde{D}_{0,2}(E_R, \chi)$ from being completely negative on the interval $\mathcal{S}_{0,1}$, for appropriate (unfeasible) E_R values.

Since $\tilde{D}_{0,2}(E_R, \chi) = \frac{\Delta_{0,2}(E_R,\chi)}{\Delta_{0,1}(E_R,\chi)}$, and the denominator has a zero at the left endpoint of the interval $\mathcal{S}_{0,1}(E_R)$, from the convexity property on this interval, we must have

$$\lim_{\chi \to \chi_{o;+}^{(0,1)}(E_R)+0^+} \tilde{D}_{0,2}(E_R, \chi) = -\infty. \tag{55}$$

With respect to the other class of HH-ratio functions, $\tilde{D}_{1,1}(E_R, \chi)$ is convex on the interval $\mathcal{S}_{1,0} = (0, 1)$ (i.e. $\Delta_{1,0}(\chi) = 1 - \chi > 0$), for any E_R. Since we know that $\Delta_{1,1}(E_R, \chi) > 0$, on the interval $\mathcal{S}_{1,1}(E_R) = \left(0, \chi_{o;-}^{(1,1)}(E_R)\right)$, the function $\tilde{D}_{1,2}(E_R, \chi)$ must be convex on this interval as well.

We also note that since $\tilde{D}_{1,2}(E_R, \chi) = \frac{\Delta_{1,2}(E_R,\chi)}{\Delta_{1,1}(E_R,\chi)}$, and the denominator has a zero at the right endpoint of the interval $\mathcal{S}_{1,1}(E_R)$, from the convexity property on this interval, we must have

$$\lim_{\chi \to \chi_{o;-}^{(1,1)}(E_R)-0^+} \tilde{D}_{1,2}(E_R, \chi) = -\infty. \tag{56}$$

Based on these properties, an alternate strategy for investigating the consequences of the 3×3 HH constraints is to determine those E_R values where either of the convex functions, $\tilde{D}_{0,2}(E_R, \chi)$ or $\tilde{D}_{1,2}(E_R, \chi)$, becomes negative on the common interval, $\mathcal{S}_{0,1}(E_R) \bigcap \mathcal{S}_{1,1}(E_R) = \left(\chi_{o;+}^{(0,1)}, \chi_{o;-}^{(1,1)}\right) = \mathcal{U}_3(E_R)$.

Because of the convexity property for each $\tilde{D}_{\sigma,2}(E_R, \chi)$, over the set $\mathcal{U}_3(E_R)$, we have the following. Given any finite number of points within the set $\mathcal{U}_3(E_R)$, $\{\chi_l | 1 \leqslant l \leqslant L\}$, the tangent lines (functions) to either one of the convex functions,

$$T_l^{(\sigma)}(E_R, \chi) \equiv \tilde{D}_{\sigma,2}(E_R, \chi_l) + (\chi - \chi_l)(\partial_\chi \tilde{D}_{\sigma,2}(E_R, \chi_l)) \tag{57}$$

will form a spline-type envelope,

$$\mathcal{T}^{(\sigma)}(E_R, \chi) \equiv \mathrm{Min}\left\{T_l^{(\sigma)}(E_R, \chi) | 1 \leqslant l \leqslant L\right\} \tag{58}$$

that bounds, from above, that convex function:

$$\tilde{D}_{\sigma,2}(E_R, \chi) \leqslant \mathcal{T}^{(\sigma)}(E_R, \chi) \tag{59}$$

for all $\chi \in \mathcal{U}_3(E_R)$.

If at a particular E_R value, one of the convex functions is completely negative over the domain $\mathcal{U}_3(E_R)$ (i.e. $\mathrm{Max}\{\tilde{D}_{\sigma,2}(E_R, \chi) | \chi \in \mathcal{U}_3(E_R)\} < 0$), the challenge is to find a finite number of points such that the corresponding spline envelope has a negative maximum; thus confirming that E_R is indeed infeasible.

Since the feasibility interval is $\mathcal{U}_3(E_R)$, and we have already established that each of the two convex functions is negatively singular at the corresponding endpoint of the $\mathcal{U}_3(E_R)$-interval, the simplest 'tangent-line' strategy is to determine the tangent line at the endpoint where $\tilde{D}_{\sigma,2}(E_R, \chi)$ is not singular. It may happen that this one tangent line, over the feasibility interval, remains completely negative; thereby establishing that the corresponding E_R is infeasible (and thus unphysical). We refer to this as the '1-tangent line strategy'.

This type of analysis can be implemented algebraically, although the formulae are too complicated to communicate in this work. Even then, one must numerically evaluate these formulae, since their algebraic structure provides no useful, algebraic, insight.

From the full EMM analysis, using the first six Stieltjes moments, for the PT-invariant case ($E_I = 0$), we find the spectral bounds (for the $a = 1$ case):

$$E_R \in (0.855, 1.470) \bigcup (1.725, \infty). \tag{60}$$

The first interval defines the lower and upper bounds for the ground state energy, as given in table 1 (i.e. $E_R^{(0)} = 1.194\,489\,9417$).

We had hoped that our '1-tangent line' approach would produce an algebraic formula verifying (approximately) this exact numerical relation. Instead, the numerical analysis of the '1-tangent line' approach yielded the lower bound $E_R > 0.614\,94$.

We now focus on an alternative analysis based on the HH determinant ratios, also exploiting convexity, but focusing on the more general case where the solution is not necessarily PT invariant.

5.2. *Algebraic relations for the PT-breaking case*

We now consider the HH determinant inequalities for the Hamburger problem corresponding to the PT-symmetry breaking solutions, with $E_I \neq 0$. We will only be able to work with Hankel moment matrices of dimension no greater than three.

Utilizing the Hamburger moment relations in equations (12) and (14), we find that the relevant HH determinants become

$$\Delta_{(0,0)}(\chi) = \chi \qquad \Delta_{(0,1)}(\chi) = \left(1 + \left(\frac{E_I}{a}\right)^2\right) \chi \left(\chi_0^{(0,1)}(a, E_I) - \chi\right) \tag{61}$$

where $\mu_0 \equiv \chi$, $\mu_1 = \frac{E_I}{a}\chi$, $\mu_2 = 1 - \chi$ and $\chi_0^{(0,1)}$ is the nontrivial zero of $\Delta_{(0,1)}(\chi)$, specified below. The required normalization condition insures that $0 < \mu_0, \mu_2 < 1$. We note that for given a and arbitrary E_R, E_I values, the first two HH determinants become positive on the interval

$$0 < \chi < \chi_o^{(0,1)}(a, E_I) \equiv \frac{a^2}{a^2 + E_I^2} \leqslant 1. \tag{62}$$

The $\Delta_{(0,2)}$ HH determinant (involving a 3×3 HH matrix) is too complicated to write down explicitly. However, it has several important properties. The first of these is that it is negative at either endpoint of the above interval:

$$\Delta_{(0,2)}(0) = -1 \qquad \Delta_{(0,2)}\big(\chi_o^{(0,1)}\big) = -\frac{16E_I^6}{(4+a^2)^2\big(a^2+E_I^2\big)^3}. \tag{63}$$

Accordingly, the ratio $D_{(0,2)}(\chi) \equiv \frac{\Delta_{(0,2)}(\chi)}{\Delta_{(0,1)}(\chi)}$ is a convex function, when restricted to the interval $\big(0, \chi_o^{(0,1)}\big)$. Furthermore, it is negatively singular at both endpoints. Because of this, we cannot implement the simplified tangent line strategy considered in the previous Stieltjes case.

Another important property is that the E_R dependence of $\Delta_{(0,2)}(\chi)$ is linear:

$$\Delta_{(0,2)}(a, E_R, E_I; \chi) = \Upsilon_{a,E_I}(\chi) + E_R \frac{3\chi}{9+a^2} \Delta_{(0,1)}(a, E_I; \chi). \tag{64}$$

Because of this, the convex function, $D_{(0,2)}(\chi) = \frac{\Upsilon_{a,E_I}(\chi)}{\Delta_{(0,1)}(\chi)} + E_R \frac{3\chi}{9+a^2}$, over the interval $\big(0, \chi_o^{(0,1)}(a, E_I)\big)$, will have the following property. If for a given E_I value, the maximum of the function, $\frac{\Upsilon_{a,E_I}(\chi)}{\Delta_{(0,1)}(\chi)}$ is negative, over the specified interval, then $E_R < 0$ is infeasible (to the HH order under consideration).

Alternatively, from the partial fraction theorem, recognizing that the numerator of $D^{(0,2)}(\chi)$ is a cubic polynomial, whereas the denominator is quadratic, we obtain the decomposition

$$D^{(0,2)}(\chi) = \Lambda_1 \chi + \Lambda_0 - \frac{A}{\chi} - \frac{B}{\chi_o^{(0,1)} - \chi} \tag{65}$$

where the various coefficients are dependent on a and E_R, E_I. Also, $A > 0$ and $B > 0$, in accordance with the negative singular nature of the convex function. More explicitly

$$A = 1 \qquad B = \frac{16E_I^6}{(4+a^2)^2\big(a^2+{E_I}^2\big)^3} \tag{66}$$

$$\Lambda_0(a, E_I) = \frac{2\begin{pmatrix} a^{10} + 60E_I^6 + a^8\big(17+3E_I^2\big) + a^6\big(88+33E_I^2+3E_I^4\big) \\ +a^2\big(216E_I^2+192E_I^4-E_I^6\big) + a^4\big(144+228E_I^2+15E_I^4+E_I^6\big) \end{pmatrix}}{(4+a^2)^2(9+a^2)\big(a^2+E_I^2\big)^2} \tag{67}$$

and

$$\Lambda_1(a, E_R, E_I)$$
$$= \frac{\begin{pmatrix} -a^{10} + 8E_I^6\big(-15+2E_I^2\big) - a^8\big(17+4E_I^2\big) - 2a^6\big(44+16E_I^2+3E_I^4\big) \\ -a^2E_I^2\big(144+312E_I^2-34E_I^4+E_I^6\big) - a^4\big(144+280E_I^2-3E_I^4+4E_I^6\big) \\ +E_R\big(3(4+a^2)^2\big(a^2+E_I^2\big)^2\big) \end{pmatrix}}{(4+a^2)^2(9+a^2)\big(a^2+E_I^2\big)^2} \tag{68}$$

where the E_R dependence is linear, and symbolized through the following implicit relation involving E_I dependent coefficients:

$$\Lambda_1(a, E_R, E_I) = \Gamma_0(a, E_I) + \Gamma_1(a, E_I)E_R \tag{69}$$

where $\Gamma_1(a, E_I) > 0$. We also note that $\Lambda_0(a, E_I) \geqslant 0$, which can be easily derived from the numerator expression in equation (67), since the following polynomial subterms define a positive expression: $(60 - a^2 + a^4)E_I^6 > 0$.

In order for E_R, E_I to correspond to a feasible pair of values, to the HH order defined (i.e. HH matrix of dimension no greater than three), we must require that $D_{(0,2)}(\chi)$ be positive on the $\left(0, \chi_o^{(0,1)}\right)$ interval. That is, it must have two roots within this interval. In other words, the cubic polynomial $\Delta_{(0,2)}(\chi)$ must have three real roots, and two of these must lie within the specified interval. Stated differently, the linear part of the partial-fraction decomposition must intersect the convex function defined by the last two terms:

$$\Lambda_1(a, E_R, E_I)\chi_{o;\eta}^{(0,2)} + \Lambda_0(a, E_I) = \frac{A(a, E_R, E_I)}{\chi_{o;\eta}^{(0,2)}} + \frac{B(a, E_R, E_I)}{\chi_o^{(0,1)} - \chi_{o;\eta}^{(0,2)}} \tag{70}$$

where $\chi_{o;\eta}^{(0,2)}$ correspond to the zeros of this relation.

In order for E_R, E_I to correspond to a feasible pair of values, the two roots must exist, and lie within the specified interval:

$$\chi_{o;\eta}^{(0,2)}(a, E_R, E_I) \in \left(0, \chi_o^{(0,1)}\right) \qquad \eta = 1, 2. \tag{71}$$

This relation is algebraically too complicated to yield a simple relation. If $E_I = 0$, one concludes that $E_R > 0$, as demonstrated in the PT-invariant case. However, if $E_I \neq 0$, to the present HH order, one cannot conclude that E_R must be positive (to the moment order considered, although from equation (8), we know it must be).

Despite these remarks, there is an alternate way to determine the viable E_R, E_I values. Consider the concaved function $f(\chi) = \frac{A}{\chi} + \frac{B}{\chi_o^{(0,1)} - \chi}$, over the interval $\left(0, \chi_o^{(0,1)}\right)$. It has an absolute minimum over this interval at the point $\chi_{\min} = \frac{\chi_o^{(0,1)}}{1+\sqrt{\frac{B}{A}}}$. The minimum value of the function is $f_{\min} = \frac{A+B+2\sqrt{AB}}{\chi_o^{(0,1)}}$.

The derivative function $f'(\chi)$ maps this interval into the entire real axis, $f'(\chi)$: $\left(0, \chi_o^{(0,1)}\right) \to (-\infty, +\infty)$, in a 1-1 manner. Therefore, there will always be a unique tangent line to the function $f(\chi)$ (at the point $(\chi_\tau, f(\chi_\tau))$) which also passes through the point $(0, \Lambda_0)$. This is given by the equation $f'(\chi_\tau) = -\frac{(\Lambda_0 - f(\chi_\tau))}{\chi_\tau}$. We note that since $f(x)$ and Λ_0 are independent of E_R, so too is $\chi_\tau(a, E_I)$.

Since $\Lambda_0(a, E_I) > 0$, and $f(x)$ is concaved, it follows that

$$0 < \chi_\tau(a, E_I) < \chi_{\min}(a, E_I). \tag{72}$$

We can now state the condition for the existence of suitable roots to equation (70). If

$$\Lambda_1(a, E_R, E_I) \geqslant -\frac{(\Lambda_0(a, E_I) - f(\chi_\tau))}{\chi_\tau(a, E_I)} \tag{73}$$

then the pair of values (E_R, E_I) is feasible, up to the HH order being considered. That is, for arbitrary a, E_I, unless E_R satisfies the relation

$$E_R > -\frac{\Gamma_0(a, E_I)}{\Gamma_1(a, E_I)} - \frac{(\Lambda_0(a, E_I) - f(\chi_\tau(a, E_I)))}{\Gamma_1(a, E_I)\chi_\tau(a, E_I)} \tag{74}$$

the pair E_R, E_I is unphysical. Note that when $E_I = 0$, this relation reproduces the condition $E_R > 0$, since $f(\chi) = \frac{1}{\chi}$, $\Lambda_0 = 2$, $\chi_\tau = 1$, $f(\chi_\tau) = 1$ and $\Lambda_1 = \Gamma_0 + \Gamma_1 E_R = -1 + \frac{3E_R}{9+a^2}$.

An alternate interpretation of the above lower bound for E_R is that for given a, E_I values, x_τ is the common zero shared by both the convex function, $\mathcal{D}^{(0,2)}_{a,E_{R,*},E_I}(\chi)$, and its derivative, $\partial_\chi \mathcal{D}^{(0,2)}_{a,E_{R,*},E_I}(\chi)$.

If (E_R, E_I) is physically possible, up to the current HH order, then so too is $(E_R, -E_I)$. Limiting $E_I \geqslant 0$, we are interested in those a, E_I regions, where the lower bound to E_R is nonnegative.

In general, it is not readily apparent how to simplify, algebraically, equation (74). Numerical experimentation, for the above relations, suggests that $E_R > 0$ for most values of a and E_I (which is consistent with equation (8)).

For the case of very small parameter values, $a \ll 1$, and working with the rescaled quantity $\epsilon \equiv \frac{E_I}{a}$, one can obtain some approximate results that sustain the general indications ensuing from numerical experimentation. Specifically, we obtain the following relations:

$$\Lambda_0(a,\epsilon) = \frac{2+3\epsilon^2}{(1+\epsilon^2)^2} + O(a^2) \tag{75}$$

$$\Gamma_j(a,\epsilon) = \begin{cases} -\frac{1}{1+\epsilon^2} + O(a^2) & j = 0 \\ \frac{1}{3} + O(a^2) & j = 1 \end{cases} \tag{76}$$

$$\chi_o^{(0,1)}(a,\epsilon) = \frac{1}{1+\epsilon^2} \tag{77}$$

$$A = 1 \qquad B = \frac{\epsilon^6}{(1+\epsilon^2)^3} \tag{78}$$

$$\chi_\tau(a,\epsilon) = \frac{2}{2+3\epsilon^2} + O(a^2) \tag{79}$$

$$\chi_\tau = \frac{2}{2+3\epsilon^2} \qquad f(\chi_\tau) = \frac{(2+3\epsilon^2)(1+2\epsilon^2+3\epsilon^4)}{2(1+\epsilon^2)^2} \tag{80}$$

which allow us to conclude

$$E_R > \frac{81}{4}\left(\frac{E_I}{a}\right)^4 + O(a^2). \tag{81}$$

For larger a values (i.e. $a > O(2)$), numerical experiments suggest that $E_R > \frac{81}{4}\left(\frac{E_I^4}{a^5}\right)$.

6. Conclusion

We have extended the moment problem quantization analysis to the non-Hermitian quartic potential studied by Bender *et al* (2001). We are able to obtain tight, converging lower and upper bounds to the real and imaginary parts of the discrete state spectrum (for the first four, low-lying, states). We also show how the formalism can be used to derive algebraic relations for the discrete state spectral values. This could only be implemented to low order, because of the underlying algebraic complexity. Nevertheless, our limited algebraic results provide useful information about the nature of the (complex) spectral values. A particular form of this, for very small Hamiltonian parameter values, is given in equation (81). Our methods are extendable to other discrete states, as well as other non-Hermitian systems, regardless of whether or not the bound states exist on the real axis, or off of it.

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