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Extension of a spectral bounding method to the PT-invariant states of the $-(\mathrm{i}X)^N$ non-Hermitian potential

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Abstract

The eigenvalue moment method (EMM) developed by Handy (*J. Phys. A: Math. Gen.* 2001 **34** L271, 5065), Handy *et al* (*J. Phys. A: Math. Gen.* 2001 **34** 5593), and Handy and Xiao-Qian Wang (*J. Phys. A: Math. Gen.* 2001 **34** 8297), which generates converging lower and upper bounds to the (complex) discrete state energies, is extended to the case of discrete states with non-Real support. In particular, Bender and Boettcher (*Phys. Rev. Lett.* 1998 **80** 5243) have argued on the reality of the discrete state spectrum for the $-(\mathrm{i}X)^N$ potential. For N (*integer*) $\geqslant 4$, such PT-invariant solutions can only exist on appropriate complex contours. We develop and apply the necessary EMM formalism to such cases. In particular, the restriction of EMM to the *anti-Stokes* angles significantly increases the convergence rate of the bounds.

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1. Introduction

There has been much interest recently in understanding the spectral properties of certain manifestly PT-invariant Schrödinger Hamiltonians with the generic potential structure: $V(x) = \mathcal{P}(\mathrm{i}x)$, where $\mathcal{P}$ is an arbitrary polynomial with real coefficients. In particular, Bender and Boettcher [1] argued, based on a conjecture by Bessis, that the discrete states (within the complex-x plane, $\mathcal{C}_x$) of the potential $-(\mathrm{i}x)^N$ must be real. This conjecture has been affirmed by Dorey *et al* [2, 3]. However, Delabaere and Trinh (2000) cautioned that manifest PT invariance of the Hamiltonian does not preclude the existence of symmetry-breaking discrete state solutions, with (necessarily) complex eigenenergies. Using asymptotic analysis methods, they studied the spectral properties of the potential $-(\mathrm{i}x)^3 + \mathrm{i}ax$ and found that for particular a-parameter regimes, there could exist PT-symmetry breaking solutions. This was also verified by Handy [4, 5], and Handy *et al* [6], through the generation of converging lower and upper bounds to the various real/complex eigenenergies. Subsequent studies by Bender *et al* [7] confirmed a similar behaviour for the potential $(\mathrm{i}x)^4 + \mathrm{i}ax$.

As noted, an important theoretical and numerical confirmation of most of these results has resulted from the spectral bounding methods of Handy, Bessis and co-workers [8, 9], referred to as the *eigenvalue moment method* (EMM). Provided the Schrödinger Hamiltonian can be transformed into a suitable non-negative representation for the desired solution, application of EMM will result in the generation of converging bounds to the corresponding (complex) eigenenergy.

In very recent work, Handy [4, 5], and Handy and Wang [10] showed that the one-dimensional Schrödinger equation, for arbitrary potential, and on any contour in the complex-x plane ($\xi \in \Re \to x(\xi) \in \mathcal{C}$), can be transformed into an equivalent, fourth-order, linear differential equation for the probability density, $S(\xi) \equiv |\Psi(x(\xi))|^2$. Restricting this to the case of rational fraction potentials, it then follows that the power moments of the bound state solution, $\mu(p) \equiv \int \mathrm{d}\xi\, \xi^p S(\xi)$, will satisfy a linear, recursive, *moment equation*.

The energy variable is a parameter in the *moment equation*. Since they are moments of a non-negative measure, one can constrain them to satisfy the necessary *moment problem* theorems [11], which in turn constrain the eigenenergy through converging lower and upper bounds (for both the real and imaginary parts of the energy). The same philosophy can be used in quantum scattering for bounding Regge poles [12].

The EMM procedure has been demonstrated to work for the complex, symmetry breaking, solutions of the $-(\mathrm{i}x)^3 + \mathrm{i}ax$ potential [5, 6]. However, in this case the bound states exist along the real axis. In their seminal work, Bender and Boettcher [1] discovered the existence of PT-invariant solutions for the $-(\mathrm{i}X)^N$ potential lying within certain wedges in the complex plane, $\mathcal{C}_x$, which do not include the real axis for (integer) $N \geqslant 4$.

Taking $x \equiv |x|\mathrm{e}^{\mathrm{i}\theta}$, the wedges within which the bound states lie are defined by

$$\theta_{L,R} - \frac{\tilde{\Delta}}{2} < \theta < \theta_{L,R} + \frac{\tilde{\Delta}}{2} \tag{1}$$

where

$$\theta_{L,R} = \begin{cases} -\pi + \frac{N-2}{N+2}\frac{\pi}{2} & \text{`L (left)'} \\ -\frac{N-2}{N+2}\frac{\pi}{2} & \text{`R (right)'} \end{cases} \tag{2}$$

and

$$\tilde{\Delta} = \frac{2\pi}{N+2}. \tag{3}$$

In this work we examine the efficiency of the EMM procedure for $N \geqslant 4$. The present analysis is important for several reasons. The first is to confirm the versatility of the EMM procedure. The second is to prepare for a more comprehensive analysis of other PT-symmetry breaking Hamiltonians corresponding to the $-(\mathrm{i}x)^N + \mathrm{i}ax$ potentials.

Our EMM analysis will involve a contour made up of the two semi-infinite rays lying within the left and right wedges, as represented by

$$\{x \mid \text{EMM complex contour}\} = \{\xi \mathrm{e}^{-\mathrm{i}\theta} \mid \xi : \infty \to 0\} \cup \{\xi \mathrm{e}^{+\mathrm{i}\theta} \mid \xi : 0 \to \infty\} \tag{4}$$

for any θ within the 'right'-handed wedge, as defined earlier.

We define moments along each of the two parts of the contour. Not surprisingly, we find that the order of the necessary moment equations reduces significantly for $\theta = \theta_R$, corresponding to the *anti-Stokes* line, along which the wavefunction decays most rapidly. Consequently, the EMM bounds converge fastest when $\theta = \theta_R$.

In the following sections we discuss in detail the necessary relations for the $N = 4$ case, and then the general theory for arbitrary N. We find that the moment equation structure for the $N =$ *even* and $N =$ *odd* is very different.

2. The $-(\mathrm{i}X)^4$ potential

2.1. The nonnegativity quantization representation

We will adopt the formalism developed by Handy and Wang [10]. Consider the Schrödinger equation

$$-\partial_x^2\Psi(x) + \mathcal{V}(x)\Psi(x) = E\Psi(x) \tag{5}$$

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:

$$x(\xi)\colon \xi \in \Re \to \mathcal{C}. \tag{6}$$

The transformed Schrödinger equation is

$$-(D(\xi)\partial_\xi)^2\Psi(\xi) + V(\xi)\Psi(\xi) = E\Psi(\xi) \tag{7}$$

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

$$A(\xi)\partial_\xi^2\Psi(\xi) + B(\xi)\partial_\xi\Psi(\xi) + C(\xi)\Psi(\xi) = 0 \tag{8}$$

where $A(\xi) \equiv -(D(\xi))^2$, $B(\xi) = -\frac{1}{2}\partial_\xi(D(\xi))^2$ and $C(\xi) = V(\xi) - E$.

We define

$$S(\xi) = \Psi^*(\xi)\Psi(\xi) \tag{9}$$

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

$$J(\xi) = \frac{\Psi(\xi)\partial_\xi\Psi^*(\xi) - \Psi^*(\xi)\partial_\xi\Psi(\xi)}{2i} \tag{11}$$

and

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

One can then transform the Schrödinger equation into four coupled differential equations for the preceding configurations (i.e. $A = A_R + \mathrm{i}A_I$, etc):

$$(S''(\xi) - 2P(\xi))A_R(\xi) + S'(\xi)B_R(\xi) + 2S(\xi)C_R(\xi) + 2(B_I(\xi) + A_I(\xi)\partial_\xi)J(\xi) = 0 \tag{13}$$

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

$$P'(\xi)A_R(\xi) + 2T(\xi)A_I(\xi) + 2P(\xi)B_R(\xi) + S'(\xi)C_R(\xi) - 2J(\xi)C_I(\xi) = 0 \tag{15}$$

and

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

Usually $A_I = 0$ and the last equation simply serves to define T. In such cases, only the first three equations are really coupled to each other. One can reduce these to one fourth-order linear differential equation for S; however, it is preferable to explicitly work with them, as given above, since in some cases they lead to additional moment constraints not readily discernable by working solely with S.

Clearly, S and P are non-negative configurations which must be bounded (i.e. L^1, since Ψ is L^2) for physical solutions. Accordingly, we refer to the above as the non-negativity quantization representation (NQR).

One can easily find a contour map that maps into the required wedges, as defined previously. Thus, $x(\xi) = \mathrm{e}^{\mathrm{i}\theta}\xi - \frac{\mathrm{e}^{-\mathrm{i}\theta}}{\xi}$, for ξ: $0 \to \infty$, will map from the left wedge into the right wedge (for an appropriate, fixed, θ value). However, this choice leads to large order polynomials in the above formulation, complicating the EMM analysis.

Alternatively, we can work with the two contour maps $x_{R,L} = \xi\, e^{\pm i\theta}$, $\xi \geqslant 0$, and for each of these generate the corresponding $\{S, P, J\}$ configurations. These configurations must then be matched at the origin. This approach leads to simpler algebraic relations, and is the one adopted throughout this work.

2.2. Obtaining the moment equations for $-(ix)^4$ within the NQR formulation

Consistent with the works of Bender and Boettcher [1] and Dorey *et al* [2, 3], we will assume that the discrete state of the $-(ix)^4$ Schrödinger equation have real eigenenergy. The corresponding differential equation is $-\Psi'' - x^4\Psi = E\Psi$. Its extension into the complex plane will be denoted as

$$-\Psi''(z) - z^4\Psi(z) = E\Psi(z) \tag{17}$$

where $z = |z|e^{i\theta} = \xi e^{i\theta}$, $|z| = \xi \geqslant 0$.

Within the right wedge the Schrödinger equation becomes

$$\Psi_R''(\xi) + \xi^4\, e^{6i\theta}\Psi_R(\xi) + E\, e^{2i\theta}\Psi_R = 0. \tag{18}$$

Similarly, within the left wedge, $z = \xi e^{-i(\pi+\theta)} = -\xi e^{-i\theta}$, the corresponding differential equation becomes

$$\Psi_L''(\xi) + \xi^4\, e^{-6i\theta}\Psi_L(\xi) + E\, e^{-2i\theta}\Psi_L(\xi) = 0. \tag{19}$$

Upon comparing with equation (8), we identify the coefficient functions as $A = 1, B = 0$, $C(\xi) = \xi^4\, e^{\pm 6i\theta} + E\, e^{\pm 2i\theta}$. Note that we do not explicitly denote the 'right-left' coefficient function $C(\xi)$, since the notation 'C_R' will be used to refer to the *real* part of the function. Thus $C(\xi) = C_R(\xi) + iC_I(\xi)$, where

$$C_R(\xi) = \xi^4 C_6 + EC_2 \tag{20}$$

and

$$C_I(\xi) = \pm\xi^4 S_6 \pm ES_2 \tag{21}$$

involving $C_n = \cos(n\theta)$ and $S_n = \sin(n\theta)$. The $\pm$ refers to the relevant expression for the R (right) and L (left) wedges, respectively.

The corresponding NQR equations become

$$S''(\xi) - 2P(\xi) + 2(\xi^4 C_6 + EC_2)S(\xi) = 0 \tag{22}$$

$$\left(\pm\xi^4 S_6 \pm ES_2\right) S(\xi) - J'(\xi) = 0 \tag{23}$$

and

$$P'(\xi) + \left(\xi^4 C_6 + EC_2\right) S'(\xi) - 2\left(\pm\xi^4 S_6 \pm ES_2\right) J(\xi) = 0. \tag{24}$$

Again, the distinction between the right and left NQR configurations is implicitly assumed.

We define the power moments for the $\{S, P, J\}$ configurations:

$$U(p) = \int_0^\infty d\xi\, S(\xi)\xi^p \tag{25}$$

$$V(p) = \int_0^\infty d\xi\, P(\xi)\xi^p \tag{26}$$

$$W(p) = \int_0^\infty d\xi\, J(\xi)\xi^p. \tag{27}$$

We multiply each of the relations in equations (22)–(24) by ξ^p and integrate over [0, ∞), making use of the integration-by-parts formulae:

$$\int_0^\infty \mathrm{d}\xi\ S''(\xi)\xi^p = -\delta_{p,0}S'(0) + \delta_{p,1}S(0) + p(p-1)U(p-2) \tag{28}$$

$$\int_0^\infty \mathrm{d}\xi\ P'(\xi)\xi^p = -\delta_{p,0}P(0) - pV(p-1) \tag{29}$$

$$\int_0^\infty \mathrm{d}\xi\ J'(\xi)\xi^p = -\delta_{p,0}J(0) - pW(p-1). \tag{30}$$

The required $\{U, V, W\}$ moment equations for $p \geqslant 0$ are

$$-\delta_{p,0}S'(0) + \delta_{p,1}S(0) + p(p-1)U(p-2) - 2V(p) + 2[C_6U(p+4) + EC_2U(p)] = 0 \tag{31}$$

$$S_6U(p+4) + ES_2U(p) \pm [\delta_{p,0}J(0) + pW(p-1)] = 0 \tag{32}$$

$$-\delta_{p,0}P(0) - pV(p-1) - C_6(p+4)U(p+3) - EC_2[\delta_{p,0}S(0) + pU(p-1)] - 2[\pm S_6W(p+4) \pm S_2W(p)] = 0. \tag{33}$$

Again, implicit reference to the R (right) and L (left) wedges is assumed (i.e. $S'_{R,L}(0)$, $U_{R,L}(p)$, etc).

With respect to equation (32), it generates two different relations. For $p = 0$ it becomes

$$S_6U(4) + ES_2U(0) = \mp J(0). \tag{34}$$

This defines a constraint on the U-moments. For $p \geqslant 1$ in equation (32) the W-moments are generated from the U-moments (i.e. take $p \to p+1$ in equation (32)):

$$W(p) = \mp\left(\frac{S_6U(p+5) + ES_2U(p+1)}{p+1}\right) \qquad p \geqslant 0. \tag{35}$$

Since equation (31) serves to generate the V-moments in terms of the U-moments, we can couple this with the previous relation and convert equation (33) into one moment equation for the U-moments. Thus we get

$$-S(0)\delta_{p,2} + \frac{S'(0)}{2}\delta_{p,1} - P(0)\delta_{p,0} - C_2ES(0)\delta_{p,0} + U(p-3)\left[-p + \frac{3p^2}{2} - \frac{p^3}{2}\right] + U(p-1)[-2pC_2E] + U(p+1)\left[\frac{2E^2{S_2}^2}{p+1}\right] + U(p+3)[-4C_6 - 2pC_6] + U(p+5)\left[\frac{2ES_2S_6}{p+1} + \frac{2ES_2S_6}{p+5}\right] + U(p+9)\left[\frac{2{S_6}^2}{p+5}\right] = 0 \tag{36}$$

for $p \geqslant 0$. This relation must be combined with the additional constraint in equation (34).

It is readily apparent that equation (36) separates into two distinct moment recursion relations for the even and odd order moments. The moment equation in equation (36) reduces to an even order moment equation for $p = 2\rho + 1$; whereas it becomes an odd order moment equation for $p = 2\rho$. In turn, the even and odd order U-moments are themselves moments of corresponding Stieltjes measures. Thus, in the first case

$$\mu(\rho) \equiv U(2\rho) = \int_0^\infty \mathrm{d}\xi\ S(\xi)\xi^{2\rho} = \int_0^\infty \mathrm{d}\eta\ \frac{1}{2\sqrt{\eta}}S(\sqrt{\eta})\ \eta^\rho \tag{37}$$

where $\rho \geqslant 0$ and $\eta \equiv \xi^2$. In the second case

$$\omega(\rho) \equiv U(2\rho+1) = \int_0^\infty \mathrm{d}\xi\ S(\xi)\xi^{2\rho+1} = \int_0^\infty \mathrm{d}\eta\ \frac{1}{2}S(\sqrt{\eta})\ \eta^\rho. \tag{38}$$

The respective moment equations become (i.e. $p = 2\rho + 1$, $\rho \geqslant 0$, in equation (36))

$$\frac{S'(0)}{2}\delta_{\rho,0} + \mu(\rho-1)\left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2}\right] + \mu(\rho)[-2C_2E(2\rho+1)]$$
$$+\mu(\rho+1)\left[\frac{E^2{S_2}^2}{\rho+1}\right] + \mu(\rho+2)[-4C_6 - 2C_6(2\rho+1)]$$
$$+\mu(\rho+3)\left[ES_2S_6\left(\frac{1}{\rho+1}+\frac{1}{\rho+3}\right)\right] + \mu(\rho+5)\left[\frac{{S_6}^2}{\rho+3}\right] = 0 \qquad (39)$$

together with equation (34)

$$S_6\mu(2) + ES_2\mu(0) = \mp J(0) \qquad (40)$$

and (i.e. $p = 2\rho$, $\rho \geqslant 0$, in equation (36))

$$-S(0)\delta_{\rho,1} - \delta_{\rho,0}[P(0) + C_2ES(0)] + \omega(\rho-2)\left[-2\rho + \frac{3(2\rho)^2}{2} - \frac{(2\rho)^3}{2}\right]$$
$$+\omega(\rho-1)[-4\rho C_2E] + \omega(\rho)\left[\frac{2E^2{S_2}^2}{2\rho+1}\right] + \omega(\rho+1)[-4C_6 - 4\rho C_6]$$
$$+\omega(\rho+2)[2ES_2S_6]\left[\frac{1}{2\rho+1}+\frac{1}{2\rho+5}\right] + \omega(\rho+4)\left[\frac{2{S_6}^2}{2\rho+5}\right] = 0. \qquad (41)$$

2.3. Relating the boundary terms for the right and left wedges

Since the NQR configurations are generated from the wavefunction, one must carefully define the correlations between the right and left wedge contributions to the respective boundary terms dependent on $\{S_{R,L}(0),\ P_{R,L}(0),\ J_{R,L}(0),\ S'_{R,L}(0)\}$. Of course, $\Psi(z)$ is analytic everywhere.

First, we have the following identities:

$$\Psi_{R,L}(\xi) = \Psi(\pm\xi \mathrm{e}^{\pm \mathrm{i}\theta}). \qquad (42)$$
$$S_{R,L}(\xi) = \Psi_{R,L}(\xi)\Psi^*_{R,L}(\xi) = |\Psi_{R,L}(\xi)|^2. \qquad (43)$$
$$S'_{R,L}(\xi) = \Psi_{R,L}(\xi)\Psi^{*'}_{R,L}(\xi) + \Psi'_{R,L}(\xi)\Psi^*_{R,L}(\xi) = 2\mathrm{Re}(\Psi_{R,L}\Psi'^*_{R,L}). \qquad (44)$$
$$P_{R,L}(\xi) = \Psi'_{R,L}(\xi)\Psi'^*_{R,L}(\xi) = |\Psi'_{R,L}(\xi)|^2. \qquad (45)$$
$$J_{R,L}(\xi) = \frac{\Psi_{R,L}(\xi)\Psi^{*'}_{R,L}(\xi) - \Psi'_{R,L}(\xi)\Psi^*_{R,L}(\xi)}{2i} = \mathrm{Im}(\Psi_{R,L}(\xi)\Psi^{*'}_{R,L}(\xi)). \qquad (46)$$

From the derivative relation

$$\Psi'_{R,L}(\xi) = \Psi'(z)(\pm \mathrm{e}^{\pm \mathrm{i}\theta}) \qquad (47)$$

it follows that

$$\Psi'_{R,L}(0) = (\pm \mathrm{e}^{\pm \mathrm{i}\theta})\Psi'(z)|_{z=0}. \qquad (48)$$

We define $\Psi'(z)|_{z=0} = \Delta$ and $\pm \mathrm{e}^{\pm \mathrm{i}\theta} = \Omega_\pm$.

From Ψ's analyticity we have $\Psi_R(0) = \Psi_L(0)$, therefore

$$S_R(0) = S_L(0). \qquad (49)$$

In addition, $P_{R,L}(0) = |\Psi'_{R,L}(0)|^2 = |\Delta\Omega_\pm|^2$ gives

$$P_R(0) = P_L(0). \qquad (50)$$

We can get S'_R, S'_L from

$$S'_R(0) = \Psi(0)\mathrm{e}^{-\mathrm{i}\theta}\Delta^* + \Psi^*(0)\mathrm{e}^{\mathrm{i}\theta}\Delta = 2C_1\mathrm{Re}(\Psi(0)\Delta^*) + 2S_1\mathrm{Im}(\Psi(0)\Delta^*) \qquad (51)$$

and

$$S'_L(0) = -\Psi(0)e^{i\theta}\Delta^* - \Psi^*(0)e^{-i\theta}\Delta = -2C_1\mathrm{Re}(\Psi(0)\Delta^*) + 2S_1\mathrm{Im}(\Psi(0)\Delta^*). \quad (52)$$

Similarly, for $J_R(0)$ and $J_L(0)$

$$J_R(0) = C_1\mathrm{Im}(\Psi(0)\Delta^*) - S_1\mathrm{Re}(\Psi(0)\Delta^*) \quad (53)$$

$$J_L(0) = -C_1\mathrm{Im}(\Psi(0)\Delta^*) - S_1\mathrm{Re}(\Psi(0)\Delta^*). \quad (54)$$

Thus, as expected, $\Psi(0)$ and $\Psi'(0)$ are the only required boundary conditions (in addition to the specification of θ). If we assume that the bound states are *PT* invariant (which is the case in this work),

$$\Psi^*(-x) = \Psi(x) \quad (55)$$

for $x \in \Re$, then from Ψ's analyticity at the origin we have

$$\Psi(0) \equiv \alpha = \mathrm{Real} \quad (56)$$

and

$$\Psi'(0) = \Delta \equiv i\beta = \mathrm{Imaginary}. \quad (57)$$

Inserting this above we have $S(0) = \alpha^2$, $P(0) = \beta^2$ and

$$S'_{R,L}(0) = -2S_1\alpha\beta \quad (58)$$

$$J_{R,L}(0) = \mp C_1\alpha\beta. \quad (59)$$

In particular, for *PT*-invariant solutions,

$$J_{R,L}(0) = \pm\left(\frac{C_1 S'_{R,L}(0)}{2S_1}\right). \quad (60)$$

2.4. *Recursive structure of the moment equation(s)*

The discussion in this section will implicitly assume that $S_6 \neq 0$ in equation (36), otherwise the order of the finite difference/moment equation is reduced. The consequences of this are examined in section 2.5.

At first sight, equation (41) seems to be the easier of the two moment equations to study within the context of the EMM analysis. However, we note that the form of this moment equation does not change for either the right or left wedge. In addition, despite the previous results, we cannot impose any constraints on $S(0)$ and $P(0)$. Thus, in fact, equation (41) cannot yield any bounds on the physical eigenenergy because it does not lead to any correlation between the right and left wedge configurations.

Instead, the collective moment equation defined by equations (39)–(40) do relate both the right- and left-hand wedges. More precisely, these moment equations depend on $S'_{R,L}(0)$ and $J_{R,L}(0)$ which in turn can be constrained in accordance with equations (58)–(59). The latter define the crucial link between the $\{S, P, J\}$ configurations in both wedges.

In the following analysis we implicitly work in terms of the right-wedge representation.

The linear, recursive structure of equation (39), tells us that all of the moments can be generated through the expression

$$\mu(\rho) = \sum_{\ell=0}^{5} \tilde{M}_{\rho,\ell}(E)\chi_\ell \qquad \rho \geqslant 0 \quad (61)$$

where

$$\chi_\ell \equiv \begin{cases} \mu(\ell) & \text{for} \quad 0 \leqslant \ell \leqslant 4 \\ S'_R(0) & \text{for} \quad \ell = 5 \end{cases} \quad (62)$$

and

$$\tilde{M}_{\ell_1,\ell_2} = \begin{cases} \delta_{\ell_1,\ell_2} & \text{for} \quad 0 \leqslant \ell_{1,2} \leqslant 4 \\ 0 & \text{for} \quad 0 \leqslant \ell_1 \leqslant 4 \quad \ell_2 = 5. \end{cases} \tag{63}$$

In addition, the $\tilde{M}_{\rho,\ell}$ matrix coefficients satisfy the moment equation in equation (39) with respect to the ρ-index, for fixed ℓ:

$$\begin{aligned} &\frac{\delta_{\ell,5}}{2}\delta_{\rho,0} + \tilde{M}_{\rho-1,\ell}(E)\left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2}\right] + \tilde{M}_{\rho,\ell}(E)[-2C_2E(2\rho+1)] \\ &\quad + \tilde{M}_{\rho+1,\ell}(E)\left[\frac{E^2{S_2}^2}{\rho+1}\right] + \tilde{M}_{\rho+2,\ell}(E)[-4C_6 - 2C_6(2\rho+1)] \\ &\quad + \tilde{M}_{\rho+3,\ell}(E)\left[ES_2S_6\left(\frac{1}{\rho+1} + \frac{1}{\rho+3}\right)\right] + \tilde{M}_{\rho+5,\ell}(E)\left[\frac{{S_6}^2}{\rho+3}\right] = 0. \end{aligned} \tag{64}$$

We can now focus on the additional constraint in equation (40). From equation (60) we can express $S_R'(0)$ in terms of $\{\mu(0), \mu(2)\}$. That is,

$$S_R'(0) = -\frac{2S_1}{C_1}(ES_2\,\mu(0) + S_6\,\mu(2)). \tag{65}$$

Substituting this relation in equation (61), we obtain

$$\mu(\rho) = \sum_{\ell=0}^{4} \tilde{M}_{\rho,\ell}(E)\,\mu(\ell) - \tilde{M}_{\rho,5}(E)\left(\frac{2S_1}{C_1}(ES_2\,\mu(0) + S_6\,\mu(2))\right). \tag{66}$$

Regrouping, we have

$$\mu(\rho) = \sum_{\ell=0}^{4} M_{\rho,\ell}(E)\,\mu_\ell \tag{67}$$

where

$$M_{\rho,\ell}(E) = \begin{cases} \tilde{M}_{\rho,\ell} & \text{for} \quad \ell \neq 0, 2 \\ \tilde{M}_{\rho,\ell} - \left(\dfrac{2ES_1S_2}{C_1}\right)\tilde{M}_{\rho,5}(E) & \text{for} \quad \ell = 0 \\ \tilde{M}_{\rho,\ell} - \left(\dfrac{2S_1S_6}{C_1}\right)\tilde{M}_{\rho,5}(E) & \text{for} \quad \ell = 2. \end{cases} \tag{68}$$

Finally, we must impose a suitable normalization. We note that all of the independent moments (i.e. the *missing moments*), $\{\mu(\ell)\,|\,0 \leqslant \ell \leqslant m_s = 4\}$, are positive quantities. We can impose the normalization

$$\sum_{\ell=0}^{m_s=4} \mu(\ell) = 1 \tag{69}$$

which is used to constrain the zeroth-order moment: $\mu(0) = 1 - \sum_{\ell=1}^{m_s}\mu(\ell)$. Incorporating this within equation (67) results in

$$\mu(\rho) = \sum_{\ell=0}^{m_s} \hat{M}_{\rho,\ell}(E)\,\hat{\mu}(\ell) \tag{70}$$

where

$$\hat{\mu}(\ell) \equiv \begin{cases} 1 & \text{if} \quad \ell = 0 \\ \mu(\ell) & \text{if} \quad \ell \geqslant 1 \end{cases} \tag{71}$$

and

$$\hat{M}_{\rho,\ell}(E) \equiv \begin{cases} M_{\rho,0}(E) & \text{if} \quad \ell = 0 \\ M_{\rho,\ell}(E) - M_{\rho,0}(E) & \text{if} \quad \ell \geqslant 1. \end{cases} \tag{72}$$

2.5. Numerical implementation of EMM for $-(\mathrm{i}x)^4$ potential

Since the $\mu(\rho)$ moments are the moments of a non-negative function, $F(\eta) \equiv \frac{1}{2\sqrt{\eta}} S(\sqrt{\eta})$, as noted in equation (37), they must satisfy the *moment problem* constraints [11]:

$$\int_0^\infty \mathrm{d}\eta\, \eta^\sigma \left(\sum_{\rho=0}^{Q} C_\rho\, \eta^\rho \right)^2 F(\eta) > 0 \tag{73}$$

for arbitrary C's (not all identically zero) and $Q \geqslant 0$. Because this is a Stieltjes function, $\sigma = 0, 1$.

The above integral expression becomes the quadratic form expression

$$\sum_{\rho_1,\rho_2=0}^{Q} C_{\rho_1}\, \mu_{\sigma+\rho_1+\rho_2}\, C_{\rho_2} > 0. \tag{74}$$

Substituting the moment equation relation in equation (70), we obtain

$$\sum_{\ell=1}^{m_s} A_\ell^{(\sigma)}[C; E]\, \mu_\ell < B^{(\sigma)}[C; E] \tag{75}$$

where

$$A_\ell^{(\sigma)}[C; E] \equiv - \sum_{\rho_1,\rho_2=0}^{Q} C_{\rho_1}\, \hat{M}_{\sigma+\rho_1+\rho_2,\ell}(E)\, C_{\rho_2} \tag{76}$$

and

$$B^{(\sigma)}[C; E] \equiv \sum_{\rho_1,\rho_2=0}^{Q} C_{\rho_1}\, \hat{M}_{\sigma+\rho_1+\rho_2,0}(E)\, C_{\rho_2}. \tag{77}$$

The physical energies, and corresponding missing moments, are those that satisfy all of the linear inequalities in equation (75), for arbitrary C's, and Q. In practice, at a given order, Q, for any E value, we can define an optimal (finite) set of *C-cutting vectors* which tell us if there exists a missing moment polytope solution, $\mathcal{U}_{C;E}$, to the corresponding linear equations. This is done through the eigenvalue moment method [8, 9], which uses basic linear programming [12] to implement this *cutting procedure*. The nonexistence of $\mathcal{U}_{C;E}$ tells us that the associated energy value is unphysical. The existence of $\mathcal{U}_{C;E}$ tells us that it may be a physical energy value. By increasing the order systematically, the feasible (i.e. physically possible) energy intervals decrease in size. Their endpoints define the lower and upper bounds to the associated discrete state energy (which must lie within the interval).

So long as $S_6 \neq 0$, all of the preceding formalism holds, and EMM must be implemented on the four-dimensional, unconstrained missing moment, formulation represented in equation (70).

The results of this analysis are noted in table 1. We only quote the results for the first two discrete states. Note that $\mathcal{P}_{\max}$ denotes the maximum number of moments used, $2Q + \sigma \leqslant \mathcal{P}_{\max}$. The data in table 1 is for $\theta \neq \theta_R \approx -0.5$. As $\theta \rightarrow \theta_R$, the presence of small denominators makes the accuracy problematic, as Q is increased. However, the tightness of the bounds does appear to increase as $\theta \rightarrow \theta_R$, which is consistent with the underlying theory. In table 2 we can cleanly (i.e. without introducing small denominators) define the moment problem theory along the anti-Stokes angle, yielding fantastically superior bounds.

If we take $S_6 = 0$, we recognize from equation (2) that this corresponds to letting θ coincide with the *anti-Stokes* line for rapid, asymptotic decrease of the wavefunction.

Table 1. Bounds for the discrete states of $P^2 - (\mathrm{i}X)^4$.

θ	$\mathcal{P}_{\max}$	$E_0^{(L)} < E_0 < E_0^{(U)}$	$E_1^{(L)} < E_1 < E_1^{(U)}$
−0.3	25	$1.477\,149\,081\,9 < E_0 < 1.477\,150\,900\,9$	$6.003\,345\,003\,1 < E_1 < 6.003\,395\,148\,0$
−0.3	30	$1.477\,149\,728\,3 < E_0 < 1.477\,149\,761\,9$	$6.003\,385\,656\,5 < E_1 < 6.003\,386\,467\,4$
−0.4	25 (23 for E_1)	$1.477\,149\,743\,1 < E_0 < 1.477\,149\,807\,1$	$6.003\,352\,613\,1 < E_1 < 6.003\,454\,992\,1$

Table 2. Bounds for the discrete states of $P^2 - (\mathrm{i}X)^4$, along anti-Stokes angle, $\theta_R = -\frac{\pi}{6}$.

$\mathcal{P}_{\max}$	$E_0^{(L)} < E_0 < E_0^{(U)}$	$E_1^{(L)} < E_1 < E_1^{(U)}$
5	$1.05 < E_0 < 1.8$	
10	$1.470 < E_0 < 1.482$	$5.6 < E_1 < 8.0$
15	$1.477\,11 < E_0 < 1.477\,19$	$5.999\,24 < E_1 < 6.012\,20$
20	$1.477\,149\,6 < E_0 < 1.477\,150\,0$	$6.003\,367 < E_1 < 6.003\,444$
25	$1.477\,149\,752 < E_0 < 1.477\,149\,756$	$6.003\,385\,96 < E_1 < 6.003\,386\,40$
30	$1.477\,149\,753\,573 < E_0 < 1.477\,149\,753\,588$	$6.003\,386\,082\,98 < E_1 < 6.003\,386\,084\,78$
	$E_2^{(L)} < E_2 < E_2^{(U)}$	$E_3^{(L)} < E_3 < E_3^{(U)}$
15	$11.6 < E_2 < 16.0$	
20	$11.8010 < E_2 < 11.806\,6$	$18.17 < E_3 < 18.65$
25	$11.802\,425 < E_2 < 11.802\,455$	$18.4572 < E_3 < 18.459\,9$
30	$11.802\,433\,57 < E_2 < 11.802\,433\,65$	$18.458\,807 < E_3 < 18.458\,827$

Now the associated moment equation reduces greatly in order, from 4 to 1! That is, equations (39)–(40) become

$$\frac{S'(0)}{2}\delta_{\rho,0} + \mu(\rho-1)\left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2}\right] + \mu(\rho)[-2C_2E(2\rho+1)] + \mu(\rho+1)\left[\frac{E^2{S_2}^2}{\rho+1}\right] + \mu(\rho+2)[-4C_6 - 2C_6(2\rho+1)] = 0$$

and

$$ES_2\mu(0) = \mp J(0) \tag{78}$$

for $S_6 = 0$, or $\theta = \theta_R = -\frac{\pi}{6}$. All of the previous formalism can be implemented, yielding the associated $\hat{M}$ coefficients.

For the special *anti-Stokes* angle case, the convergence rate of the bounds is much faster, as shown in table 2.

3. The general $-(\mathrm{i}X)^N$ potential

We now consider the generic case for the $-(\mathrm{i}x)^N$ Schrödinger equation, extended into the complex-z plane

$$-\Psi''(z) - (\mathrm{i}z)^N\Psi(z) = E\Psi(z). \tag{79}$$

Along the $z = \xi\mathrm{e}^{\pm\mathrm{i}\theta}$ rays ($\xi \geqslant 0$), the Schrödinger equation becomes

$$\Psi_R''(\xi) + \mathrm{i}^N\xi^N\mathrm{e}^{\mathrm{i}(N+2)\theta}\Psi_R(\xi) + E\,\mathrm{e}^{2\mathrm{i}\theta}\Psi_R = 0 \tag{80}$$

and

$$\Psi_L''(\xi) + (-\mathrm{i})^N\xi^N\mathrm{e}^{-\mathrm{i}(N+2)\theta}\Psi_L(\xi) + E\mathrm{e}^{-2\mathrm{i}\theta}\Psi_L(\xi) = 0 \tag{81}$$

along the R (right) and L (left) wedges, respectively.

In accordance with the representation in equation (8), $\Psi(\xi) \equiv A(\xi)\Psi''(\xi) + B(\xi)\Psi'(\xi) + C(\xi)\Psi(\xi) = 0$, we have $A = 1$, $B = 0$, $C(\xi) = \xi^N e^{\pm i[(N+2)\theta + \frac{N\pi}{2}]} + Ee^{\pm 2i\theta}$. The real and imaginary parts of the $C(\xi)$ coefficient function become

$$C_R(\xi) = \xi^N C^+_{N+2} + EC_2 \tag{82}$$

and

$$C_I = \pm\xi^N S^+_{N+2} \pm ES_2. \tag{83}$$

We define $C^+_{N+2} = \cos\left[(N+2)\theta + \frac{N\pi}{2}\right]$, and $S^+_{N+2} = \sin\left[(N+2)\theta + \frac{N\pi}{2}\right]$, where, as before, $C_n = \cos(n\theta)$, $S_n = \sin(n\theta)$ ($\pm$ is for R (right) and L (left)).

When N is even, $C^+_{N+2} = (-1)^{\frac{N}{2}} C_{N+2}$ and $S^+_{N+2} = (-1)^{\frac{N}{2}} S_{N+2}$. When N is odd, $C^+_{N+2} = (-1)^{\frac{N+1}{2}} S_{N+2}$ and $S^+_{N+2} = (-1)^{\frac{N-1}{2}} C_{N+2}$.

The S, P, J equations become

$$S''(\xi) - 2P(\xi) + 2\left(\xi^N C^+_{n+2} + EC_2\right) S(\xi) = 0 \tag{84}$$

$$\left(\pm\xi^N S^+_{N+2} \pm ES_2\right) S(\xi) - J'(\xi) = 0 \tag{85}$$

and

$$P'(\xi) + (\xi^N C^+_{n+2} + EC_2)S'(\xi) - 2\left(\pm\xi^N S^+_{N+2} \pm ES_2\right) J(\xi) = 0. \tag{86}$$

The U, V, W moment equations become

$$\begin{aligned} -\delta_{p,0}S'(0) + \delta_{p,1}S(0) + p(p-1)U(p-2) - 2V(p) \\ + 2[C^+_{N+2}U(p+N) + EC_2U(p)] = 0 \end{aligned} \tag{87}$$

$$\pm S^+_{N+2}U(p+N) \pm ES_2U(p) + [\delta_{p,0}J(0) + pW(p-1)] = 0 \tag{88}$$

and

$$\begin{aligned} -\delta_{p,0}P(0) - pV(p-1) + C^+_{N+2}[-(p+N)U(p+N-1)] + EC_2[-\delta_{p,0}S(0) \\ - pU(p-1)] - 2[\pm S^+_{N+2}W(p+N) \pm ES_2W(p)] = 0. \end{aligned} \tag{89}$$

As before, equation (88) really contains two separate relations. One, when $p = 0$, serves to constrain the U moments

$$S^+_{N+2}U(N) + ES_2U(0) = \mp J(0) \tag{90}$$

the other, when $p \geqslant 1$, serves to generate the W moments from the U's (i.e. take $p \to p+1$ in equation (88))

$$W(p) = \mp\frac{\left(S^+_{N+2}U(p+N+1) + ES_2U(p+1)\right)}{p+1}. \tag{91}$$

We can substitute for V (i.e. equation (87)) and W (i.e. equation (91)), in equation (89), reducing it into one moment equation for the U's (in addition to equation (90))

$$\begin{aligned} -S(0)\delta_{p,2} + \frac{S'(0)}{2}\delta_{p,1} - P(0)\delta_{p,0} - C_2ES(0)\delta_{p,0} + U(p-3)\left[-p + \frac{3p^2}{2} - \frac{p^3}{2}\right] \\ + U(p-1)[-2pC_2E] + U(p+1)\left[\frac{2E^2{S_2}^2}{p+1}\right] + U(p+N-1)\left[-NC^+_{N+2}\right. \\ \left. - 2pC^+_{N+2}\right] + U(p+N+1)\left[\frac{2ES_2S^+_{N+2}}{p+1} + \frac{2ES_2S^+_{N+2}}{p+N+1}\right] \\ + U(p+2N+1)\left[\frac{2{S^+_{N+2}}^2}{p+N+1}\right] = 0. \end{aligned} \tag{92}$$

When $N = 2m = even$, the U moment equation separates into distinct relations for the even and odd order moments. When $N = odd$, this separation does not happen, and one must work with the U-moment equation directly.

For the $N = 2m$ case, as explained in the context of the $-(\mathrm{i}x)^4$ potential, only the even order moment relations will yield eigenenergy bounds. Taking $\mu(\rho) \equiv U(2\rho)$, as before, the μ-moment equation becomes (i.e. take $p = 2\rho + 1$ in equation (92))

$$\frac{S'(0)}{2}\delta_{\rho,0} + \mu(\rho-1)\left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2}\right] + \mu(\rho)[-2C_2E(2\rho+1)]$$
$$+\mu(\rho+1)\left[\frac{E^2{S_2}^2}{\rho+1}\right] + \mu(\rho+m)\left[-NC^+_{N+2} - 2C^+_{N+2}(2\rho+1)\right] + \mu(\rho+m+1)$$
$$\times\left[ES_2S^+_{N+2}\left(\frac{1}{\rho+m+1} + \frac{1}{\rho+1}\right)\right] + \mu(\rho+2m+1)\left[\frac{{S^+_{N+2}}^2}{\rho+m+1}\right] = 0. \tag{93}$$

We note that through equation (60), $J_{R,L}(0)$ and $S'_{R,L}(0)$ are linearly related (a consequence of assuming PT invariance). However, through the constraint in equation (90), $J_{R,L}(0)$ is determined by the corresponding U-moments. Thus, these boundary terms are completely determined by the $\{U(0), U(N)\}$ moments.

If $S^+_{N+2} \neq 0$, and $N = odd$, taking note of the previous remarks, the independent variables become $\{U(0), \ldots, U(2N), S(0), P(0)\}$, which are $2N + 3$ in number (before imposing any normalization).

Similarly, if $S^+_{N+2} \neq 0$, and $N = 2m$, then the number of independent variables is $2m + 1$ (i.e. the moments $\{\mu(0), \ldots, \mu(2m)\}$).

By taking $\theta = \theta_R$ (i.e. equation (2)), or $S^+_{N+2} = 0$, we can significantly reduce the number of independent variables; and thereby increase the convergence rate of the generated bounds. Under this simplification, the U moment equation now involves the $N+1$ independent variables $\{U(0), \ldots, U(N-2), S(0), P(0)\}$, before normalization; and the μ moments involve m independent variables, $\{\mu(0), \ldots, \mu(m-1)\}$ (before imposing the normalization condition which brings it down to $m - 1$).

The corresponding moment equations become

$$-S(0)\delta_{p,2} + \frac{S'(0)}{2}\delta_{p,1} - P(0)\delta_{p,0} - C_2ES(0)\delta_{p,0} + U(p-3)\left[-p + \frac{3p^2}{2} - \frac{p^3}{2}\right]$$
$$+U(p-1)[-2pC_2E] + U(p+1)\left[\frac{2E^2{S_2}^2}{p+1}\right]$$
$$+U(p+N-1)[-NC^+_{N+2} - 2pC^+_{N+2}] = 0 \tag{94}$$

and

$$\frac{S'(0)}{2}\delta_{\rho,0} + \mu(\rho-1)\left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2}\right] + \mu(\rho)[-2C_2E(2\rho+1)]$$
$$+\mu(\rho+1)\left[\frac{E^2{S_2}^2}{\rho+1}\right] + \mu(\rho+m)[-NC^+_{N+2} - 2C^+_{N+2}(2\rho+1)] = 0. \tag{95}$$

These equations hold both for the right and left wedges, provided we make explicit the reference to a particular wedge. Thus, $S(0) \to S_{R,L}(0)$, $P(0) \to P_{R,L}(0)$, $S'(0) \to S'_{R,L}(0)$, and $U(p) \to U_{R,L}(p)$, etc.

3.1. Recursive expression for N = odd, U-moment equation

For completeness, we detail the generation of the moment-missing moment relation required in implementing the EMM algorithm for generating bounds. We focus only on the moment formulation represented in equation (94), for $\theta = \theta_R$. As noted, the ensuing EMM analysis will generate the fastest bounds in this case.

From equation (94), all of the moments are explicitly, linearly, dependent on the $\{U_R(0), \ldots, U_R(N-2)\}$ moments, and the boundary terms $\{S_R(0), P_R(0), S'_R(0)\}$

$$U_R(p) = \sum_{\ell=0}^{N+1} \tilde{M}_{p,\ell}(E)\chi_\ell \tag{96}$$

where

$$\chi_\ell = \begin{cases} U_R(\ell) & 0 \leqslant \ell \leqslant N-2 \\ S_R(0) & \ell = N-1 \\ P_R(0) & \ell = N \\ S'_R(0) & \ell = N+1. \end{cases} \tag{97}$$

The $\tilde{M}$ coefficients satisfy equation (94) with respect to the p-index, for fixed ℓ

$$\begin{aligned} -\delta_{\ell,N-1}\delta_{p,2} + \frac{\delta_{\ell,N+1}}{2}\delta_{p,1} - \delta_{\ell,N}\delta_{p,0} - C_2 E\delta_{\ell,N-1}\delta_{p,0} + \tilde{M}_{p-3,\ell}(E)\left[-p + \frac{3p^2}{2} - \frac{p^3}{2}\right] \\ + \tilde{M}_{p-1,\ell}(E)\left[-2pC_2E\right] + \tilde{M}_{p+1,\ell}(E)\left[\frac{2E^2{S_2}^2}{p+1}\right] \\ + \tilde{M}_{p+N-1,\ell}(E)\left[-NC^+_{N+2} - 2pC^+_{N+2}\right] = 0 \end{aligned} \tag{98}$$

$p \geqslant 0$.

In addition, the $\tilde{M}$'s must satisfy the initialization conditions

$$\tilde{M}_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2} \tag{99}$$

for $0 \leqslant \ell_1 \leqslant N-2$ and $0 \leqslant \ell_2 \leqslant N+1$.

From equation (60) $S'_R(0) = \frac{2S_1}{C_1} J_R(0)$, and from equation (90), $J_R(0) = -ES_2\, U_R(0)$, under the assumption $S^+_{N+2} = 0$. Combining these, and substituting into equation (96) yields

$$U_R(p) = \sum_{\ell=0}^{N} M_{p,\ell}(E)\chi_\ell \tag{100}$$

where

$$M_{p,\ell}(E) = \begin{cases} \tilde{M}_{p,0} - \dfrac{2ES_1S_2}{C_1}\tilde{M}_{p,N+1} & \text{if} \quad \ell = 0 \\ \tilde{M}_{p,\ell} & \text{if} \quad \ell \neq 0. \end{cases} \tag{101}$$

One can now proceed as in the $-(ix)^4$ case and impose a similar normalization and EMM implementation. Note that all of the χ_ℓ's in the above linear relation are positive quantities.

In table 3 we give bounds on the first two discrete states for $N = 3, 5, 7$. We have included $N = 3$ in order to compare with the result of Handy [4], and Handy and Wang [10], which corresponds to a different complex-rotation EMM implementation. The results here are superior by at least two decimal places.

Table 3. Bounds for the discrete states of $P^2 - (\mathrm{i}X)^N$, along anti-Stokes angle, $\theta_R = -\frac{N-2}{N+2}\frac{\pi}{2}$.

N	$\mathcal{P}_{\max}$ (for E_1)	$E_0^{(L)} < E_0 < E_0^{(U)}$	$E_1^{(L)} < E_1 < E_1^{(U)}$
3	28 (27)	$1.156\,267\,065\,7 < E_0 < 1.156\,267\,077\,2$	$4.109\,227 < E_1 < 4.109\,231$
5	24 (22)	$1.908\,244 < E_0 < 1.908\,273$	$8.5837 < E_1 < 8.5902$
7	25 (20)	$3.068\,43 < E_0 < 3.068\,73$	$15.01 < E_1 < 16.59$

Table 4. Bounds for the discrete states of $P^2 - (\mathrm{i}X)^N$, along anti-Stokes angle, $\theta_R = -\frac{N-2}{N+2}\frac{\pi}{2}$.

N	$\mathcal{P}_{\max}$ (for E_1)	$E_0^{(L)} < E_0 < E_0^{(U)}$	$E_1^{(L)} < E_1 < E_1^{(U)}$
6	30 (28)	$2.439\,346\,483\,9 < E_0 < 2.439\,346\,488\,3$	$11.881\,564\,834 < E_1 < 11.881\,564\,915\,6$
8	30 (23)	$3.796\,474\,882\,2 < E_0 < 3.796\,474\,885\,8$	$20.735\,611 < E_1 < 20.735\,854$
10	29 (22)	$5.553\,309\,963\,9 < E_0 < 5.553\,310\,069\,8$	$32.807\,78 < E_1 < 32.814\,56$

3.2. Recursive expression for N = 2m (even), μ moment equation

In this case, we have

$$\mu_R(\rho) = \sum_{\ell=0}^{m} \tilde{M}_{\rho,\ell}(E)\chi_\ell \tag{102}$$

where

$$\chi_\ell = \begin{cases} \mu_R(\ell) & 0 \leqslant \ell \leqslant m-1 \\ S'_R(0) & \ell = m. \end{cases} \tag{103}$$

The $\tilde{M}$'s must satisfy equation (95) with respect to the ρ-index

$$\frac{\delta_{\ell,m}}{2}\delta_{\rho,0} + \tilde{M}_{\rho-1,\ell}(E)\left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2}\right] + \tilde{M}_{\rho,\ell}(E)\,[-2C_2E(2\rho+1)] + \tilde{M}_{\rho+1,\ell}(E)\left[\frac{E^2{S_2}^2}{\rho+1}\right] + \tilde{M}_{\rho+m,\ell}(E)\left[-NC^+_{N+2} - 2C^+_{N+2}(2\rho+1)\right] = 0 \tag{104}$$

in addition to the initialization conditions

$$\tilde{M}_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2} \tag{105}$$

for $0 \leqslant \ell_1 \leqslant m-1$ and $0 \leqslant \ell_2 \leqslant m$.

Finally, incorporating the constraint of $S'_R(0)$ on $\mu(0)$ (i.e. $S'_R(0) = -\frac{2ES_1S_2}{C_1}\mu(0)$), we obtain

$$\mu_R(\rho) = \sum_{\ell=0}^{m-1} M_{\rho,\ell}\,\mu_R(\ell) \tag{106}$$

where

$$M_{\rho,\ell}(E) = \begin{cases} \tilde{M}_{\rho,0} - \dfrac{2ES_1S_2}{C_1}\tilde{M}_{\rho,m} & \text{if} \quad \ell = 0 \\ \tilde{M}_{\rho,\ell} & \text{if} \quad \ell \neq 0. \end{cases} \tag{107}$$

In table 4 we give bounds on the first two discrete states for $N = 6, 8, 10$. As is clear, upon comparing with the data in table 3, the bounds for the $N = \textit{even}$ case, based upon the

μ-EMM formalism, converge much faster than those for the $N = odd$ case, based on the U-EMM analysis. This cannot be avoided.

4. Conclusion

We have extended the EMM formalism to the case of discrete states with non-Real support. The primary focus of this work is to emphasize the theoretical/analytical modifications of the original work by Handy [4], in order to accomodate bound state problems on complex contours.

Bounding methods are generally more difficult to formulate, and apply, than do estimation methods (i.e. numerical integration). Furthermore, the 'tightness' of the bounds can be inferior (at a comparable 'expansion' order) than the numbers generated by estimation methods. However, bounding methods are inherently more reliable in terms of their theoretical predictions, than estimation methods, since they clearly impose constraints on the physical answer. Such properties are useful in dealing with strong coupling/singular perturbation-type systems, where different computational methodologies can yield very different answers. The most famous of these is the quadratic Zeeman effect for superstrong magnetic fields [9]. Application of EMM to this problem confirmed the estimation methods of LeGuillou and Zinn-Justin [13], in comparison to many other methods.

Whereas several bounding theories have been developed over the last few decades, there are very few that yield converging bounds to the physical answer (albeit for the low-lying states). Further still, there are even fewer such methods that can yield converging bounds to non-Hermitian Hamiltonians. A very recent example of the interest in such problems is the work of Abramov *et al* [14], which focuses on bounding complex energies and resonant states. By way of contrast, the more recent work of Handy [5], and Handy *et al* [6], generates converging eigenenergy bounds to various, non-Hermitian, complex energy problems. Still more recent works extend the EMM philosophy to generate converging bounds to complex Regge-pole solutions [15].

The use of a moments' representation makes EMM suitable for solving singular perturbation-type problems. This is because its linear programming formulation (i.e. equations (73)–(75)) is inherently an affine map invariant variational procedure [16], making EMM sensitive to delicate multiscale dependencies inherent to singular systems. This also underscores its deep connection with wavelet analysis [16, 17].

With regard to the problems examined here, other, estimation-analysis type, works have recently appeared yielding excellent results for the eigenenergies. These include the works by Bender and Wang [18], Dorey *et al* [2, 3] and Shin [19].

These works notwithstanding, from a purely numerical perspective, EMM can offer impressive accuracy. The numerical implementation can be done to any desired precision, although our results were done only to fifteen decimal place accuracy (which does not necessarily coincide with the tightness of the bounds). We could have easily doubled the accuracy of all the results appearing in the tables.

The tightness of the bounds, at a fixed $P_{\max}$, decreases with increasing energy level. This is a practical limitation which makes the method relevant for the low-lying states; although with the advent of more powerful computers, one can easily examine progressively higher energy level states.

Another fundamental feature of the EMM procedure is its dependency on a non-negative ('positivity') formulation of quantum mechanics. The novel use of the differential system in equations (9)–(16), introduces a significant variation to conventional formulations of quantum mechanics (in one dimension). We believe that the focus on 'positivity' as a quantization tool will impact other areas as well, particularly in the context of certain Wigner-transform-related issues currently under consideration.

We believe that EMM theory, despite its current limitation to multidimensional rational fraction potential systems (which, nevertheless, correspond to a significantly large class of problems), represents a radically new, and powerful, alternative quantization formulation, of particular relevance to singular systems.

The formalism developed here now opens up the extension of EMM to symmetry breaking solutions for such potentials as $-(\mathrm{i}X)^N + \mathrm{i}aX$, and any other rational fraction complex potential.

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