ABSTRACT

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EXTENSION OF A SPECTRAL BOUNDING METHOD TO THE PT-INVARIANT STATES OF THE $-(ix)^N$ NON-HERMITIAN POTENTIAL

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The research objective of this thesis is to extend the Eigenvalue Moment Method (EMM) to bound state problems for non-Hermitian potentials, extended to the complex plane in configuration space. The confirmation of this objective enables the generation of converging lower and upper bounds to the discrete state energies, thereby, defining a very accurate computational tool for analyzing such difficult problems. The basic approach adopted here combines several important developments. The first is that one can transform the one dimensional Schrödinger equation, on any complex contour, into a fourth order, linear differential equation for the probability density. This then defines a Nonnegativity Quantization Representation (NQR) in which the physical solution is uniquely associated with a nonnegative, bounded, configuration/solution. For the problems of interest, one can then transform the NQR differential representation into a *Moment Equation* representation (involving the moments of the physical solution) which assumes the form of a linear recursion relation in which the energy appears as an unknown parameter. Because of the underlying nonnegativity (positivity) of the physical solution, it is then possible to impose the positivity constraints emanating from the famous *Moment Problem* theorems in mathematics. Its linear programming implementation defines the algorithmic structure of

the EMM approach. The generated constraints then serve to define a converging sequence of approximants which define lower and upper bounds for the physical values of the discrete state energies.

EXTENSION OF A SPECTRAL BOUNDING METHOD TO THE
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LIST OF ABBREVIATIONS

EMM	Eigenvalue Moment Method
ME	Moment Equation
HH	Hankel-Hadamard
DIP	Deep Interior Point
c.c.	Complex Conjugate
PT	Parity/time reversal
NQR	Nonnegativity Quantization Representation

CHAPTER 1

INTRODUCTION

Over the last several years, there has been a considerable amount of work [1-21] focusing on the existence of bound (L^2) states for non-Hermitian Schrödinger equation problems of the type

$$-\frac{\hbar^2}{2m}\Psi''(x) + V(x)\Psi(x) = E\Psi(x), \quad (1.1)$$

for potential functions of the class

$$V(x) = \sum_{j=0}^J C_j x^j, \quad (1.2)$$

where the C_j coefficients are complex numbers, and the domain of definition is allowed to extend into the complex- x plane.

For simplicity, we will henceforth assume that the above system is rescaled, $x \rightarrow sx$, so that the ratio $\frac{\hbar^2}{2m} \equiv s^2$ is effectively factored out.

The prototype of the above class of problems is the $-(ix)^N$ potential, for arbitrary N , as first studied by Bender and Boettcher [1]. Their focus was to confirm a conjecture by Bessis that the bound state eigenenergies of the ix^3 potential are real, for bound states on the real axis, $\Re$. More generally, they proved that for arbitrary N , there exist bound states along infinite contours in the complex- x plane, all having real eigenenergies, E . It was conjectured by Bender and Boettcher that the reality of the bound state (discrete) spectrum was due to the parity/time reversal (PT) invariance of the system in question. This has been subsequently disproved through the analysis of PT invariant systems with complex eigenenergy states. The first example of this was discovered by Delabaere and Trinh [7], and reconfirmed by Handy [13] and Handy et al. [14].

The objective of this thesis is to confirm the (WKB-asymptotic analysis [1]) results of Bender and Boettcher through the implementation of an alternative

computational method developed by Handy and colleagues. This approach has several distinctive, and important, components.

The first involves rewriting the Schrödinger equation, for complex potentials, as a fourth order, linear differential equation, for the probability density, $S(x) \equiv |\Psi(x)|^2$, as first recognized by Handy [12] and subsequently refined by Handy and Wang [15]. Within this representation, the physical solutions are bounded (exponentially vanish, at infinity, along the required complex contours), and correspond to nonnegative configurations, $S(x) \geq 0$.

A second feature, for the potentials of interest, is that the fourth order representation for $S(x)$ admits a Moment Equation representation (to be discussed subsequently).

Because of this we can recast the quantization problem into a Moment Problem [22] formulation and exploit the applicability of the Eigenvalue Moment Method (EMM), as originally developed by Handy and Bessis [23], and its subsequent, linear programming based, reformulation by Handy et al. [24]. The remarkable feature of the EMM approach is that the physical eigenenergies are obtained through a convergent sequence of lower and upper bound approximants. Thus, one can obtain very accurate and reliable estimates of the physical energies.

In the subsequent discussion, we first introduce the Moment Problem and the EMM formalism. We highlight its nonlinear (through the Hankel-Hadamard formulation) and linear programming computational implementation, through an important pedagogic example, the sextic anharmonic oscillator, $V(x) = c_2x^2 + c_6x^6$. We then derive the fourth order representation for $S(x)$, and proceed with the details of our analysis as applied to the non-Hermitian potential $V(x) = -(ix)^N$, for integer N values. The numerical results of this investigation have been published [21] and, for the most part, the published work is directly incorporated in this thesis, forming the body of Chapter 4.

CHAPTER 2

OVERVIEW OF THE MOMENT PROBLEM AND THE EIGENVALUE MOMENT METHOD

2.1 The Moment Problem

Before the development of Quantum Mechanics, mathematicians were interested in understanding the relationship between a positive function, $f(x) > 0$, and its (power) moments,

$$\mu_p = \int_{\mathcal{D}} dx \, x^p f(x), \quad (2.1)$$

$p \geq 0$ and integer. The basic question was, what properties must all of the moments have in order to conclude that the underlying function is positive, or nonnegative (i.e., $f(x) \geq 0$). This is referred to as the *Moment Problem* [22].

Depending on the nature of the domain, $\mathcal{D}$, on which the function is defined, the corresponding Moment Problem is given different names. Thus, if $\mathcal{D} \equiv \mathbb{R}$, the entire real axis, we call this the Hamburger moment problem, in recognition of the mathematician Hamburger who proved a particular theorem, quoted below. If $\mathcal{D} = \mathbb{R}^+$, the nonnegative real axis (including zero), then we refer to the Stieltjes Moment Problem, in recognition of Stieltjes. This particular form of the Moment Problem is very important because it is related to the theory of Pade approximants. If $\mathcal{D} = [0, 1]$, the closed unit interval, then we say that we have a Hausdorff Moment Problem. Finally, if one deals with periodic functions, $f(\theta + 2\pi) = f(\theta)$, then one has the Trigonometric moment problem, in which the moments are defined in terms of periodic functions

$$\nu_p = \int_0^{2\pi} d\theta \, e^{ip\theta} f(\theta). \quad (2.2)$$

As already stated, in all these cases, one wants to know what properties the moments must satisfy in order for the underlying function to be (nonnegative) positive.

We emphasize that a nonnegative function can take on a zero value. In the present work, we shall use the words *nonnegative* and *positive* interchangeably, because the subset of points on which any physical function is zero is of measure zero, and thus does not affect the corresponding moments.

Another issue is, suppose one is given the infinite set of numbers, $\{\mu_p | p \geq 0\}$, when are these the moments of a unique positive function? That is, when can we guarantee that there are no other positive functions having the same moments? This is an important concern, and leads to the Carleman conditions for uniqueness [25].

Although the Stieltjes moment problem was solved in the 1800s, and the Hamburger moment problem was solved in 1922, we shall take things in reverse order and discuss the latter first.

A necessary (but not sufficient) condition for the Hamburger moments to correspond to the moments of a positive function (i.e., the following conditions are required, but by themselves are not sufficient to prove that the underlying function is positive, or even unique) is that

$$\int_{-\infty}^{+\infty} dx \left| \sum_{j=0}^J C_j x^j \right|^2 f(x) > 0, \quad (2.3)$$

for arbitrary (complex) C_j 's, except all identically zero (i.e., if all the C 's are zero, then we get zero). Also, $J \geq 0$.

The above is clearly true if $f(x)$ is a positive function which decays asymptotically ($|x| \rightarrow \infty$) fast enough so that all the moments are finite.

We can transform the preceding integral inequality into the quadratic form expression:

$$\sum_{j_1=0, j_2=0}^{J, J} C_{j_1} \mu_{j_1+j_2} C_{j_2} > 0, \quad (2.4)$$

upon interchanging the summation and integration operations. This corresponds to a matrix expectation value $\langle \vec{C} | \mathcal{M} | \vec{C} \rangle > 0$, where the moment matrix, $\mathcal{M}_{j_1, j_2} = \mu_{j_1+j_2}$, admits '0' as a row-column index value.

The $\mathcal{M}$ matrix is real-symmetric, thus its $J+1$ dimensional finite projection, $\mathcal{M}^{(J)}$, on the corresponding vector space can only admit real eigenvalues. That is,

$$\sum_{j_2=0}^J \mu_{j_1+j_2} \tilde{C}_{j_2} = \lambda \tilde{C}_{j_1}, \quad (2.5)$$

for $0 \leq j_1 \leq J$, can only have real eigenvalues, $\lambda \in \mathbb{R}$, for normalized eigenvectors, $\langle \tilde{C} | \tilde{C} \rangle = 1$. Thus, the positive quadratic form expression in Eq.(2.4), restricted to these eigenvectors, requires that the eigenvalues themselves be positive, $\lambda > 0$.

A fundamental property is that the determinant of the $J+1$ dimensional matrix, $\mathcal{M}^{(J)}$, is given by the product of all its eigenvalues:

$$\text{Det}(\mathcal{M}^{(J)}) = \prod_{j=0}^J \lambda_j > 0, \quad (2.6)$$

and this must be positive.

Now consider increasing J . Let $\lambda_j^{(J)}$ denote the above eigenvalues for the $J+1$ dimensional $\mathcal{M}^{(J)}$ matrix (i.e., $0 \leq j_{1,2} \leq J$). The eigenvalues for the $J+2$ dimensional $\mathcal{M}^{(J+1)}$ matrix, $\lambda_j^{(J+1)}$ (i.e., $0 \leq j \leq J+1$) must interlace the previous one:

$$\begin{aligned} \lambda_0^{(J+1)} &\leq \lambda_0^{(J)} \leq \lambda_1^{(J+1)} \\ \lambda_1^{(J+1)} &\leq \lambda_1^{(J)} \leq \lambda_2^{(J+1)} \\ \lambda_2^{(J+1)} &\leq \lambda_2^{(J)} \leq \lambda_3^{(J+1)} \\ &\vdots \\ \lambda_J^{(J+1)} &\leq \lambda_J^{(J)} \leq \lambda_{J+1}^{(J+1)}. \end{aligned} \quad (2.7)$$

Thus, we come to the Hamburger Moment Problem theorem which states that a necessary condition for an infinite sequence of moments to correspond to a positive function, on the entire real axis, is that the Hankel-Hadamard (HH) determinants be positive:

$$\Delta_{m,n}(\mu) \equiv \text{Det}(\mu_{m+j_1+j_2}) > 0, \quad (2.8)$$

for $0 \leq j_{1,2} \leq n \rightarrow \infty$, and $m = 0$. We include the ‘ m ’ generalization for future reference.

We note that the HH determinants are nonlinear in the moments.

In the Stieltjes moment case, one is interested in similar conditions as applied to a function restricted to the nonnegative real axis, $\mathfrak{R}^+$. However, in deriving the necessary HH constraints, we will pretend that the function can be extended to the entire real axis, by assuming that $f(x) = 0$, for $x < 0$.

Given a function with the property that it is identically zero on the negative real axis, and positive elsewhere, we ask: how must the Hamburger moment problem conditions be modified so as to conclude that the moments must correspond to the type of function just defined? To this extent, we note that the Hamburger Moment Problem conditions force $f(x) \geq 0$ for all x . If we also consider the Hamburger Moment Problem conditions on the function $xf(x)$, then we would also force $xf(x) \geq 0$, for all $x \in \mathfrak{R}$. However, the only way that $f(x) \geq 0$, and $xf(x) \geq 0$, for $x \in \mathfrak{R}$, is for $f(x) = 0$, for $x < 0$. Thus, the Stieltjes moment problem HH condition becomes

$$\Delta_{m,n}(\mu) > 0, \quad (2.9)$$

for $m = 0, 1$ and $n \geq 0$. Since $f(x) = 0$ for $x < 0$, the moments are implicitly Stieltjes moments, that is: $\mu_p = \int_0^\infty dx x^p f(x)$.

We can continue with the above intuitive analysis for the case of the Hausdorff moment problem. Thus, we can pretend that $f(x) = 0$ both for $x < 0$ and $x > 1$. Consistent with the previous reasoning, we extend the Hamburger conditions to the functions $xf(x)$ and $(1-x)f(x)$. The only way all three functions $\{f(x), xf(x), (1-x)f(x)\}$ can be nonnegative (≥ 0) throughout the entire real axis is if $f(x) = 0$ outside of the unit interval, $[0, 1]$. Therefore, in addition to Eq.(2.9), we would also need $Det(\mu_{j_1, j_2} - \mu_{j_1+1, j_2}) > 0$.

2.2 Moment Equation Representation

Consider the (rescaled) Schrödinger equation

$$-\partial_x^2 \Psi(x) + V(x)\Psi(x) = E\Psi(x), \quad (2.10)$$

in one space dimension. We allow the potential function, $V(x)$, to be a rational fraction potential

$$V(x) = \frac{\sum_{n=0}^T N_n x^n}{\sum_{b=0}^B D_b x^b}. \quad (2.11)$$

One is interested in generating the physical, L^2 , eigensolutions for the above differential equation, and in particular, the corresponding eigenenergies, E . The Hamburger moments for the physical solution must exist, since the physical wavefunction solution, Ψ , will usually correspond to a decaying exponential type configuration.

Multiplying both sides of the Schrödinger equation by the potential denominator function (provided the denominator does not have a zero at a point where $\Psi \neq 0$), multiplying again by x^p , and performing the necessary integration by parts, one can transform the Schrödinger equation into a Moment Equation (ME) [12, 13, 15] for the Hamburger moments. We emphasize that the Moment Equation is derived by implicitly assuming that one is working only with the physical solutions, which, by definition, are bounded (in the L^2 sense) and have finite moments. All of the other solutions of the Schrödinger equation are unbounded, and thus do not have finite moments.

The ME relation corresponds to a linear, homogeneous, finite difference equation of order $1 + m_s$, where $m_s = \text{Max}\{B, T\} - 1$. Thus $1 + m_s$ initialization moments, otherwise known as *missing moments*, must be specified before all of the other moments can be generated through the ME relation. The energy, E , appears as an arbitrary parameter (although our ultimate objective is to determine the physical energy values).

After some rewriting, the Moment Equation can be shown to take on the form

$$\mu_p = \sum_{\ell=0}^{m_s} M_{p,\ell}(E) \mu_\ell, \quad (2.12)$$

where the energy dependent coefficients $M_{p,\ell}(E)$ must satisfy the moment equation, with respect to the p -index, and in addition satisfy the initialization conditions:

$$M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}, \quad (2.13)$$

for $0 \leq \ell_1, \ell_2 \leq m_s$.

We note that the above ME expression shows that all of the moments are linearly dependent on the missing moments. The homogeneous character of this relation demands the imposition of some normalization condition. Usually, we can take

$$\sum_{\ell=0}^{m_s} \mu_\ell = 1, \quad (2.14)$$

and solve for μ_0 in terms of the other missing moments. We can incorporate this into the ME relation by substituting, $\mu_0 = 1 - \sum_{\ell=1}^{m_s} \mu_\ell$, and regrouping the terms:

$$\mu_p = \hat{M}_{p,0} + \sum_{\ell=1}^{m_s} \hat{M}_{p,\ell}(E) \mu_\ell, \quad (2.15)$$

for $p \geq 0$, and

$$\hat{M}_{p,\ell} = \begin{cases} M_{p,0}(E), \ell = 0 \\ M_{p,\ell}(E) - M_{p,0}(E), 1 \leq \ell \leq m_s \end{cases}. \quad (2.16)$$

2.3 Positivity and Eigenenergy Bounds

A fundamental theorem in quantum mechanics tells us that the ground (lowest eigenenergy) state must be positive:

$$\Psi_{gr}(x) > 0. \quad (2.17)$$

Thus, given that a moment equation exists, and the ground state is positive, it is natural to ask if the physical ground state energy can be determined by constraining the moments to satisfy the corresponding Moment Problem conditions. This is Handy's great discovery (although first realized in the context of the nesting property of Pade approximants, not discussed here). Handy and Bessis realized that the best formulation of this would be in terms of the Hankel-Hadamard (HH) inequality relations. They were the first to consider combining three important theorems into one computational program, referred to as the Eigenvalue Moment Method (EMM) [23, 24]: (1) Moment Problem HH-constraints; (2) existence of ME relation; and (3) the positivity of the ground state wavefunction.

The EMM procedure achieves two important results. The first, as motivated by Handy's earlier interest in singular-perturbation theory and the moment problem (and the eventual overlap with wavelet theory [26,27]), is that an EMM formulation of quantum mechanics is ideally suited for analyzing strong coupling problems (i.e., where the potential function is influenced by "strong coupling" terms, for instance $V(x) = x^2 + gx^4$, and $g \gg 1$). Secondly, one of the more remarkable achievements of the work of Handy and Bessis is that the EMM formulation generates converging lower and upper bounds to the ground state energy (or any other eigenenergy whose signature properties are known):

$$E_{lower}^{(J)} \leq E_{lower}^{(J+1)} \leq \dots < E_{gr} < \dots \leq E_{upper}^{(J+1)} \leq E_{upper}^{(J)}. \quad (2.18)$$

Many singular perturbation/strong coupling problems are so delicate that different numerical schemes can yield significantly varying results. Having a method that can generate converging bounds enables one to rigorously ascertain the true value of a physical quantity. The most important example of this is the famous Quadratic Zeeman effect [28] for hydrogenic atoms in superstrong magnetic fields [28]. In 1988 Handy et al. [24] applied the EMM procedure to this notoriously difficult problem, generating tight bounds on the binding energy of one electron systems in intense magnetic fields (i.e., neutron stars, etc.) of the order of 10^9 Gauss and higher.

We outline the essentials of the EMM approach in the following section.

2.4 Hamburger Moment Problem Formulation of the Eigenvalue Moment Method

Although one prefers to work within a Stieltjes moment problem representation in order to explain the EMM procedure (because one can directly present the necessary relations), for consistency, and greater generality, we develop this within the context of the Hamburger moment representation.

We prefer to work with positive (missing moment) variables. This requires that we convert the general, Hamburger, missing moment problem into an equivalent

representation that only works with the first $1 + m_s$ even order initialization moment variables. This is discussed below.

We first note that just because a function is positive, $f(x) > 0$, does not imply that all of its Hamburger moments are positive. Clearly, the even order Hamburger moments must be positive $\mu_{2\rho} > 0$; however, the odd order moments, $\mu_{2\rho+1}$, need not be. Assuming that the ME relation does not separate into two relations, one for the even moments, and the other for the odd moments, we can always have even order moments as independent variables. Thus, simply invert the relation in Eq.(2.12), as applied to even order moments, $\mu_{2\rho} = \sum_{\ell=0}^{m_s} M_{2\rho,\ell}(E) \mu_\ell$, for $0 \leq \rho \leq m_s$. Therefore, all of the odd order missing moments, $\mu_{\ell=\text{odd}}$, can be expressed in terms of the first $1 + m_s$ even order moments. Let us express this as

$$\mu_p = \sum_{\ell=0}^{m_s} \tilde{M}_{p,\ell}(E) \chi_\ell, \quad (2.19)$$

where $\chi_\ell \equiv \mu_{2\ell}$. We can then go on to impose a normalization prescription as before, $\sum_{\ell=0}^{m_s} \chi_\ell = 1$, obtaining

$$\mu_p = \hat{M}_{p,0} + \sum_{\ell=1}^{m_s} \hat{M}_{p,\ell}(E) \chi_\ell. \quad (2.20)$$

The importance of this change of notation is that since the even order moments are positive, the choice of normalization condition ensures that the χ -moments are restricted to lie within the unit, $1 + m_s$ dimensional, hypercube: $(\chi_0, \dots, \chi_{m_s}) \in [0, 1]^{1+m_s}$.

We can now substitute the above ME relation into the HH inequalities:

$$\Delta_{m,n}(E; \chi_1, \dots, \chi_{m_s}) > 0, \quad (2.21)$$

for $m = 0$ and $n \geq 0$. If we take $n \leq N$, then all of the moments $\{\mu_p | p \leq 2N\}$ are required.

At a given E value, and order N , we want to know if there exists any χ -values, within the unit hypercube, satisfying the above HH inequalities. It can be argued that the χ -solution set to the above nonlinear inequalities, if it exists, must correspond to a convex set.

In practice, at a low expansion order, N , one picks a large energy interval, and partitions it. At each energy value, within the partition, one must determine the existence or non-existence of a χ -solution set to the (nonlinear) inequality relations in Eq.(2.21). Those E -partition points that admit a χ -solution solution define the updated (smaller) feasible energy interval. The entire procedure is repeated at the next higher moment order ($N \rightarrow N+1$). This process is continued, thereby generating the aforementioned converging lower and upper bounds to the ground state energy, symbolized in Eq.(2.18).

2.5 The Linear Programming EMM Formulation: *The Cutting Method*

The fact that the HH inequalities involve nonlinear expressions with respect to the χ 's made the above procedure very difficult to implement, numerically, except for problems where $m_s \geq 2$. In order to circumvent this algorithmic difficulty, Handy realized that the linear (in the moments) relation in Eq.(2.4) was very important. He developed a linear programming reformulation [29] of the nonlinear, Hankel-Hadamard, EMM procedure. This is referred to as the *Cutting Method* [24].

If we substitute the missing-moment moment relation in Eq.(2.4) we obtain

$$\sum_{\ell=1}^{m_s} \mathcal{A}_{C,\ell} \chi_\ell < \mathcal{B}_C, \quad (2.22)$$

where

$$\begin{aligned} \mathcal{A}_{C,\ell} &= - \sum_{j_1, j_2=0}^{J,J} C_{j_1} \hat{M}_{j_1+j_2,\ell}(E) C_{j_2} \\ \mathcal{B}_C &= \sum_{j_1, j_2=0}^{J,J} C_{j_1} \hat{M}_{j_1+j_2,0}(E) C_{j_2}. \end{aligned} \quad (2.23)$$

For a given energy value, E , consider all the possible $J+1$ dimensional C -vectors, and the corresponding linear inequality relations they generate. Let us denote the χ -solution set to all of them by $\mathcal{U}^{(J)}$. If it exists, then the particular

energy value chosen is a possible physical value for the ground state energy. The set of all such *feasible* energy values, at order J , defines an updated interval whose endpoints correspond to lower and upper bounds for the physical answer.

The solution set $\mathcal{U}^{(J)}$ is the same solution set for the HH nonlinear inequality relations $\Delta_{0,j}(\chi) > 0$, for $j \leq J$, as given in Eq.(2.21).

In order to know that $\mathcal{U}^{(J)}$ exists, all that is required is that we generate just one missing moment tuple (i.e., $(\chi_1, \dots, \chi_{m_s})$) satisfying the above inequalities for all possible C 's. We describe below a procedure for doing this, in a finite number of steps.

The definition of a convex set, $\mathcal{U}$, is that for any two elements in the set, $\vec{\chi}_{1,2} \in \mathcal{U}$, the straight line connecting the two elements must also lie in the set, $\vec{\chi}_1 + s \vec{\chi}_2 \in \mathcal{U}$, for $0 \leq s \leq 1$.

A convex set whose boundary is made up of hyperplanes (i.e., straight lines, in two dimensions), is referred to as a *polytope*. If the boundary consists of curved hyperplanes (i.e., curved lines, in two dimensions), it is considered to be a *nonlinear* convex set. Any nonlinear convex set can be thought of as the intersection of infinitely many polytopes. Thus, all of the linear inequality constraints in Eq.(2.22) define the nonlinear convex set solution for the corresponding HH relations.

The linear constraints in Eq.(2.22) are ideally suited for linear programming (LP) considerations. The EMM-LP reformulation of the HH relations corresponds to a *Cutting Procedure* by which an optimal, finite sequence (to each J -order), of C -vectors is generated in order to determine if $\mathcal{U}^{(J)}$ exists or not. Each generated C -vector defines a linear inequality relation within the missing moment space, as represented by the $\mathcal{A}_C$ and $\mathcal{B}_C$ coefficients. At each step in the sequential procedure, the increasing set of linear coefficients define a nested sequence of sub-polytopes all lying within the original hypercube (i.e., $[0, 1]^{1+m_s}$).

For each of the sequentially generated polytopes, we can define its *Deep Interior Point* (DIP). The DIP is the center of the largest inscribed hypersphere (i.e., circle, in two dimensions).

At each DIP we can generate the appropriate moment matrix, $\mathcal{M}$ (two such moment matrices must be generated in the Stieltjes formulation). This matrix (matrices) will either be positive or not (either or both, in the Stieltjes case). If it is not positive, then by definition, it must have a C -eigenvector of negative eigenvalue. The eigenvector with the smallest negative eigenvalue (one or two such eigenvectors in the Stieltjes case, depending on whether one or both moment matrices are not positive) is used to define the next, sequentially generated, cutting-vector. If the moment matrix is positive (both, in the Stieltjes case), then the DIP establishes the existence of the solution set $\mathcal{U}^{(J)}$.

One of two things must happen after a finite number of steps in the above sequential process. Either the DIP corresponds to a positive matrix, or, after a finite number of cuts, the original hypercube is completely eliminated, thereby confirming that $\mathcal{U}^{(J)}$ does not exist.

We repeat the previous procedure in terms of the relevant mathematical expressions.

Pick an arbitrary E value. We assume that $\mathcal{U}^{(J)}$ exists.

We are going to generate a set of polytopes which bound $\mathcal{U}^{(J)}$.

The starting polytope is the unit m_s dimensional hypercube, $\mathcal{P} = [0, 1]^{m_s}$. We use linear programming to find the DIP, denoted as $(\chi_{o;1}, \dots, \chi_{o;m_s})$. At the DIP we find any non-positive eigenvector for the matrix (refer to Eq.(2.20))

$$\mathcal{M}_{j_1, j_2}(\chi_o) \equiv \sum_{\ell=0}^{m_s} \hat{M}_{j_1+j_2, \ell} \hat{\chi}_{o\ell}, \quad (2.24)$$

where

$$\hat{\chi}_{o\ell} = \begin{cases} 1, & \text{if } \ell = 0 \\ \chi_{o\ell}, & \text{if } \ell \geq 1 \end{cases}. \quad (2.25)$$

If we cannot find any non-positive eigenvector, it tells us that the quadratic form inequalities in Eq.(2.4) are satisfied for arbitrary C , hence $\mathcal{U}^{(J)}$ must exist, because the DIP lies in $\mathcal{U}^{(J)}$.

Let us, therefore, assume that such a non-positive eigenvector exists, satisfying

$$\langle \tilde{C} | \mathcal{M}(\chi_o) | \tilde{C} \rangle \leq 0. \quad (2.26)$$

We now emphasize the following simple observation. The scalar function

$$\Lambda(\chi_1, \dots, \chi_{m_s}) \equiv \langle \tilde{C} | \mathcal{M}(\chi) | \tilde{C} \rangle = \sum_{\ell=1}^{m_s} \chi_\ell \langle \tilde{C} | \hat{M}_\ell | \tilde{C} \rangle, \quad (2.27)$$

divides the $1+m_s$ dimensional missing moment space into two halves, one positive, the other negative. They are separated by the hyperplane on which the function is zero. In the non-positive DIP case (that is, when the associated moment matrix, evaluated at DIP, is non-positive), the DIP lies in the non-positive region. The solution set $\mathcal{U}^{(J)}$ must lie in the positive half. Accordingly, the $\mathcal{U}^{(J)}$ nonlinear convex set must lie within the intersection of the following two sets:

$$\mathcal{U}^{(J)} \subset \mathcal{P} \cap \left\{ \sum_{\ell=1}^{m_s} \mathcal{A}_{\tilde{C},\ell} \chi_\ell < \mathcal{B}_{\tilde{C}} \right\}. \quad (2.28)$$

That is, the $\mathcal{A}_{\tilde{C},\ell}$'s define a hyperplane (line, in two dimensions) that cuts up the polytope, $\mathcal{P}$, resulting in a smaller polytope:

$$\mathcal{P} \rightarrow \mathcal{P}' \equiv \mathcal{P} \cap \left\{ \sum_{\ell=1}^{m_s} \mathcal{A}_{\tilde{C},\ell} \chi_\ell < \mathcal{B}_{\tilde{C}} \right\}. \quad (2.29)$$

If $\mathcal{P}' = \emptyset$, it then means that $\mathcal{U}^{(J)}$ does not exist. If it does, then we use linear programming to find the new DIP, and repeat the entire procedure. In this manner, we can quickly generate an optimal, finite set of cutting vectors (i.e., the corresponding $\mathcal{A}$ -coefficients) that quickly yield a DIP where no non-positive eigenvectors can be found; thereby establishing the existence of $\mathcal{U}^{(J)}$. Alternatively, if $\mathcal{U}^{(J)}$ does not exist, then after a finite number of steps, one will have cut up the starting polytope (i.e., the unit hypercube) into the null set!

This is the Cutting Procedure for numerically implementing EMM. So far, it has been used in multidimensional problems with missing moment index values $m_s \leq 12$.

The above cutting procedure is performed, at low order, on a large energy interval. The feasible energy partition points (i.e., those admitting a $\mathcal{U}$ solution set) then define a smaller energy interval, which is subsequently repartitioned, and analyzed through the cutting algorithm, at a higher moment order. In this manner, as previously stated, converging bounds are generated.

In order to illustrate the above, we discuss one example, that of the sextic anharmonic oscillator, which corresponds to an $m_s = 2$ problem.

CHAPTER 3

THE SEXTIC ANHARMONIC OSCILLATOR: A PEDAGOGIC EXAMPLE

3.1 Generation of Relevant Formulas

3.1.1 *Deriving the Stieltjes Moment Equation*

We present a pedagogic example of the Eigenvalue Moment Method [23, 24] with respect to the ground state of the quantum, sextic anharmonic oscillator potential, $x^2 + x^6$. The relevant Schrödinger equation is

$$-\Psi'' + (x^2 + x^6)\Psi = E\Psi. \quad (3.1)$$

Since this is an Hermitian operator problem, the domain of definition is the entire real axis, $x \in \mathbb{R}$.

As noted before, the ground state wavefunction must be positive, $\Psi_{gr}(x) > 0$, and exponentially bounded at infinity, becoming asymptotically zero; therefore, its Hamburger moments exist:

$$\mu_p = \int_{-\infty}^{+\infty} \Psi(x) x^p dx, \quad (3.2)$$

where $p \geq 0$, and an integer.

An important relation that facilitates the ensuing analysis is that because the potential function is a symmetric function (i.e., is invariant under the parity operator), $V(-x) = V(x)$, the ground state must also be symmetric. Accordingly, the odd order Hamburger moments must be zero. Only the even order Hamburger moments are nonzero for the physical solution. Thus we have:

$$\mu_p = \begin{cases} > 0, & \text{if } p = \text{even} \\ = 0, & \text{if } p = \text{odd} \end{cases} \quad (3.3)$$

For future reference, we note the integration by parts relation:

$$\int_{-\infty}^{+\infty} \Psi''(x) x^p dx = x^p \Psi'|_{-\infty}^{+\infty} - p x^{p-1} \Psi|_{-\infty}^{+\infty} + p(p-1) \mu_{p-2}. \quad (3.4)$$

Because the physical, bounded, solution must satisfy the boundary conditions $\Psi(x) = 0$ at $\pm\infty$, the previous relation becomes:

$$\int_{-\infty}^{+\infty} \Psi''(x) x^p dx = p(p-1) \mu_{p-2}. \quad (3.5)$$

Integrating both sides of Eq.(3.1) with respect to x^p , we obtain

$$\int_{-\infty}^{+\infty} (-\Psi'' + (x^2 + x^6) \Psi) x^p dx = \int_{-\infty}^{+\infty} E \Psi x^p dx, \quad (3.6)$$

which becomes the moment equation:

$$p(p-1) \mu_{p-2} - \mu_{p+6} - \mu_{p+2} + E \mu_p = 0. \quad (3.7)$$

We can now exploit the symmetric nature of the desired wavefunction. The even order Hamburger moments become ordinary Stieltjes moments for a modified function. Thus, for $p \rightarrow 2p$, we have:

$$\mu_{2p} = \int_{-\infty}^{+\infty} \Psi(x) x^{2p} dx = 2 \int_0^{+\infty} \frac{\Psi(\sqrt{x^2})}{2\sqrt{x^2}} x^{2p} dx^2, \quad (3.8)$$

or, upon defining $y \equiv x^2$,

$$u_p \equiv \int_{-\infty}^{+\infty} \frac{\Psi(\sqrt{y})}{2\sqrt{y}} y^p dy. \quad (3.9)$$

These are the Stieltjes moments for the integrand function given. In summary:

$$\mu_{2p} = u_p. \quad (3.10)$$

Making the appropriate substitution in the Hamburger moment equation, we obtain the Stieltjes moment equation:

$$2p(2p-1) u_{p-1} - u_{p+3} - u_{p+1} + E u_p = 0. \quad (3.11)$$

3.1.2 Missing Moment Dependence of the Stieltjes Moment Equation

We can rewrite Eq.(3.11) as

$$u_{p+3} = 2p(2p-1)u_{p-1} + Eu_p - u_{p+1}, \quad (3.12)$$

for $p \geq 0$. This recursive moment equation involves the initialization (missing) moment variables : u_0, u_1, u_2 . That is, any other moment can be expressed as a linear combination of the missing moments:

$$u_p = \sum_{l=0}^2 M_{p,l}(E)u_l. \quad (3.13)$$

Substituting this relation into the moment equation, and recognizing that the missing moments are independent variables, yields the recursion relation for the M -coefficients (the E dependence is implicitly assumed):

$$M_{p+3,l} = 2p(2p-1)M_{p-1,l} + EM_{p,l} - M_{p+1,l} \quad l = 0, 1, 2. \quad (3.14)$$

In order to quantize the system, we must impose some normalization. Since we are dealing with positive (missing) moment variables, we can take

$$u_0 + u_1 + u_2 = 1. \quad (3.15)$$

Clearly, this constraint limits the missing moments to lie within the unit hypercube, $0 \leq u(0), u(1), u(2) \leq 1$. We can now generate (for instance) the zeroth order moment in terms of the other missing moments: $u_0 = 1 - u_1 - u_2$. Thus, there are actually only two unconstrained missing moments, and (u_1, u_2) must lie within the unit square.

In terms of the unconstrained missing moment variables, the moment/missing moment relation becomes

$$u_p = \sum_{l=0}^2 M_{p,l}(E)u_l = M_{p,0}(E) + (M_{p,1}(E) - M_{p,0}(E))u_1 + (M_{p,2}(E) - M_{p,0}(E))u_2, \quad (3.16)$$

or, more succinctly,

$$u_p = \sum_{l=0}^2 \hat{M}_{p,l}(E) \hat{u}_l, \quad (3.17)$$

where

$$\hat{M}_{p,l} = \begin{cases} M_{p,0}, & \text{if } l = 0 \\ M_{p,l} - M_{p,0}, & \text{if } l = 1, 2 \end{cases}, \quad (3.18)$$

and

$$\hat{u}_l = \begin{cases} 1, & \text{if } l = 0 \\ u_l, & \text{if } l = 1, 2 \end{cases}. \quad (3.19)$$

The $\hat{M}$ coefficients satisfy the same recursive relation structure with respect to the p - index:

$$\hat{M}_{p+3,l} = 2p(2p-1)\hat{M}_{p-1,l} + E\hat{M}_{p,l} - \hat{M}_{p+1,l} \quad l = 0, 1, 2 \quad (3.20)$$

although the required initialization conditions are different (as expected):

$$\begin{aligned} \hat{M}_{0,0} &= 1, & \hat{M}_{1,0} &= 0, & \hat{M}_{2,0} &= 0, \\ \hat{M}_{0,1} &= -1, & \hat{M}_{1,1} &= 1, & \hat{M}_{2,1} &= 0, \\ \hat{M}_{0,2} &= -1, & \hat{M}_{1,2} &= 0, & \hat{M}_{2,2} &= 1, \end{aligned} \quad (3.21)$$

3.2 Numerical Implementation of the EMM Formalism

Since the Stieltjes moments are linearly dependent on the corresponding missing moments, and nonlinearly dependent on the energy, we can substitute this relation into the HH determinantal inequality relations

$$\Delta_{m,n}(u) = \text{Det}(u_{m+n_1+n_2}) > 0, \quad 0 \leq n_{1,2} \leq n \rightarrow \infty, \quad (3.22)$$

for $m = 0, 1$. The impacted moment matrix is

$$\mathcal{M}_m^{(n)}(u_1, u_2; E) = \begin{pmatrix} u_m & u_{m+1} & \cdot & \cdot & \cdot & u_{m+n} \\ u_{m+1} & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ u_{m+n} & \cdot & \cdot & \cdot & \cdot & u_{m+2n} \end{pmatrix}, \quad (3.23)$$

where the missing moment (i.e., $u_{1,2}$) and energy (E) dependence ensues upon substituting the appropriate moment equation relation (i.e., Eq.(3.17)) for the corresponding moment-matrix element.

Computationally, in order to determine the physical ground state energy, one first starts at some low moment order (i.e., $u_{p \leq \mathcal{P}_{max}}$) and determines the energy interval, such that for every energy value within that interval there exists a u_1, u_2 solution set to Eq.(3.22). Numerically, this entails partitioning a given (arbitrarily large) energy interval, $[E_1^{(\mathcal{P}_{max})}, E_2^{(\mathcal{P}_{max})}]$, and at each partition point, $E_i \in [E_1^{(\mathcal{P}_{max})}, E_2^{(\mathcal{P}_{max})}]$, determining what (unconstrained) missing moment values generate moments, $\{u_{p \leq \mathcal{P}_{max}}\}$, that satisfy the HH inequalities in Eq.(3.22).

If one wants to implement the above in terms of the HH relations, then one must also define a sufficiently fine grid within the unit square in the missing moment space, and at each (u_1, u_2) point assessing the compliance of the HH positivity relations. The numerically generated set of missing moment coordinate pairs that satisfy the HH inequalities (for the given E_i energy partition value) define a non-linear convex missing moment solution set, $\mathcal{U}^{(\mathcal{P}_{max})}(E_i)$. All of the energy partition points for which $\mathcal{U}^{(\mathcal{P}_{max})}(E_i) \neq \emptyset$, in turn define a new (smaller) energy interval, for which the entire procedure is repeated at the next moment order, $\mathcal{P}_{max} \rightarrow \mathcal{P}_{max} + 1$. As the moment order increases, the feasible energy interval decreases, and the corresponding endpoints define the lower and upper values for the ground state energy.

We summarize the procedure below.

- i. Pick starting (low order) value for $\mathcal{P}_{max}$.
- ii. Pick arbitrary starting energy interval, $[E_1, E_2]$.

- iii. Partition energy interval. At each partition point, E_i , determine existence or nonexistence of (u_1, u_2) missing moment set, $\mathcal{U}^{(\mathcal{P}_{max})}$, for which the generated moments, up to order $\mathcal{P}_{max}$, satisfy the HH determinantal inequalities in Eq.(3.22). This process requires one to partition the unit square (i.e., generate a mesh set of grid points), and at each coordinate pair on the grid, determine if Eq.(3.22) is satisfied.
- iv. If for a given E_i no $u_{1,2}$ can be found, that is $\mathcal{U}^{(\mathcal{P}_{max})} = \emptyset$, then that E_i is not a possible physical value for the ground state energy. This assumes that the missing moment grid is sufficiently fine so that no possible solution points to Eq.(3.22) are missed.

If for a given energy partition value, E_i , there exists a missing moment solution set, $\mathcal{U}^{(\mathcal{P}_{max})} \neq \emptyset$, then that E_i is a possible physical value.

- v. The updated (reduced) set of energy partition points which are physically possible, define a new energy interval on which the entire procedure is repeated, at the next higher order, $\mathcal{P}_{max} \rightarrow \mathcal{P}_{max} + 1$. The new energy interval can be noted as $[E_1^{(\mathcal{P}_{max}+1)}, E_2^{(\mathcal{P}_{max}+1)}]$.
- vi. The generated set of feasible energy interval endpoints define the converging lower and upper bounds to the physical ground state energy:

$$E_1^{(\mathcal{P}_{max})} \leq E_1^{(\mathcal{P}_{max}+1)} \leq \dots \leq E_{gr} \leq \dots \leq E_2^{(\mathcal{P}_{max}+1)} \leq E_2^{(\mathcal{P}_{max})}. \quad (3.24)$$

The numerical implementation of the above EMM-HH approach is discussed in Section (2.2.1).

Clearly, the above procedure is tedious to implement on larger missing moment order problems (i.e., $m_s \geq 3$), since defining a grid within the unit hypercube is prohibitively expensive. An alternative procedure, which is much more elegant and efficient, is to implement a linear programming (LP) based, *cutting method* analysis, by which to determine the existence of the $\mathcal{U}$ convex sets, and thereby, the physical ground state energy [23, 24]. The numerical details are in Section (2.2.2). We refer to this as the EMM-LP approach. It is completely equivalent to the EMM-HH, although much easier to implement for large missing moment order problems. Using

this approach, Handy and co-workers have been able to analyze systems with an effective missing moment order of $m_s \leq 12$. Further algorithmic/numerical improvements on the LP based EMM procedure enable one to investigate larger missing moment systems.

3.2.1 Computational Implementation of EMM-HH

In this section, we use the HH-determinants to compute the energy bounds for the Schrödinger equation with potential $V(x) = x^2 + x^6$.

The author wrote a program in Mathematica. We briefly describe the essentials of our program.

(1). First, we obtain the recursive formula for generating the Stieltjes moments, u_p , in terms of the unconstrained missing moments, u_1, u_2 , and the energy E (e in program), using Eq.(3.16)-(3.19).

(2). Next, defining $\mathcal{P}_{max}$ as the maximum moment number, we generate all the determinants $\Delta_{m,n}(u)$, with $m = 0$ or 1 , satisfying $m + 2n \leq \mathcal{P}_{max}$. For example, if $\mathcal{P}_{max} = 6$, then we generate $\Delta_{0,0}(u)$, $\Delta_{0,1}(u)$, $\Delta_{0,2}(u)$, $\Delta_{0,3}(u)$, $\Delta_{1,0}(u)$, $\Delta_{1,1}(u)$, $\Delta_{1,2}(u)$.

(3). We must then consider a “do loop” in order to sample all of the energy partition values (e) lying within an arbitrary energy interval. In the numerical example, we take: $0 \leq e \leq 3$, with a partition size of $\delta e = 0.1$. For each partition point energy value (i.e., $e = 0, 0.1, 0.2, \dots$), we write another double “do-loop” structure in order to sample (unconstrained) missing moment coordinate pairs, $(u(1), u(2))$, lying within the unit square: $0 < u(1), u(2) < 1$. Here we take the grid size to be $\delta u = 0.01$.

(4). For each energy partition value, e , we test all of the missing moment grid points to determine which of these generate moments that have positive HH determinants, $\Delta_{m,n}(u_1, u_2; e) > 0$. These points are then stored in a file and plotted.

In Figure 1 through 8 we show the missing moment grid points that generate positive HH determinants up to the $\mathcal{P}_{max}$ order indicated. Clearly, as more moments

are used, the size of the missing moment solution set quickly becomes smaller, requiring that we increase the energy partition point resolution (that is, make δe smaller). As $\mathcal{P}_{max}$ increases, the set of energy points admitting HH solutions shrinks. Finally, in Figure 8, at $\mathcal{P}_{max} = 7$ order, we obtain energy bounds $1.380 \leq E_g \leq 1.460$. In Table 1, we give the numerical bounds for the energy, corresponding to the various figures. In addition, we show the results for higher moment orders than those represented in the figures.

If one proceeds to order $\mathcal{P}_{max} = 30$, one obtains the result $1.4356246190092 < E_{gr} < 1.43562461901777$, with E_{gr} determined to within one part in 10^{12} .

We expound upon the various figures below.

Figure 1. $\mathcal{P}_{max} = 0, 1$, and $0 < e < 3$, with $\delta e = 0.1$. All energies are feasible.

Figure 2. $\mathcal{P}_{max} = 2$, and $0 < e < 3$, with $\delta e = 0.1$. All energies are feasible.

Figure 3. $\mathcal{P}_{max} = 3$, and $0 < e < 3$, with $\delta e = 0.1$. All energies in this interval are feasible; however, at $e = 0.1$, the size of the missing moment feasible region is very small, in comparison to the missing moment feasible regions for other energy values.

Figure 4. $\mathcal{P}_{max} = 4$, and $0 < e < 3$, with $\delta e = 0.1$. Now the size of the feasible missing moment solution is significantly small near the end point energy values (i.e., 0 and 3).

Figure 5. $\mathcal{P}_{max} = 5$, and $0 < e < 3$, with $\delta e = 0.1$. The previous manifestation becomes more pronounced. Indeed, there is no discernable missing moment solution set for $0 < e < 1.3$. It is clear that we must increase the energy resolution (i.e., partition) size.

Figure 6. $\mathcal{P}_{max} = 6$, and $0 < e < 3$, with $\delta e = 0.1$. The results here confirm the previous observation.

Figure 7. $\mathcal{P}_{max} = 6$, and $1.3 < e < 1.6$, with $\delta e = 0.01$. No discernable missing moment solution sets found for energy values outside of the reduced interval. Even at this level, for $1.49 < e < 1.6$, there is no discernable missing moment solution either.

Figure 1. Distribution of (u_1, u_2) with $\mathcal{P}_{max} = 0.1$, $0 < e < 3$, $\delta e = 0.1$

Figure 2. Distribution of (u_1, u_2) with $\mathcal{P}_{max} = 2$, $0 < e < 3$, $\delta e = 0.1$

Figure 8. $\mathcal{P}_{max} = 7$, and $1.340 < e < 1.510$, with $\delta e = 0.05$.

When $\mathcal{P}_{max}$ increases, the (u_1, u_2) area became smaller, and its points density is related to step length of u_1, u_2 ,

Figure 3. Distribution of (u_1, u_2) with $\mathcal{P}_{max} = 3$, $0 < e < 3$, $\delta e = 0.1$

Figure 4. Distribution of (u_1, u_2) with $\mathcal{P}_{max} = 4$, $0 < e < 3$, $\delta e = 0.1$

Figure 5. Distribution of (u_1, u_2) with $\mathcal{P}_{max} = 5$, $0 < e < 3$, $\delta e = 0.1$

Figure 6. Distribution of (u_1, u_2) with $\mathcal{P}_{max} = 6$, $0 < e < 3$, $\delta e = 0.1$

Figure 7. Distribution of (u_1, u_2) with $\mathcal{P}_{max} = 6$, $1.30 < e < 1.60$, $\delta e = 0.01$

Figure 8. Distribution of (u_1, u_2) with $\mathcal{P}_{max} = 7$, $1.340 < e < 1.510$, $\delta e = 0.05$

Table 1. Ground State Energy Bounds with the Increase of $\mathcal{P}_{max}$ using HH Method

$\mathcal{P}_{max}$	e interval	e step	e bounds
0,1,2	$0.1 \leq e \leq 2.9$	0.1	$0.1 \leq e \leq 2.9$
3	$0.1 \leq e \leq 2.9$	0.1	$0.1 \leq e \leq 2.9$
4	$0.1 \leq e \leq 2.9$	0.1	$0.1 \leq e \leq 2.9$
5	$0.1 \leq e \leq 2.9$	0.1	$1.3 \leq e \leq 2.9$
6	$0.1 \leq e \leq 2.9$	0.1	$1.3 \leq e \leq 2.9$
6	$1.30 \leq e \leq 1.59$	0.01	$1.33 \leq e \leq 1.48$
7	$1.340 \leq e \leq 1.510$	0.005	$1.385 \leq e \leq 1.455$
8	$1.385 \leq e \leq 1.460$	0.002	$1.411 \leq e \leq 1.459$
9	$1.410 \leq e \leq 1.460$	0.002	$1.432 \leq e \leq 1.452$

In Table 1 we show how the ground state energy bounds change with increasing $\mathcal{P}_{max}$. Clearly, the bounds become tighter as the order increases. One should compare the entries with the corresponding figures previously given. One can see that when $\mathcal{P}_{max}$ becomes 6, the bounds become $1.33 < e < 1.48$, and are then used at the next moment order.

So clearly we can see that the e bounds become tighter as $\mathcal{P}_{max}$ increases.

3.2.2 Computational Implementation of EMM-LP

In this section we will show how to apply the *Cutting Method* linear programming (LP) analysis for the EMM approach. This will yield exactly the same result as that discussed previously for the EMM-HH analysis. The illustration in Figure 9 and Table 2, combined with a description of the EMM-LP procedure, will facilitate the understanding of the present approach.

In the EMM-LP implementation, one uses linear programming to define an optimal, finite, sequence of lines, in the (two dimensional) missing moment plane, which can quickly determine the existence, or non-existence, of the $\mathcal{U}^{(\mathcal{P}_{max})}$ missing moment solution set. These lines are referred to as *cutting lines*, since they quickly

slice up the starting unit square into either the null set (thereby confirming that $\mathcal{U}^{(\mathcal{P}_{max})} = \emptyset$), or a finite polytope (i.e., a convex set whose boundary is made up of intersecting straight lines) which contains the missing moment solution (thereby determining that the associated energy partition point is feasible).

The center of the indicated polytope is very important. In the EMM-LP algorithm, the center, referred to as the *Deep Interior Point* (DIP) is defined as the center of the largest inscribed circle within the polytope. At the DIP, one determines the negative eigenvectors of the moment matrices (i.e., $m = 0, 1$) in Eq.(3.23) (if they exist, otherwise the DIP must lie within $\mathcal{U}^{(\mathcal{P}_{max})}$, which in turn implies its existence). These negative eigenvectors, in turn, define the cutting vectors, when projected into the missing moment plane.

We give a brief overview of the numerical implementation of the above, corresponding to the Mathematica program developed by the author.

- (1). As in the EMM-HH approach, we pick a low $\mathcal{P}_{max}$ moment order.
- (2). For $m = 0, 1$, we generate the maximum moment matrix $\mathcal{M}_m^{(n)}(u_1, u_2; E)$ consistent with the chosen $\mathcal{P}_{max}$ value. For example, when $\mathcal{P}_{max} = 6$, we work with $\mathcal{M}_0^{(3)}(u_1, u_2; E)$ and $\mathcal{M}_1^{(2)}(u_1, u_2; E)$.
- (3). Having picked an arbitrary (large) energy interval, we define a sufficiently small partition, and loop on each E_i energy partition value (e in the program).
- (4). As before, for each E_i , we must determine the existence or non-existence of $\mathcal{U}^{(\mathcal{P}_{max})}$. Within the EMM-LP, this determination is made by generating a finite number of cutting vectors which either admit a common region, or have no such region. The region in question is a polytope, if it exists. This polytope, $\mathcal{P}$, will either satisfy, $\mathcal{U}^{(\mathcal{P}_{max})} \subset \mathcal{P} \neq \emptyset$, or $\mathcal{U}^{(\mathcal{P}_{max})} \subset \mathcal{P} = \emptyset$. Clearly, the first means that the associated missing moment solution set exists, the second indicates that the missing moment solution set does not exist.
- (5). The generation of $\mathcal{P}$ is done iteratively. At each step, the updated DIP must be located. For each generated DIP, two sets of cutting vectors are generated, one for the $m = 0$ moment matrix, and the other for the $m = 1$ moment matrix, as defined above. This procedure continues until no cutting vectors can be found. This

means that both moment matrices are positive (i.e, have no negative eigenvectors). Hence the DIP must lie within $\mathcal{U}^{(\mathcal{P}_{max})}$; thereby establishing the existence of the missing moment solution set. Alternatively, one might find that the generated, finite sequence, of cutting vectors completely eliminates the starting unit square. This means that no polytope is possible. That is, $\mathcal{U}^{(\mathcal{P}_{max})} = \emptyset$.

The following is a detailed description for $\mathcal{P}_{max} = 6$ and $E = e = 1.430$. We know from the EMM-HH analysis that there must exist a missing moment solution set for this case. By examining the features depicted in Figure 9, the *cutting* aspect of the EMM-LP approach becomes transparent.

Cell# 1 in Figure 9.

From the (positive) unit square (normalization) constraints we obtain the starting polytope as defined by the linear inequalities:

$$u_1 < 1, -u_1 < 0, u_2 < 1, -u_2 < 0. \quad (3.25)$$

The center of the largest inscribed circle defines the *deep interior point* (DIP): $(\frac{1}{2}, \frac{1}{2})$. The eigenvalues for the $\mathcal{M}_0^{(3)}(u_1, u_2; E)$ -moment matrix (Eq.(3.23)) are: 17.1485, -3.11748, 0.812586, -0.0590889; whereas, the eigenvalues for the $\mathcal{M}_1^{(2)}(u_1, u_2; E)$ -moment matrix are: 7.25663, -0.726547, 0.685419.

The presence of at least one non-positive eigenvalue tells us that the DIP cannot lie within $\mathcal{U}^{(\mathcal{P}_{max})}$, if the latter exists. Each non-positive eigenvalue generates a *cut* within the (two dimensional) missing moment space. If $\mathcal{U}^{(\mathcal{P}_{max})}$ exists, it must lie on the positive side of this cut.

Cell # 2 in Figure 9.

For each set of eigenvalues, one only need consider the algebraically smallest eigenvalue. In the present case, we must consider both the -3.11748 eigenvalue, and the -0.726547 eigenvalue. The corresponding eigenvectors are denoted by $\vec{C}_0$ and $\vec{C}_1$, respectively. Upon considering the expected value formed from the corresponding eigenvector and moment-matrix, we can generate the cuts corresponding to the following linear inequalities (refer to the discussion in the context of Eq.(2.27)):

$$\begin{aligned}
& -(2.98472 - 11.6864u_1 - 0.518313u_2) < 0, \\
& -(1.07573 - 1.90011u_1 - 1.70453u_2) < 0.
\end{aligned} \tag{3.26}$$

Combining these inequalities (cuts) with the original ones in Eq.(3.25) gives us an updated polytope. For completeness, we make explicit the derivation of the above inequalities.

We consider the two scalar functions associated with each of the eigenvectors (refer to Eqs.(3.17-19)):

$$\Lambda_m(u_1, u_2) \equiv \langle \vec{C}_m | \hat{M}_{m,0} | \vec{C}_m \rangle + \sum_{\ell=1}^2 u_\ell \langle \vec{C}_m | \hat{M}_{m;\ell} | \vec{C}_m \rangle, \tag{3.27}$$

for $m = 0, 1$, and adopting the definition for the indicated matrices: $(\hat{M}_{m;\ell})_{j_1, j_2} \equiv \hat{M}_{m+j_1+j_2, \ell}$, for $0 \leq \ell \leq m_s$.

At the DIP, the scalar functions are negative, as determined by the previous negative eigenvalues: $\Lambda_0(\frac{1}{2}, \frac{1}{2}) = -3.11748$ and $\Lambda_1(\frac{1}{2}, \frac{1}{2}) = -0.726547$.

Because each of the two moment matrices, evaluated at the DIP, has a negative eigenvalue, we know that if the $\mathcal{U}^{(\mathcal{P}_{max}=6)}$ convex set exists, it must lie in the missing moment region making the scalar functions positive. This is how Eq.(3.26) comes about.

We can repeat the entire process, and find the updated DIP, which now becomes: (0.12487, 0.12487). The entire process is repeated.

In Figure 9 we detail the above process step by step. In Table 2 we give the numerical values for the generated cuts, the corresponding DIP, and the relevant eigenvalues. We note that the last entry for the eigenvalues shows them all to be positive. This confirms that at the chosen energy partition value, $e = 1.430$, to maximum moment order, $\mathcal{P}_{max} = 6$, there exists a missing moment solution set. That is, the indicated energy value is a possible physical value for the ground state energy.

Table 2. Constraints, DIPs, Eigenvalues Step by Step Using Cutting Method

No.	Constraints	DIP	Eigenvalues
1	$u_1 < 1, -u_1 < 0, u_2 < 1, -u_2 < 0$	(1/2, 1/2)	-3.1175, -0.7265
2	$-(2.9847 - 11.6864u_1 - 0.5183u_2) < 0$ $-(1.0757 - 1.9001u_1 - 1.7045u_2) < 0$	(0.1248, 0.1249)	-0.6988, -1.0760
3	$-(-2.7640 + 8.8315u_1 + 4.6871u_2) < 0$ $-(-2.0437 + 4.2625u_1 + 6.5080u_2) < 0$	(0.1887, 0.3437)	-0.0441
4	$-(0.5338 - 0.4953u_1 - 1.4091u_2) < 0$	(0.2091, 0.2689)	-0.0127
5	$-(-0.5884 + 1.1946u_1 + 1.2117u_2) < 0$	0.2276, 0.2826	<i>all positive</i>

The plots in Figure 9 depict the numerical results contained in Table 2. If we compare the subplots No. 5 and No. 6 with that given for the EMM-HH approach, we see that the indicated polytopes in Figure 9 contain the missing moment solution set region given in Figure 7. Both methods give identical results and verify the high level of precision possible through EMM [23, 24].

Table 3 shows the tighter and tighter energy bounds as $\mathcal{P}_{max}$ increases. It can be compared with Table 1.

Actually when implementing the computation, the EMM-LP Cutting Method is much faster than EMM-HH Method because one does not have to partition the unit square. The DIP is automatically generated, and it, in turn, allows us to automatically locate the possible location of the missing moment solution set.

Figure 9. Cutting Lines, DIPs of Cutting Method and Comparison with HH Method
($\mathcal{P}_{max} = 6$, $e = 1.43$)

Table 3. Ground State Energy Bounds with the Increase of $\mathcal{P}_{max}$ using Cutting Method

$\mathcal{P}_{max}$	e interval	e step	e bounds
1,2,3,4,5	$0.1 \leq e \leq 2.9$	0.1	$0.1 \leq e \leq 2.9$
6	$0.1 \leq e \leq 2.9$	0.1	$e = 1.4$
8	$1.3 \leq e \leq 1.5$	0.01	$1.41 \leq e \leq 1.47$
10	$1.4 \leq e \leq 1.48$	0.005	$1.43 \leq e \leq 1.435$
12	$1.425 \leq e \leq 1.44$	0.001	$1.428 \leq e \leq 1.438$
14	$1.427 \leq e \leq 1.439$	0.001	$1.430 \leq e \leq 1.435$
16	$1.429 \leq e \leq 1.438$	0.0002	$1.4352 \leq e \leq 1.4368$
18	$1.435 \leq e \leq 1.4368$	0.0001	$1.4354 \leq e \leq 1.4360$
20	$1.4352 \leq e \leq 1.460$	0.001	$1.4354 \leq e \leq 1.4355$

The value of the preceding pedagogic example is that we see the practicality of the EMM-LP approach once a nonnegativity representation of the physical problem is realized. This is referred to, in the next chapter, as the Nonnegativity Quantization Representation (NQR). As indicated at the outset, our ultimate objective is to apply this NQR computational formalism to the $-(ix)^N$ potential. This is the basic focus of the next chapter.

CHAPTER 4

GENERATION OF CONVERGING BOUNDS FOR THE GROUND AND EXCITED STATES OF THE $-(IX)^N$ POTENTIAL

In their seminal work, Bender and Boettcher [1] discovered the existence of PT invariant, bounded, solutions for the $-(ix)^N$ potential, lying within certain wedges in the complex plane, $\mathcal{C}_x$, which do not include the real axis for (integer) $N \geq 4$. These bounded (exponentially vanishing at infinity, along the complex contours) solutions are, necessarily, complex.

Since our interest is to test the effectiveness of the EMM-LP approach, we must transform the above system into one for which the desired solutions are uniquely nonnegative and bounded. This is made possible by utilizing the Nonnegativity Quantization Representation (NQR) developed by Handy [12, 13], and Handy and Wang [14]. In these works, it is shown that the one dimensional Schrödinger equation, for arbitrary (complex) potential, and on any contour in the complex- x plane ($\xi \in \mathfrak{R} \rightarrow x(\xi) \in \mathcal{C}$), can be transformed into an equivalent, fourth order, linear differential equation for the probability density, $S(\xi) \equiv |\Psi(x(\xi))|^2$.

Returning to the Bender and Boettcher formalism, upon adopting the polar complex number representation $x \equiv |x|e^{i\theta}$, the “boundedness” wedges (within which the bound states lie) are defined by

$$\theta_{L,R} - \frac{\tilde{\Delta}}{2} < \theta < \theta_{L,R} + \frac{\tilde{\Delta}}{2}, \quad (4.1)$$

where

$$\theta_{L,R} = \begin{cases} -\pi + \frac{N-2}{N+2} \frac{\pi}{2}, & \text{“}L \text{ (left)}\text{”} \\ -\frac{N-2}{N+2} \frac{\pi}{2}, & \text{“}R \text{ (right)}\text{”} \end{cases}, \quad (4.2)$$

and

$$\tilde{\Delta} = \frac{2\pi}{N+2}. \quad (4.3)$$

Our interest is to examine the efficiency of the EMM-LP procedure for $N \geq 4$.

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

$$\{x|EMM \text{ complex contour}\} = \{\xi e^{-i\theta}|\xi : \infty \rightarrow 0\} \cup \{\xi e^{+i\theta}|\xi : 0 \rightarrow \infty\}, \quad (4.4)$$

for any θ within the “Right” handed wedge, as defined above.

We will 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 $N \in \text{even}$ and $N \in \text{odd}$ are very different.

4.1 The $-(ix)^4$ Potential

4.1.1 The Nonnegativity Quantization Representation

We will adopt the formalism developed by Handy and Wang [15]. Consider the Schrödinger equation

$$-\partial_x^2 \Psi(x) + \mathcal{V}(x)\Psi(x) = E\Psi(x), \quad (4.5)$$

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:

$$x(\xi) : \xi \in \mathfrak{R} \rightarrow \mathcal{C}. \quad (4.6)$$

The transformed Schrödinger equation is

$$-\left(D(\xi)\partial_\xi\right)^2\Psi(\xi)+V(\xi)\Psi(\xi)=E\Psi(\xi), \quad (4.7)$$

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

$$A(\xi)\partial_\xi^2\Psi(\xi)+B(\xi)\partial_\xi\Psi(\xi)+C(\xi)\Psi(\xi)=0, \quad (4.8)$$

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

Define

$$S(\xi) = \Psi^*(\xi)\Psi(\xi), \quad (4.9)$$

$$P(\xi) = \Psi'^*(\xi)\Psi'(\xi), \quad (4.10)$$

$$J(\xi) = \frac{\Psi(\xi)\partial_\xi\Psi^*(\xi) - \Psi^*(\xi)\partial_\xi\Psi(\xi)}{2i}, \quad (4.11)$$

and

$$T(\xi) = \frac{\partial_\xi\Psi(\xi)\partial_\xi^2\Psi^*(\xi) - \partial_\xi\Psi^*(\xi)\partial_\xi^2\Psi(\xi)}{2i}. \quad (4.12)$$

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

$$(S''(\xi) - 2P(\xi))A_R(\xi) + S'(\xi)B_R(\xi) + 2S(\xi)C_R(\xi) + 2(B_I(\xi) + A_I(\xi)\partial_\xi)J(\xi) = 0, \quad (4.13)$$

$$(S''(\xi) - 2P(\xi))A_I(\xi) + S'(\xi)B_I(\xi) + 2S(\xi)C_I(\xi) - 2(B_R(\xi) + A_R(\xi)\partial_\xi)J(\xi) = 0, \quad (4.14)$$

$$P'(\xi)A_R(\xi) + 2T(\xi)A_I(\xi) + 2P(\xi)B_R(\xi) + S'(\xi)C_R(\xi) - 2J(\xi)C_I(\xi) = 0, \quad (4.15)$$

and

$$P'(\xi)A_I(\xi) - 2T(\xi)A_R(\xi) + 2P(\xi)B_I(\xi) + S'(\xi)C_I(\xi) + 2J(\xi)C_R(\xi) = 0. \quad (4.16)$$

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 nonnegative configurations that must be bounded (i.e., L^1 , since Ψ is L^2) for physical solutions. Accordingly, we refer to the above as the nonnegativity quantization representation (NQR).

One can easily find a contour map that maps into the required wedges, as defined previously. Thus, $x(\xi) = e^{i\theta}\xi - \frac{e^{-i\theta}}{\xi}$, for $\xi : 0 \rightarrow \infty$, 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 $x_{R,L} = \xi e^{i\theta}$, $\xi \geq 0$, 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.

4.1.2 Obtaining the Moment Equations for $-(ix)^4$ Within the NQR Formulation

Consistent with the works of Bender and Boettcher [1], and Dorey et al. [19, 20], we will assume that the discrete states 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

$$-\Psi''(z) - z^4\Psi(z) = E\Psi(z). \quad (4.17)$$

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

Within the right wedge the Schrödinger equation becomes

$$\Psi_R''(\xi) + \xi^4 e^{6i\theta} \Psi_R(\xi) + E e^{2i\theta} \Psi_R = 0. \quad (4.18)$$

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

$$\Psi_L''(\xi) + \xi^4 e^{-6i\theta} \Psi_L(\xi) + E e^{-2i\theta} \Psi_L(\xi) = 0. \quad (4.19)$$

Upon comparing with Eq.(4.8), we identify the coefficient functions as $A = 1$, $B = 0$, $C(\xi) = \xi^4 e^{6i\theta} + E e^{2i\theta}$. 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

$$C_R(\xi) = \xi^4 C_6 + E C_2, \quad (4.20)$$

and

$$C_I(\xi) = \xi^4 S_6 E S_2, \quad (4.21)$$

involving $C_n = \text{Cos}(n\theta)$, $S_n = \text{Sin}(n\theta)$.

The corresponding NQR equations become

$$S''(\xi) - 2P(\xi) + 2(\xi^4 C_6 + E C_2)S(\xi) = 0, \quad (4.22)$$

$$(\xi^4 S_6 E S_2)S(\xi) - J'(\xi) = 0, \quad (4.23)$$

and

$$P'(\xi) + (\xi^4 C_6 + E C_2)S'(\xi) - 2(\xi^4 S_6 E S_2)J(\xi) = 0. \quad (4.24)$$

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

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

$$U(p) = \int_0^\infty d\xi S(\xi) \xi^p, \quad (4.25)$$

$$V(p) = \int_0^\infty d\xi P(\xi) \xi^p, \quad (4.26)$$

$$W(p) = \int_0^\infty d\xi J(\xi) \xi^p. \quad (4.27)$$

We multiply each of the relations in Eq.(4.22-24) by ξ^p and integrate over $[0, \infty)$, making use of the integration-by-parts formulae:

$$\int_0^\infty d\xi S''(\xi) \xi^p = -\delta_{p,0} S'(0) + \delta_{p,1} S(0) + p(p-1)U(p-2), \quad (4.28)$$

$$\int_0^\infty d\xi P'(\xi) \xi^p = -\delta_{p,0} P(0) - pV(p-1), \quad (4.29)$$

$$\int_0^\infty d\xi J'(\xi)\xi^p = -\delta_{p,0}J(0) - pW(p-1). \quad (4.30)$$

The required $\{U, V, W\}$ moment equations are

$$-\delta_{p,0}S'(0) + \delta_{p,1}S(0) + p(p-1)U(p-2) - 2V(p) + 2[C_6U(p+4) + EC_2U(p)] = 0, \quad (4.31)$$

$$S_6U(p+4) + ES_2U(p)[\delta_{p,0}J(0) + pW(p-1)] = 0, \quad (4.32)$$

$$\begin{aligned} -\delta_{p,0}P(0) - pV(p-1) - C_6(p+4)U(p+3) - EC_2[\delta_{p,0}S(0) + pU(p-1)] \\ - 2[S_6W(p+4)S_2W(p)] = 0, \end{aligned} \quad (4.33)$$

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

Eq.(4.32) generates two different relations. For $p = 0$ it becomes

$$S_6U(4) + ES_2U(0) = J(0). \quad (4.34)$$

This defines a constraint on the U -moments. For $p \geq 1$ in Eq.(4.32) the W -moments are generated from the U -moments (i.e., take $p \rightarrow p+1$ in Eq.(4.32)):

$$W(p) = \left(\frac{S_6U(p+5) + ES_2U(p+1)}{p+1} \right), \quad (4.35)$$

where $p \geq 0$.

Since Eq.(4.31) serves to generate the V -moments in terms of the U -moments, we can couple this with the previous relation and convert Eq.(4.33) into one moment equation for the U -moments. Thus we get:

$$\begin{aligned} -S(0)\delta_{p,2} + \frac{S'(0)}{2}\delta_{p,1} - P(0)\delta_{p,0} - C_2ES(0)\delta_{p,0} + U(p-3)\left[-p + \frac{3p^2}{2} - \frac{p^3}{2}\right] \\ + U(p-1)[-2pC_2E] + U(p+1)\left[\frac{2E^2S_2^2}{p+1}\right] + U(p+3)[-4C_6 - 2pC_6] \\ + U(p+5)\left[\frac{2ES_2S_6}{p+1} + \frac{2ES_2S_6}{p+5}\right] + U(p+9)\left[\frac{2S_6^2}{p+5}\right] = 0, \end{aligned} \quad (4.36)$$

for $p \geq 0$. This relation must be combined with the additional constraint in Eq.(4.34).

It is readily apparent that Eq.(4.36) separates into two distinct moment recursion relations for the even and odd order moments. The moment equation in Eq.(4.36) 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:

$$\mu(\rho) \equiv U(2\rho) = \int_0^\infty d\xi S(\xi) \xi^{2\rho} = \int_0^\infty d\eta \frac{1}{2\sqrt{\eta}} S(\sqrt{\eta}) \eta^\rho, \quad (4.37)$$

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

$$\omega(\rho) \equiv U(2\rho + 1) = \int_0^\infty d\xi S(\xi) \xi^{2\rho+1} = \int_0^\infty d\eta \frac{1}{2} S(\sqrt{\eta}) \eta^\rho. \quad (4.38)$$

The respective moment equations become (i.e., $p = 2\rho + 1$, $\rho \geq 0$, in Eq.(4.36)):

$$\begin{aligned} & \frac{S'(0)}{2} \delta_{\rho,0} + \mu(\rho - 1) [-(2\rho + 1) + \frac{3(2\rho + 1)^2}{2} - \frac{(2\rho + 1)^3}{2}] \\ & + \mu(\rho) [-2C_2 E(2\rho + 1)] + \mu(\rho + 1) \left[\frac{E^2 S_2^2}{\rho + 1} \right] + \mu(\rho + 2) [-4C_6 - 2C_6(2\rho + 1)], \\ & + \mu(\rho + 3) \left[E S_2 S_6 \left(\frac{1}{\rho + 1} + \frac{1}{\rho + 3} \right) \right] + \mu(\rho + 5) \left[\frac{S_6^2}{\rho + 3} \right] = 0, \end{aligned} \quad (4.39)$$

together with Eq.(4.34)

$$S_6 \mu(2) + E S_2 \mu(0) = J(0); \quad (4.40)$$

and (i.e., $p = 2\rho$, $\rho \geq 0$, in Eq.(4.36)):

$$\begin{aligned} & -S(0) \delta_{\rho,1} - \delta_{\rho,0} [P(0) + C_2 E S(0)] + \omega(\rho - 2) \left[-2\rho + \frac{3(2\rho)^2}{2} - \frac{(2\rho)^3}{2} \right] \\ & + \omega(\rho - 1) [-4\rho C_2 E] + \omega(\rho) \left[\frac{2E^2 S_2^2}{2\rho + 1} \right] + \omega(\rho + 1) [-4C_6 - 4\rho C_6] \\ & + \omega(\rho + 2) [2E S_2 S_6] \left[\frac{1}{2\rho + 1} + \frac{1}{2\rho + 5} \right] + \omega(\rho + 4) \left[\frac{2S_6^2}{2\rho + 5} \right] = 0. \end{aligned} \quad (4.41)$$

4.1.3 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:

$$\Psi_{R,L}(\xi) = \Psi(\xi e^{i\theta}). \quad (4.42)$$

$$S_{R,L}(\xi) = \Psi_{R,L}(\xi) \Psi_{R,L}^*(\xi) = |\Psi_{R,L}(\xi)|^2. \quad (4.43)$$

$$S'_{R,L}(\xi) = \Psi_{R,L}(\xi) \Psi_{R,L}'^*(\xi) + \Psi_{R,L}'(\xi) \Psi_{R,L}^*(\xi) = 2\text{Re}(\Psi_{R,L} \Psi_{R,L}'^*). \quad (4.44)$$

$$P_{R,L}(\xi) = \Psi_{R,L}'(\xi) \Psi_{R,L}'^*(\xi) = |\Psi_{R,L}'(\xi)|^2. \quad (4.45)$$

$$J_{R,L}(\xi) = \frac{\Psi_{R,L}(\xi) \Psi_{R,L}'^*(\xi) - \Psi_{R,L}'(\xi) \Psi_{R,L}^*(\xi)}{2i} = \text{Im}(\Psi_{R,L}(\xi) \Psi_{R,L}'^*(\xi)). \quad (4.46)$$

From the derivative relation

$$\Psi_{R,L}'(\xi) = \Psi'(z)(e^{i\theta}) \quad (4.47)$$

it follows that

$$\Psi_{R,L}'(0) = (e^{i\theta}) \Psi'(z)|_{z=0}. \quad (4.48)$$

Define $\Psi'(z)|_{z=0} = \Delta$, and $e^{i\theta} = \Omega$.

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

$$S_R(0) = S_L(0). \quad (4.49)$$

In addition, $P_{R,L}(0) = |\Psi_{R,L}'(0)|^2 = |\Delta \Omega|^2$ gives

$$P_R(0) = P_L(0). \quad (4.50)$$

We can get S'_R , S'_L from:

$$S'_R(0) = \Psi(0) e^{-i\theta} \Delta^* + \Psi^*(0) e^{i\theta} \Delta$$

$$= 2C_1 \text{Re}(\Psi(0)\Delta^*) + 2S_1 \text{Im}(\Psi(0)\Delta^*), \quad (4.51)$$

and

$$\begin{aligned} S'_L(0) &= -\Psi(0)e^{i\theta}\Delta^* - \Psi^*(0)e^{-i\theta}\Delta \\ &= -2C_1 \text{Re}(\Psi(0)\Delta^*) + 2S_1 \text{Im}(\Psi(0)\Delta^*). \end{aligned} \quad (4.52)$$

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

$$J_R(0) = C_1 \text{Im}(\Psi(0)\Delta^*) - S_1 \text{Re}(\Psi(0)\Delta^*), \quad (4.53)$$

$$J_L(0) = -C_1 \text{Im}(\Psi(0)\Delta^*) - S_1 \text{Re}(\Psi(0)\Delta^*). \quad (4.54)$$

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

$$\Psi^*(-x) = \Psi(x), \quad (4.55)$$

for $x \in \mathfrak{R}$, then from Ψ 's analyticity at the origin we have

$$\Psi(0) \equiv \alpha \in \text{Real}, \quad (4.56)$$

and

$$\Psi'(0) = \Delta \equiv i\beta \in \text{Imaginary}. \quad (4.57)$$

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

$$S'_{R,L}(0) = -2S_1\alpha\beta, \quad (4.58)$$

$$J_{R,L}(0) = -C_1\alpha\beta, \quad (4.59)$$

in particular, for PT invariant solutions:

$$J_{R,L}(0) = \left(\frac{C_1 S'_{R,L}(0)}{2S_1} \right). \quad (4.60)$$

4.1.4 Recursive Structure of the Moment Equation(s)

The discussion in this section will implicitly assume that $S_6 \neq 0$ in Eq.(4.36), otherwise the order of the finite difference/moment equation is reduced. The consequences of this are examined in Subsection E.

At first sight, Eq.(4.41) 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, Eq.(4.41) 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 Eqs.(39-40) do relate 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 Eqs.(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 Eq.(4.39), tells us that all of the moments can be generated through the expression

$$\mu(\rho) = \sum_{\ell=0}^5 \tilde{M}_{\rho,\ell}(E) \chi_{\ell}, \quad (4.61)$$

$\rho \geq 0$, where

$$\chi_{\ell} \equiv \begin{cases} \mu(\ell), & \text{for } 0 \leq \ell \leq 4 \\ S'_R(0), & \text{for } \ell = 5 \end{cases}, \quad (4.62)$$

and

$$\tilde{M}_{\ell_1,\ell_2} = \begin{cases} \delta_{\ell_1,\ell_2}, & \text{for } 0 \leq \ell_{1,2} \leq 4 \\ 0, & \text{for } 0 \leq \ell_1 \leq 4, \ell_2 = 5 \end{cases}. \quad (4.63)$$

In addition, the $\tilde{M}_{\rho,\ell}$ matrix coefficients satisfy the moment equation in Eq.(4.39) with respect to the ρ -index, for fixed ℓ :

$$\frac{\delta_{\ell,5}}{2} \delta_{\rho,0} + \tilde{M}_{\rho-1,\ell}(E) \left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2} \right]$$

$$\begin{aligned}
& + \tilde{M}_{\rho,\ell}(E) [-2C_2 E(2\rho+1)] + \tilde{M}_{\rho+1,\ell}(E) \left[\frac{E^2 S_2^2}{\rho+1} \right] + \tilde{M}_{\rho+2,\ell}(E) [-4C_6 - 2C_6(2\rho+1)] \\
& + \tilde{M}_{\rho+3,\ell}(E) [ES_2 S_6 (\frac{1}{\rho+1} + \frac{1}{\rho+3})] + \tilde{M}_{\rho+5,\ell}(E) \left[\frac{S_6^2}{\rho+3} \right] = 0.
\end{aligned} \tag{4.64}$$

We can now focus on the additional constraint in Eq.(4.40). From Eq.(4.60) we can express $S'_R(0)$ in terms of $\{\mu(0), \mu(2)\}$. That is,

$$S'_R(0) = -\frac{2S_1}{C_1} (ES_2 \mu(0) + S_6 \mu(2)). \tag{4.65}$$

Substituting this relation in Eq.(4.61), we obtain

$$\mu(\rho) = \sum_{\ell=0}^4 \tilde{M}_{\rho,\ell}(E) \mu(\ell) - \tilde{M}_{\rho,5}(E) \left(\frac{2S_1}{C_1} (ES_2 \mu(0) + S_6 \mu(2)) \right). \tag{4.66}$$

Regrouping, we have

$$\mu(\rho) = \sum_{\ell=0}^4 M_{\rho,\ell}(E) \mu_\ell, \tag{4.67}$$

where

$$M_{\rho,\ell}(E) = \begin{cases} \tilde{M}_{\rho,\ell}, & \text{for } \ell \neq 0, 2 \\ \tilde{M}_{\rho,\ell} - \left(\frac{2ES_1 S_2}{C_1} \right) \tilde{M}_{\rho,5}(E), & \text{for } \ell = 0 \\ \tilde{M}_{\rho,\ell} - \left(\frac{2S_1 S_6}{C_1} \right) \tilde{M}_{\rho,5}(E), & \text{for } \ell = 2 \end{cases} \tag{4.68}$$

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

$$\sum_{\ell=0}^{m_s=4} \mu(\ell) = 1, \tag{4.69}$$

which is used to constrain the zeroth order moment: $\mu(0) = 1 - \sum_{\ell=1}^{m_s} \mu(\ell)$. Incorporating this within Eq.(4.67) results in

$$\mu(\rho) = \sum_{\ell=0}^{m_s} \hat{M}_{\rho,\ell}(E) \hat{\mu}(\ell), \tag{4.70}$$

where

$$\hat{\mu}(\ell) \equiv \begin{cases} 1, & \text{if } \ell = 0 \\ \mu(\ell), & \text{if } \ell \geq 1 \end{cases}, \tag{4.71}$$

and

$$\hat{M}_{\rho,\ell}(E) \equiv \begin{cases} M_{\rho,0}(E), & \text{if } \ell = 0 \\ M_{\rho,\ell}(E) - M_{\rho,0}(E), & \text{if } \ell \geq 1 \end{cases}. \tag{4.72}$$

4.1.5 Numerical Implementation of EMM for $-(ix)^4$ Potential

Since the $\mu(\rho)$ moments are the moments of a nonnegative function, $F(\eta) \equiv \frac{1}{2\sqrt{\eta}}S(\sqrt{\eta})$, as noted in Eq.(4.37), they must satisfy the *Moment Problem* constraints (Shohat and Tamarkin [22]):

$$\int_0^\infty d\eta \eta^\sigma \left(\sum_{\rho=0}^Q C_\rho \eta^\rho \right)^2 F(\eta) > 0, \quad (4.73)$$

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

The above integral expression becomes the quadratic form expression:

$$\sum_{\rho_1, \rho_2=0}^Q C_{\rho_1} \mu_{\sigma+\rho_1+\rho_2} C_{\rho_2} > 0. \quad (4.74)$$

Substituting the moment equation relation in Eq.(4.70), we obtain

$$\sum_{\ell=1}^{m_s} A_\ell^{(\sigma)}[C; E] \mu_\ell < B^{(\sigma)}[C; E], \quad (4.75)$$

where

$$A_\ell^{(\sigma)}[C; E] \equiv - \sum_{\rho_1, \rho_2=0}^Q C_{\rho_1} \hat{M}_{\sigma+\rho_1+\rho_2, \ell}(E) C_{\rho_2}, \quad (4.76)$$

and

$$B^{(\sigma)}[C; E] \equiv \sum_{\rho_1, \rho_2=0}^Q C_{\rho_1} \hat{M}_{\sigma+\rho_1+\rho_2, 0}(E) C_{\rho_2}. \quad (4.77)$$

The physical energies, and corresponding missing moments, are those that satisfy all of the linear inequalities in Eq.(4.75), 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 (Handy and Bessis [23], Handy et al. [23, 24]), which uses basic linear programming [29] 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

Table 4. Bounds for the Discrete States of $P^2 - (ix)^4$

θ	$\mathcal{P}_{max}$	$E_0^{(L)} < E_0 < E_0^{(U)}$	$E_1^{(L)} < E_1 < E_1^{(U)}$
-.3	25	$1.4771490819 < E_0 < 1.4771509009$	$6.0033450031 < E_1 < 6.0033951480$
-.3	30	$1.4771497283 < E_0 < 1.4771497619$	$6.0033856565 < E_1 < 6.0033864674$
-.4	25	$1.4771497431 < E_0 < 1.4771498071$	$6.0033526131 < E_1 < 6.0034549921$

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 Eq.(4.70).

The results of this analysis are noted in Table 4. We only quote the results for the first two discrete states. Note that $\mathcal{P}_{max}$ denotes the maximum number of moments used, $2Q + \sigma \leq \mathcal{P}_{max}$. The data in Table 4 are for $\theta \neq \theta_R \approx -.5$. 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 5 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 Eq.(4.2) that this corresponds to letting θ coincide with the *anti-Stokes* line for rapid, asymptotic decrease of the wavefunction. Now the associated moment equation reduces greatly in order, from 4 to 1! That is, Eqs.(39-40) become

$$\begin{aligned} & \frac{S'(0)}{2} \delta_{\rho,0} + \mu(\rho-1) \left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2} \right] \\ & + \mu(\rho) [-2C_2 E(2\rho+1)] + \mu(\rho+1) \left[\frac{E^2 S_2^2}{\rho+1} \right] + \mu(\rho+2) [-4C_6 - 2C_6(2\rho+1)] = 0, \end{aligned}$$

and

$$ES_2\mu(0) = J(0), \quad (4.78)$$

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 5.

Table 5. Bounds for the Discrete States of $P^2 - (ix)^4$, 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	$1.47711 < E_0 < 1.47719$	$5.99924 < E_1 < 6.01220$
20	$1.4771496 < E_0 < 1.4771500$	$6.003367 < E_1 < 6.003444$
25	$1.477149752 < E_0 < 1.477149756$	$6.00338596 < E_1 < 6.00338640$
30	$1.477149753573 < E_0 < 1.477149753588$	$6.00338608298 < E_1 < 6.00338608478$

4.2 The General $-(ix)^N$ Potential

We now consider the generic case for the $-(ix)^N$ Schrödinger equation, extended into the complex- z plane:

$$-\Psi''(z) - (iz)^N \Psi(z) = E\Psi(z). \quad (4.79)$$

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

$$\Psi_R''(\xi) + i^N \xi^N e^{i(N+2)\theta} \Psi_R(\xi) + E e^{2i\theta} \Psi_R = 0, \quad (4.80)$$

and

$$\Psi_L''(\xi) + (-i)^N \xi^N e^{-i(N+2)\theta} \Psi_L(\xi) + E e^{-2i\theta} \Psi_L(\xi) = 0, \quad (4.81)$$

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

In accordance with the representation in Eq.(4.8),

$$H(\xi) \equiv A(\xi) \Psi''(\xi) + B(\xi) \Psi'(\xi) + C(\xi) \Psi(\xi) = 0,$$

we have $A = 1$, $B = 0$, $C(\xi) = \xi^N e^{i[(N+2)\theta + \frac{N\pi}{2}]} + Ee^{2i\theta}$. The real and imaginary parts of the $C(\xi)$ coefficient function become:

$$C_R(\xi) = \xi^N C_{N+2}^+ + EC_2, \quad (4.82)$$

and

$$C_I = \xi^N S_{N+2}^+ ES_2. \quad (4.83)$$

We define $C_{N+2}^+ = \text{Cos}[(N+2)\theta + \frac{N\pi}{2}]$, and $S_{N+2}^+ = \text{Sin}[(N+2)\theta + \frac{N\pi}{2}]$, where, as before, $C_n = \text{Cos}(n\theta)$, $S_n = \text{Sin}(n\theta)$.

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

$$S''(\xi) - 2P(\xi) + 2(\xi^N C_{N+2}^+ + EC_2)S(\xi) = 0, \quad (4.84)$$

$$(\xi^N S_{N+2}^+ ES_2)S(\xi) - J'(\xi) = 0, \quad (4.85)$$

and

$$P'(\xi) + (\xi^N C_{N+2}^+ + EC_2)S'(\xi) - 2(\xi^N S_{N+2}^+ ES_2)J(\xi) = 0. \quad (4.86)$$

The U, V, W moment equations become

$$-\delta_{p,0}S'(0) + \delta_{p,1}S(0) + p(p-1)U(p-2) - 2V(p) + 2[C_{N+2}^+U(p+N) + EC_2U(p)] = 0, \quad (4.87)$$

$$S_{N+2}^+U(p+N)ES_2U(p) + [\delta_{p,0}J(0) + pW(p-1)] = 0, \quad (4.88)$$

and

$$\begin{aligned} -\delta_{p,0}P(0) - pV(p-1) + C_{N+2}^+[-(p+N)U(p+N-1)] + EC_2[-\delta_{p,0}S(0) - pU(p-1)] \\ - 2[S_{N+2}^+W(p+N)ES_2W(p)] = 0. \end{aligned} \quad (4.89)$$

As before, Eq.(4.88) really contains two separate relations. One, when $p = 0$, serves to constrain the U moments:

$$S_{N+2}^+U(N) + ES_2U(0) = J(0); \quad (4.90)$$

the other, when $p \geq 1$, serves to generate the W moments from the U 's (i.e., take $p \rightarrow p + 1$ in Eq.(4.88)):

$$W(p) = -\frac{(S_{N+2}^+ U(p + N + 1) + ES_2 U(p + 1))}{p + 1}. \quad (4.91)$$

We can substitute for V (i.e., Eq.(4.87)) and W (i.e., Eq.(4.91)), in Eq.(4.89), reducing it to one moment equation for the U 's (in addition to Eq.(4.90)):

$$\begin{aligned} & -S(0)\delta_{p,2} + \frac{S'(0)}{2}\delta_{p,1} - P(0)\delta_{p,0} - C_2 ES(0)\delta_{p,0} + U(p-3)[-p + \frac{3p^2}{2} - \frac{p^3}{2}] \\ & + U(p-1)[-2pC_2 E] + U(p+1)[\frac{2E^2 S_2^2}{p+1}] + U(p+N-1)[-NC_{N+2}^+ - 2pC_{N+2}^+] \\ & + U(p+N+1)[\frac{2ES_2 S_{N+2}^+}{p+1} + \frac{2ES_2 S_{N+2}^+}{p+N+1}] + U(p+2N+1)[\frac{2S_{N+2}^{+2}}{p+N+1}] = 0. \end{aligned} \quad (4.92)$$

When $N = 2m$ (*even*), the U moment equation separates into distinct relations for the even and odd order moments. When $N \in \text{odd}$, 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 $-(ix)^4$ potential, only the even order moment relations 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 Eq. (92))

$$\begin{aligned} & \frac{S'(0)}{2}\delta_{\rho,0} + \mu(\rho-1)[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2}] \\ & + \mu(\rho)[-2C_2 E(2\rho+1)] + \mu(\rho+1)[\frac{E^2 S_2^2}{\rho+1}] + \mu(\rho+m)[-NC_{N+2}^+ - 2C_{N+2}^+(2\rho+1)] \\ & + \mu(\rho+m+1)[ES_2 S_{N+2}^+(\frac{1}{\rho+m+1} + \frac{1}{\rho+1})] + \mu(\rho+2m+1)[\frac{S_{N+2}^{+2}}{\rho+m+1}] = 0. \end{aligned} \quad (4.93)$$

We note that through Eq.(4.60), $J_{R,L}(0)$ and $S'_{R,L}(0)$ are linearly related (a consequence of assuming PT invariance). However, through the constraint in Eq.(4.90), $J_{R,L}(0)$ 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 is *odd*, taking note of the previous remarks, the independent variables become $\{U(0), \dots, U(2N), S(0), P(0)\}$, 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 $\{\mu(0), \dots, \mu(2m)\}$).

By taking $\theta = \theta_R$ (i.e., Eq.(4.2)), 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 $\{U(0), \dots, U(N - 2), S(0), P(0)\}$, before normalization; and the μ moments involve m independent variables, $\{\mu(0), \dots, \mu(m - 1)\}$ (before imposing the normalization condition which brings it down to $m - 1$).

The corresponding moment equations become:

$$\begin{aligned} -S(0)\delta_{p,2} + \frac{S'(0)}{2}\delta_{p,1} - P(0)\delta_{p,0} - C_2ES(0)\delta_{p,0} + U(p-3)\left[-p + \frac{3p^2}{2} - \frac{p^3}{2}\right] \\ + U(p-1)[-2pC_2E] + U(p+1)\left[\frac{2E^2S_2^2}{p+1}\right] \\ + U(p+N-1)[-NC_{N+2}^+ - 2pC_{N+2}^+] = 0, \end{aligned} \quad (4.94)$$

and

$$\begin{aligned} \frac{S'(0)}{2}\delta_{\rho,0} + \mu(\rho-1)\left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2}\right] \\ + \mu(\rho)[-2C_2E(2\rho+1)] + \mu(\rho+1)\left[\frac{E^2S_2^2}{\rho+1}\right] \\ + \mu(\rho+m)[-NC_{N+2}^+ - 2C_{N+2}^+(2\rho+1)] = 0. \end{aligned} \quad (4.95)$$

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

4.2.1 Recursive Expression for $N \in \text{odd}$, U -Moment Equation

For completeness, we detail the generation of the moment-missing moment relation in implementing the EMM algorithm for generating bounds. We focus only on the moment formulation represented in Eq.(4.94), for $\theta = \theta_R$. As noted, the ensuing EMM analysis will generate the fastest bounds in this case.

From Eq.(4.94), all of the moments are explicitly, linearly, dependent on the $\{U_R(0), \dots, U_R(N-2)\}$ moments, and the boundary terms $\{S_R(0), P_R(0), S'_R(0)\}$:

$$U_R(p) = \sum_{\ell=0}^{N+1} \tilde{M}_{p,\ell}(E) \chi_\ell, \quad (4.96)$$

where

$$\chi_\ell = \begin{cases} U_R(\ell), 0 \leq \ell \leq N-2 \\ S_R(0), \ell = N-1 \\ P_R(0), \ell = N \\ S'_R(0), \ell = N+1 \end{cases}. \quad (4.97)$$

The $\tilde{M}$ coefficients satisfy Eq.(4.94) with respect to the p -index, for fixed ℓ :

$$\begin{aligned} & -\delta_{\ell,N-1} \delta_{p,2} + \frac{\delta_{\ell,N+1}}{2} \delta_{p,1} - \delta_{\ell,N} \delta_{p,0} - C_2 E \delta_{\ell,N-1} \delta_{p,0} + \tilde{M}_{p-3,\ell}(E) \left[-p + \frac{3p^2}{2} - \frac{p^3}{2}\right] + \tilde{M}_{p-1,\ell}(E) \\ & [-2pC_2E] + \tilde{M}_{p+1,\ell}(E) \left[\frac{2E^2 S_2^2}{p+1}\right] + \tilde{M}_{p+N-1,\ell}(E) [-NC_{N+2}^+ - 2pC_{N+2}^+] = 0, \end{aligned} \quad (4.98)$$

where $p \geq 0$.

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

$$\tilde{M}_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}, \quad (4.99)$$

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

From Eq.(4.60) $S'_R(0) = \frac{2S_1}{C_1} J_R(0)$, and from Eq.(4.90), $J_R(0) = -ES_2 U_R(0)$, under the assumption $S_{N+2}^+ = 0$. Combining these, and substituting into Eq.(4.96) yields

$$U_R(p) = \sum_{\ell=0}^N M_{p,\ell}(E) \chi_\ell, \quad (4.100)$$

where

$$M_{p,\ell}(E) = \begin{cases} \tilde{M}_{p,0} - \frac{2ES_1S_2}{C_1} \tilde{M}_{p,N+1}, & \text{if } \ell = 0 \\ \tilde{M}_{p,\ell}, & \text{if } \ell \neq 0 \end{cases}. \quad (4.101)$$

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 6 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 [12], and Handy and Wang [15], which corresponds to a different complex-rotation EMM implementation. The results here are superior by at least two decimal places.

Table 6. Bounds for the Discrete States of $P^2 - (ix)^N$, along Anti-Stokes angle, $\theta_R = -\frac{N-2}{N+2}\frac{\pi}{2}$

N	$\mathcal{P}_{max}(\text{for } E_1)$	$E_0^{(L)} < E_0 < E_0^{(U)}$	$E_1^{(L)} < E_1 < E_1^{(U)}$
3	28(27)	$1.1562670657 < E_0 < 1.1562670772$	$4.109227 < E_1 < 4.109231$
5	24(22)	$1.908244 < E_0 < 1.908273$	$8.5837 < E_1 < 8.5902$
7	25(20)	$3.06843 < E_0 < 3.06873$	$15.01 < E_1 < 16.59$

4.2.2 Recursive Expression for $N = 2m$ (even), μ Moment Equation

In this case, we have

$$\mu_R(\rho) = \sum_{\ell=0}^m \tilde{M}_{\rho,\ell}(E) \chi_\ell, \quad (4.102)$$

where

$$\chi_\ell = \begin{cases} \mu_R(\ell), & 0 \leq \ell \leq m-1 \\ S'_R(0), & \ell = m \end{cases}. \quad (4.103)$$

The $\tilde{M}$'s must satisfy Eq.(4.95) with respect to the ρ -index:

$$\begin{aligned} \frac{\delta_{\ell,m}}{2} \delta_{\rho,0} + \tilde{M}_{\rho-1,\ell}(E) \left[-(2\rho+1) + \frac{3(2\rho+1)^2}{2} - \frac{(2\rho+1)^3}{2} \right] + \tilde{M}_{\rho,\ell}(E) \left[-2C_2 E(2\rho+1) \right] \\ + \tilde{M}_{\rho+1,\ell}(E) \left[\frac{E^2 S_2^2}{\rho+1} \right] + \tilde{M}_{\rho+m,\ell}(E) \left[-NC_{N+2}^+ - 2C_{N+2}^+(2\rho+1) \right] = 0, \end{aligned} \quad (4.104)$$

in addition to the initialization conditions

$$\tilde{M}_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}, \quad (4.105)$$

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

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

$$\mu_R(\rho) = \sum_{\ell=0}^{m-1} M_{\rho,\ell} \mu_R(\ell), \quad (4.106)$$

where

$$M_{\rho,\ell}(E) = \begin{cases} \tilde{M}_{\rho,0} - \frac{2ES_1S_2}{C_1} \tilde{M}_{\rho,m}, & \text{if } \ell = 0 \\ \tilde{M}_{\rho,\ell}, & \text{if } \ell \neq 0 \end{cases}. \quad (4.107)$$

In Table 7 we give bounds on the first two discrete states for $N = 6, 8, 10$. As is clear, upon comparing with the data in Table 6, the bounds for the $N \in \text{even}$ case, based upon the μ -EMM formalism, converge much faster than those for the $N \in \text{odd}$ case, based on the U -EMM analysis. This cannot be avoided.

Table 7. Bounds for the Discrete States of $P^2 - (iX)^N$, Along Anti-Stokes Angle, $\theta_R = -\frac{N-2}{N+2}\frac{\pi}{2}$

N	$\mathcal{P}_{max}(\text{for } E_1)$	$E_0^{(L)} < E_0 < E_0^{(U)}$	$E_1^{(L)} < E_1 < E_1^{(U)}$
6	30(28)	$2.4393464839 < E_0 < 2.4393464883$	$11.881564834 < E_1 < 11.8815649156$
8	30(23)	$3.7964748822 < E_0 < 3.7964748858$	$20.735611 < E_1 < 20.735854$
10	29(22)	$5.5533099639 < E_0 < 5.5533100698$	$32.80778 < E_1 < 32.81456$

CHAPTER 5

CONCLUSION

We have extended the EMM formalism to the case of discrete states with non-Real support. The numerical implementation can be done to any desired accuracy, although our results were done only to fifteen decimal place accuracy (which does not have to coincide with the tightness of the bounds). We could have easily doubled the accuracy of all the results appearing in the tables. The formalism developed here now opens up the extension of EMM to symmetry breaking solutions for such potentials as $-(ix)^N + iax$, and any other rational fraction complex potential.

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