Exact Christoffel-Darboux expansions: A new, multidimensional, algebraic, eigenenergy bounding method

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Abstract
Although the Christoffel-Darboux representation (CDR) plays an important role within the theory of orthogonal polynomials, and many important bosonic and fermionic, multidimensional, Hermitian and Non-Hermitian, systems can be transformed into a moment equation representation (MER), the union of the two into an effective, algebraic, eigenenergy bounding method has been overlooked. This particular fusion of the two representations (CDR and MER), defines the Orthonormal Polynomial Projection Quantization—Bounding Method (OPPQ-BM), as developed here. We use it to analyze several one dimensional and two dimensional systems, including the quadratic Zeeman effect for strong-superstrong magnetic fields. For this problem, we match or surpass the excellent, but intricate, results of Kravchenko et al (1996 Phys. Rev. A 54 287) for a broad range of magnetic fields, without the need for any truncations or approximations. The methods developed here apply to any linear, partial differential equation eigen-parameter problem, hermitian or non-hermitian.

1. Introduction

1.1. The Importance of eigenvalue bounding methods: hilbert space versus moment representation-positivity formulations
One important class of problems in mathematical physics corresponds to the development of effective methods for generating tight, converging, bounds to the eigenvalue problem associated with linear partial differential equations (LPDEs), including linear ordinary differential equations. If $\lambda_{\text{phys}}$ denotes the physical eigenvalue (real, for simplicity) corresponding to an $L^2$ integrable solution, satisfying the required boundary conditions, then the objective is to define a systematic procedure for generating converging lower and upper bounds, $\lambda^{(l)} < \lambda_{\text{phys}} < \lambda^{(U)}$, such that $\lim_{j \to \infty} (\lambda^{(l)}_j - \lambda^{(U)}_j) = 0^+$, converges rapidly, or sufficiently fast.

Different types of problems will recommend particular bounding methods. For hermitian quantum operators of the Sturm-Liouville (SL) type (i.e. the, rescaled, Schrodinger equation),

$$-\nabla^2\Psi(\vec{r}) + V(\vec{r})\Psi(\vec{r}) = E\Psi(\vec{r}),$$

with real potential function, $V(\vec{r})$, the generation of upper bounds to the eigenenergy, $E$, is straightforward; and obtainable through the Rayleigh-Ritz (RR) variational procedure [1, 2].

The difficult part is generating converging lower bounds. A general framework for this exists, as defined by the Temple lower bound method, which is usually slowly converging [3, 4]. The recent work by Martinazzo and Pollak [5], entitled Lower bounds to the eigenvalues of the Schrodinger equation by a solution of a 90 y challenge presents a major improvement in conventional bounding methods, as applied to hermitian quantum operators, by significantly improving upon the Temple lower bound procedure. Their work underscores the importance of the traditional eigenvalue bounding problem, which has been the focus of much study since the discovery of quantum mechanics and the development of its mathematical (differential) foundation [6].

Despite the achievements of the Martinazzo-Pollak eigenvalue bounding procedure, their methods do not apply to non-hermitian linear operators, particularly those associated with PT (i.e. parity-time) invariant, pseudo-hermitian systems. These have come to prominence over the last twenty-five years [7–9]. Indeed, the use
of complex-eigenvalue bounding methods was important in one of the first confirmations of PT-symmetry breaking, corresponding to the SL potential $V(x) = ix^3 + iax$. The complex-eigenvalue bounding capabilities of the Eigenvalue Moment Method (EMM), accurately predicted the ‘a’ parameter regimes where the system admitted complex conjugate eigenenergy pairs, as opposed to having real eigenenergies [10, 11]. These results disproved certain inaccurate predictions based on asymptotic analysis [12]. The interest in these types of non-hermitian operators is that they expand the possible class of operators corresponding to physical processes.

Another important difference between the traditional Martinazzo–Pollak bounding formulation and bounding methods such as EMM [13, 14], is that the first requires two separate formalisms (i.e. RR and the Temple related approach); whereas the second can generate geometrically converging, lower and upper bounds, within the same formalism.

Despite these important differences, of greatest significance is the EMM bounding philosophy exploits the use of one of the most important tools in analysis: the Moment Problem (MP) [15]. Historically, the Stieltjes moment problem, and the use of Padé approximants to bound the Stieltjes integral [16], are some of the most well known bounding theorems in mathematical physics. These structures are also used to understand the implications of large order perturbation theory [17, 18]. Also, MP is intimately tied to the theory of orthogonal polynomials [19]; and many exactly solvable quantum systems involve solutions corresponding to the orthogonal polynomials of the classic weights (i.e. Laguerre, Hermite, etc.) [20]. Methods, such as those associated with the Nikiforov–Uvarov formalism [21], can be used to identify these systems; so too can supersymmetric quantum mechanics be used to identify many more systems that are exactly solvable [22]. Orthogonal polynomials are also relevant in the study of quasi-exactly solvable quantum systems [23]. Finally, until the development of EMM, it was not known that all versions of the Moment Problem (i.e. the Hausdorff, Stieltjes, Hamburger, etc.), could be used to generate converging eigenenergy bounds to an important and large class of multidimensional SL systems, hermitian and non-hermitian (i.e. those transformable into MER form, as explained below).

The EMM methodology [13, 14] involves identifying a nonnegative configuration space representation for the physical solution $s$, $\psi(\vec{r}) \to F(\vec{r}) \geq 0$ wherein the power moments of $F$, $\nu(\vec{p}) \equiv \int_{\mathbb{R}^3} \vec{p}^i F(x_1, x_2, x_3) \, d^3r$, satisfy a linear recursion relation, referred to as a Moment Equation Representation (MER). The MER is parameterized by $\lambda$. One then imposes the MP positivity constraints on the moment solutions to the MER relation; thereby constraining the $\lambda$ parameter, and generating geometrically converging bounds.

The existence of a MER relation depends on whether or not $F$ satisfies a linear, partial/ordinary, differential equation with function coefficients corresponding to rational polynomials of the coordinate variables. If so, then the MER relation ensues through an appropriate integration by parts analysis. This is clarified below and through the various examples considered in this work.

The actual EMM implementation involves nonlinear convex optimization analysis, through semidefinite programming (SDP) algorithms [24, 25]. This can be relaxed through an equivalent, but slower, linear convex optimization analysis involving linear programming (LP) algorithms [14, 26, 27]. For MER type systems, EMM can be used to generate bounds to the multidimensional bosonic ground state, and to arbitrary states for one dimensional SL problems (hermitian or non-hermitian). Each of these readily admits a nonnegativity representation. However, identifying suitable (easy to use) nonnegativity representations is not straightforward for the case of multidimensional bosonic excited states [28], for reasons clarified below. The same difficulties apply to vector/spinorial field models.

The first application of SDP analysis to quantum operators was through the EMM formalism developed by Handy and Bessis [13, 14, 26]. Since SDP algorithms were not well developed in the 1980’s, an equivalent computational implementation was done using LP methods [14, 26]. These developments are acknowledged in the recent work by Lasserre [25]. The EMM formalism was used to generate tight bounds on the one dimensional and multidimensional bosonic ground state energy, involving the positivity representation: $F(\vec{r}) \equiv \Psi_0(\vec{r}) > 0$ [13, 14, 29]. This is because of the well known theorem that the multidimensional bosonic ground state must be of uniform signature, which can be taken to be positive.

EMM was also used to generate tight real/complex eigenenergy bounds to arbitrary $L^2$ states of the one dimensional SL problem for real/complex potentials, exploiting the natural nonnegativity of the probability density, $F(x) \equiv S(x) = \Psi^*(x)\Psi(x) \geq 0$ [10, 30–32]. It can readily be shown that the probability density will satisfy a third or fourth order linear differential (eigen-parameter) equation, depending on the nature of the potential function, $V(x)$ (i.e. real or complex, respectively). An important aspect of this is that through the Herglotz theorem, the complex extension of the one dimensional probability density is made possible. Depending on the rational polynomial form of the ensuing differential coefficient functions, a MER relation can be obtained, and EMM implemented. This procedure was used to solve the PT symmetry breaking problem referenced earlier (i.e. $V(x) = ix^3 + iax$).
The multidimensional probability density does not satisfy an LPDE relation, let alone generate a MER representation; therefore it cannot be exploited within EMM. However, through the methods developed here, we can circumvent this problem, and effectively implement a bounding theory based on the multidimensional probability density, \( S(\vec{r}) = |\Psi(\vec{r})|^2 \geq 0 \).

1.2. Generating converging eigenvalue bounds: A novel use of positivity constraints and moment representations
In keeping with the versatility of the Moment Problem, we have discovered a powerful reformulation of the basic EMM methodology of combining MERs with positivity constraints. It is referred to as the Orthonormal Polynomial Projection Quantization—Bounding Method (OPPQ-BM). It offers two very important advantages over the EMM formulation. First, its computational structure is purely algebraic (i.e. no SDP/LP analysis required). Second, its theoretical structure greatly expands the class of problems that can be studied through the generation of tight, converging, eigenenergy/eigenvalue bounds; specifically: arbitrary \( L^2 \) solutions of low dimension LPDEs, hermitian or non-hermitian, including vector/spinorial field configurations.

In this work we develop and apply OPPQ-BM to some representative problems, including the multidimensional quadratic Zeeman (QZM) effect for electrons in superstrong magnetic fields [14, 33–35], as found on neutron stars (\( B = O(10^9) \) T). The bounding of electrons in even stronger magnetic fields [36], approaching that of magnetars (\( B = O(10^{15}) \) T), requires the study of the relativistic Dirac equation involving spinorial fields, \( \Psi \rightarrow \tilde{\Psi} \). This is very difficult to do within EMM; however, it becomes relatively straightforward using OPPQ-BM, although not considered here. This also extends to relativistic, non-hermitian, problems of low dimension.

The impetus for OPPQ-BM originates from a related, eigenvalue estimation, formalism by Handy and Vrinceanu (HV) [37, 38]. A closer examination of its structure, particularly with respect to their, novel, non-orthogonal basis expansion, strongly suggested that it could be used to develop an eigenvalue bounding formalism, as presented here. We will refer to the HV formalism as the Orthonormal Polynomial Projection Quantization—Approximation Method (OPPQ-AM) in this work. Both formalisms, OPPQ-AM and OPPQ-BM, use the same non-orthogonal basis expansion, as explained below.

The generation of tight eigenvalue bounds is not solely motivated by computational reasons. The ability to accurately determine the physical values, through tight bounds, allows us to assess which theories and methodologies are correct. Most computational strategies for solving physical systems involve approximation methods. If the underlying physical dynamics are sensitive, such estimations can lead to significantly inaccurate results in predicting the true physical values.

Strong coupling—singular perturbation (SCSP) problems [39] are of this type. That is, not only are the physical interactions significant, but they occur over short, multi, scales. These are best handled through non-local, extensive, configuration space representations (i.e. power moments [40] wavelets [41-43], etc) in order to better control/understand their contributions. The strong (nuclear) forces are of this type. So too is the QZM problem involving the electromagnetic interactions that govern the bound state behavior of electrons in highly ionized (i.e. hydrogenic) atoms, with superstrong magnetic field interactions [14, 34, 35].

Historically, the QZM problem was one of the most difficult, low dimension, problems to solve accurately due to its SCSP character [14, 34, 35]. The lowest eigenenergy state, the ground state, was the most singular and strongly coupled bound state. Different theories and computational strategies yielded greatly varying results, until the specialized approximation methods of Le Guillou and Zinn-Justin (LG-ZJ) were applied (i.e. order dependent conformal transformations) [34]. Through the EMM bounding methods of Handy and Bessis (HB), relatively tight bounds for the ground state binding energy were obtained, confirming the LG-ZJ results [14]. No other, recent, bounding study for the QZM problem has been published, until now; although excellent approximation methods have been developed, such as those by Kravchenko et al [35]. The QZM problem continues to be important for benchtesting other methods, such as the recent B-spline analysis of QZM by Schimarecz and Wunner [36].

1.3. Essentials of the orthonormal polynomial projection quantization—bounding method (OPPQ-BM)
The OPPQ-BM formalism is applicable to any homogeneous, hermitian or non-hermitian, LPDE, eigenparameter problem of the form:

\[
\sum_{\vec{r}} \mathcal{C}(\lambda; \vec{r}) \partial^{\alpha_1}_{\lambda_1} \partial^{\alpha_2}_{\lambda_2} \partial^{\alpha_3}_{\lambda_3} \Psi(\vec{r}) = 0, \tag{2}
\]

where \( \vec{r} \equiv (\chi_1, \chi_2, \chi_3) \in \mathcal{D} \subset \mathbb{R}^d \) (i.e. \( d = 3 \) for simplicity). The domain is any compact, or unbounded, continuous subset of \( \mathbb{R}^3 \). The \( \mathcal{C}(\lambda; \vec{r}) \) depend on the eigen-parameter, \( \lambda \) and must be (or can be transformed into) rational polynomials in the coordinate variables (i.e. \( \chi_i \)). The coefficients of these rational polynomials depend on \( \lambda \) (either linearly or nonlinearly, although the first is the more prevalent case). We note that the
terminology ‘eigen-parameter’ and ‘eigenvalue/eigenenergy’ will be used, interchangeably, to refer to \( \lambda \). This is because equation (2) includes both types of problems.

We assume that the physical solutions to equation (2) are \( L^2 \)-integrable; whereas the unphysical solutions are either not \( L^2 \)-integrable (on unbounded domains) or do not satisfy the required boundary conditions on compact domains. An alternate characterization is that on unbounded domains, the physical solutions are exponentially bounded in all asymptotic directions; and their power moments are finite. The unphysical solutions are exponentially unbounded, in all, or some, asymptotic directions; and all their power moments are divergent [44, 45]. This is summarized below for unbounded domains:

\[
\mu(\vec{p}) = \int \int_D \int_0^{3} \prod_{j=1}^{\infty} \chi^j_{\ell} \Psi(\vec{r}) \, d^3r = \begin{cases} \text{finite} & \iff \Psi = \Psi_{\text{phys}} \\ \pm \infty & \iff \Psi = \Psi_{\text{unphys}} \end{cases}
\]  

(3)

for unbounded \( D \) domains, and all nonnegative integer vector values, \( \vec{p} \geq 0 \).

Due to the form of equation (2) it generally follows that the LPDE can be transformed into a linear recursion, multidimensional finite difference equation for the power moments (of the physical solutions, implicitly). This is accomplished by factoring out the denominators of the LPDE coefficients in equation (2), multiplying the resulting equation by \( \prod_{j=1}^{\infty} \chi^j_{\ell} \), and integrating by parts, implicitly assuming that \( \Psi = \Psi_{\text{phys}} \). The resulting expression is of the form:

\[
\mathcal{M}_\mu(\vec{p}) = \sum_{\vec{q} \in \mathcal{Q}} C_\mu(\vec{p}, \vec{q}) \mu(\vec{p} + \vec{q}) = 0,
\]  

(4)

for \( \vec{p} \geq 0 \). This is referred to as a moment equation representation (MER). The class of important quantum operators transformable into MER form is large.

Up to any finite expansion order, the MER relation will divide the power moments into two finite sets \( \{ \mu(\vec{p}) | \vec{p} \geq 0 \} = \{ \mu(\vec{p}_f) \} \cup \{ \mu(\vec{p}_u) \} \) the initialization moments (or missing moments), \( \{ \mu_c \equiv \mu(\vec{p}_f) \} \); and those generated by them, \( \{ \mu(\vec{p}_u) \} \), through a linear relation of the form:

\[
\mu(\vec{p}_u) = \sum_{\ell} M_{\ell}(\vec{p}, \ell) \mu_c.
\]  

(5)

Within the OPPQ-BM formulation, the physical solutions are expanded in terms of a special basis

\[
\Psi(\vec{r}) = \sum_n c_n B_n(\vec{r}),
\]  

(6)

where \( B_n(\vec{r}) \equiv P_n(\vec{r}) R(\vec{r}) \), involving the multidimensional orthonormal polynomials \( \{ P_n(\vec{r}) \} \), of a properly selected, nonnegative, weight, \( R \geq 0 \):

\[
\langle P_m | R | P_n \rangle = \delta_{m,n}
\]  

(7)

where the bra-ket notation is used symbolically. Note that the polynomials are orthonormal to the weight, \( R \), and not \( R^2 \). Because of this, the basis \( \{ B_n \} \) is non-orthogonal:

\[
\langle B_m | B_n \rangle = \delta_{m,n} \text{ if } m = n.
\]  

(8)

Normally, the expansion in equation (6) is referred to as a weighted polynomial expansion [46]. The problem with this characterization is that it is not clear if the polynomials are orthonormal with respect to \( R \) or \( R^2 \). Since the well studied theory of Christoffel-Darboux Kernels [47] involves weighted, orthonormal, polynomial expansions with respect to \( R \), and not \( R^2 \), we refer to equation (6) as the Christoffel-Darboux Expansion/Representation (CDE/R).

For MER type systems, this particular non-orthogonal basis expansion yields exact, closed form, expressions for the expansion coefficients of the physical solutions, \( \{ c_n \} \). That is, these coefficients involve, known, rational polynomial functions in \( \lambda \), and are linearly dependent on the initialization moments:

\[
c_n(\lambda, \mu) = \langle P_n | \Psi \rangle = \sum_{\ell} \Lambda^n_{\ell}(\lambda) \mu_c,
\]  

(9)

where the \( \Lambda^{n\ell}(\lambda) \) are known, rational polynomials of \( \lambda \).

The asymptotic form of the physical and unphysical solutions are readily determined through methods such as WKB analysis, etc [39, 48]. One can choose the weight’s asymptotic form based on the asymptotic form of the physical and unphysical solutions so that following, positive, integral conditions/constraints are satisfied:

\[
0 < T[\Psi, R] \equiv \int \int_D d^3r \frac{|\Psi(\vec{r})|^2}{R(\vec{r})} = \begin{cases} \text{finite} & \iff \Psi = \Psi_{\text{phys}} \\ \infty & \iff \Psi = \Psi_{\text{unphys}} \end{cases}
\]  

(10)

We also want \( \text{Inf}_r \{ R^{-1}(\vec{r}) \} \equiv \text{Const}_r > 0 \), so that \( 0 < \int \int_D d^3r \ |\Psi(\vec{r})|^2 \leq \frac{T[\Psi, R]}{\text{Const}_r} \). For configurations, \( \Psi \), which are solutions to equation (2), this criteria, combined with equation (10), will distinguish the physical
(\(L^2\) integrable) solutions from the unphysical ones (i.e. not \(L^2\) integrable, on unbounded domains). The asymptotic properties of the weight, \(R\), are specified in section 2.

We note that on unbounded domains, the weight will generally be positive, \(R > 0\); however, on compact domains, the weight will have to take on the physical boundary condition (i.e. \(R(\text{boundary}) = 0\)) so that equation (10) holds; therefore, the weight must be nonnegative on compact domains: \(R \geq 0\). We demonstrate this in the appendix through an illustrative problem corresponding to the infinite square well potential problem. Also, on compact domains the MER relation can be generated so as not to involve boundary terms This is also discussed in the appendix.

It is assumed \(\Psi_{\text{phys}}\) satisfies some normalization condition, \(C_{\text{Norm}}(\Psi_{\text{phys}}) = 1\), independent of \(R\).

Due to the orthonormal polynomial dependence of the \(\{B_n\}\) basis functions, equation (10) can be transformed into a positive series involving the moduli-squared of the CDE expansion coefficients:

\[
0 < I[\Psi, R] = \sum_{n=0}^{\infty} |c_n(\lambda; \mu_c)|^2 = \begin{cases} \text{finite} & \iff \lambda = \lambda_{\text{phys}} \text{ and } \mu_c = \mu_{\epsilon_{\text{phys}}} \\ \infty & \iff \lambda = \lambda_{\text{phys}} \text{ or } \mu_c = \mu_{\epsilon_{\text{phys}}}. \end{cases}
\]

The physical eigenvalues can be estimated, by approximating the vanishing asymptotic terms that define the converging, positive, series:

\[
\lim_{n \to \infty} c_n(\lambda_{\text{phys}} \mu_{\epsilon_{\text{phys}}}) = 0.
\]

This quantization condition defines the Orthonormal Polynomial Projection Quantization-Approximation Method (OPPQ-AM), as will be referred to in this work, corresponding to the Handy and Vrinceanu formalism [37, 38]. It will reduce to a determinantal, secular equation, condition solely involving the eigenparameter, since the \(c_n\)'s are linear in the initialization moments (i.e. equation (9)). Very good eigenvalue estimation results were obtained, both for hermitian and non-hermitian, multidimensional LPDEs [37, 38]. Furthermore, the better the weight imitates the asymptotic properties of the physical solution, the faster the convergence for the OPPQ-AM eigenenergy estimates. The same applies for OPPQ-BM, although we do not investigate these properties.

The OPPQ-AM formalism solely focused on the use of the above analysis as an eigen-parameter estimation/approximation ansatz. Here we examine the full implications of equation (11), including the unphysical solutions. Clearly, equation (11) has the structure of a shooting method formalism within the \(\{\lambda, \mu_c\}\) parameter space. This is inefficient to implement, since the number of initialization moments can be large, even for one dimensional systems. Fortunately, the formalism outlined in section 2 (and further specialized to the individual problems considered in sections 3–5) can convert this suggestive interpretation into an algebraic bounding formalism for the physical eigen-parameter values.

In summary, EMM requires the identification of a nonnegativity representation, \(\Psi \to F \geq 0\), that also admits a MER relation for the power moments of \(F\). One then imposes positivity constraints on the MER representation arising from the positivity conditions (not given here) associated with the Moment Problem, in order to generate eigen-parameter bounds.

EMM works very well on multidimensional bosonic ground states, and arbitrary one dimensional SL systems (hermitian or non-hermitian) since these admit readily identifiable nonnegativity representations transformable into MER form: \(\psi_{\text{p}}(\tau) > 0\) [49] and \(S(x) = \Psi^*(\Psi)x \geq 0\) [10]. However, to extend EMM to multidimensional excited states, the only available formalism involves working with the expression \(\Phi(\tau) = (\Psi(\tau) + C)R(\tau)\) [28] involving an exponentially decaying regulating factor, \(R(\tau) > 0\), and a sufficiently positive constant, \(C \geq \sup_{\tau}[–\Psi(\hat{\tau})] \geq 0\). Although this approach works, it is not elegant. In this regard, we note that there exists a formalism for factoring out the \(C\)-constant [50], although it can only be used to estimate the eigen-parameter. However, recent results suggest that this can be transformed into a bounding procedure as well.

Regardless, EMM is not suitable for vector/spinorial systems, \(\Psi \to \hat{\Psi}\). Working with the multidimensional probability density would be the recommended approach; however, the multidimensional probability density \(S(\tau) \equiv |\Psi(\tau)|^2\) does not have an LPDE representation through which a MER relation could be generated. As such, this approach cannot be implemented within EMM. Fortunately, OPPQ-BM does allow us to work with \(S(\tau)\), and does not require a MER for it, but instead allows us to use the easier to generate MER for the \(\Psi(\tau)\) configuration.

Within OPPQ-BM, the expression \(F(\tau) \equiv \frac{|\Psi(\tau)|^2}{R(\tau)}\) becomes the natural nonnegativity representation. This involves the multidimensional probability density, \(S(\tau)\), and the nonnegative weight used for generating the CDE expansion. The MER relation is only required for the power moments of \(\Psi\): \(\{\mu(\hat{p})\}\). Through the positivity of the integral expressions in equation (10) one can impose constraints on the eigen-parameter and power moments, through equation (11). This approach will generate eigen-parameter converging bounds. Its effectiveness is suggested through the OPPQ-AM eigen-parameter estimation ansatz, which exploits one aspect
of equation (11), as expressed in equation (12). OPPQ-BM is a more flexible formalism than EMM, and easily lends itself to spinorial/vector fields, since it involves the nonnegativity of the probability density.

In the following section we show how to convert equation (11) into an eigen-parameter bounding formalism, devoid of any explicit moment contributions.

2. The Algebraic Implementation of OPPQ-BM

In section 1 we introduced the essential structure of the multidimensional Orthonormal Polynomial Projection Quantization—Bounding Method (OPPQ-BM). In this section we show how to transform the positivity quantization constraints in equation (11), into an algebraic bounding analysis for the desired eigenvalues/eigenenergies. The formalism used here is that for one dimensional systems, for greater clarity. The basic structure is unchanged for multidimensional systems, unless noted otherwise.

The presentation below is given in the most general way possible, emphasizing the broad class of physical and applied problems that can be solved. In sections 3–5 we apply this formalism to various Sturm-Liouville (SL) problems, including the one dimensional quantum harmonic oscillator problem; the one dimensional quartic anharmonic (double well) oscillator; and the three dimensional quadratic Zeeman effect, although symmetry considerations reduce the effective dimensionality to two. Included with each of these examples are proofs of particular aspects of the OPPQ-BM approach specific to the case being studied. Other proofs of key steps appear in the appendix.

The OPPQ-BM formalism is made up of two parts. The first exploits the formalism developed by Handy and Vrinceanu, referred to in this work as the Orthonormal Polynomial Projection Quantization-Approximation Method (OPPQ-AM), as discussed in section 1. It is an estimation method. The OPPQ-BM formalism is a first principles eigenenergy bounding method suitable for low dimension systems, within the class of problems identified below.

2.1. The Class of 1-dimensional problems amenable to OPPQ-BM

Consider the following homogeneous, linear ordinary differential equation (LODE), problem involving coefficient functions that are (or can be transformed into) rational polynomials in $x$, in addition to their dependence on the eigen-parameter, $E$:

$$\frac{d^n}{dx^n}\Psi(x) + \sum_{n=0}^{N-1} C_n(E; x) \frac{d^n}{dx^n}\Psi(x) = 0. \quad (13)$$

We choose to denote the eigen-parameter by $E$, and not $\lambda$, since the Sturm-Liouville version of equation (13) involves the eigenenergy notation $E$. To simplify the presentation, we assume that $x \in \mathbb{R}$, corresponding to the entire real line. Also, we make no assumptions as to the hermitian or non-hermitian character of the system. Due to the homogeneous nature of the system, the physical solutions are required to satisfy some normalization condition, as symbolized by:

$$\mathcal{C}_{\text{Norm}}(\Psi) = 1. \quad (14)$$

The traditional, physical, normalization is $\int_{\mathbb{R}} |\Psi(x)|^2 = 1$, which is nonlinear in $\Psi$, and all physical states can satisfy it. Any other linear or nonlinear normalization will also be acceptable for determining the physical, discrete, $E$, values so long as the desired physical solution(s) satisfy $\mathcal{C}_{\text{Norm}}(\Psi) \neq 0$. Within our formalism there are many possible normalization prescriptions. Some can be satisfied by all physical solutions; others can only be satisfied by the targeted solutions, usually due to symmetry conditions.

We assume that the physical solutions are $L^2$ integrable and exponentially bounded (i.e. $|\Psi_{\text{phys}}(x)| < \mathcal{N} \exp(-|x|^Q)$, for $|x| \to \infty$, and some $Q > 0$), with finite power moments. The unphysical solutions are not $L^2$ integrable, and are exponentially unbounded in one, or both, asymptotic directions; furthermore, their power moments are divergent:

$$\mu(p) \equiv \int_{\mathbb{R}} |x|^p \Psi(x) \, dx = \begin{cases} \text{finite} & \Psi = \Psi_{\text{phys}}; \\ \pm \infty & \Psi = \Psi_{\text{unphys}}. \end{cases} \quad (15)$$

Power moments defined on $\mathbb{R}$ are referred to as Hamburger moments. Those defined on the nonnegative real line are referred to as Stieltjes moments.

As noted in section 1, OPPQ-BM is only applicable to systems for which the physical power moments satisfy a linear recursion relation, referred to as the Moment Equation Representation (MER). This corresponds to a finite difference equation of order $1 + m$. The initialization moments are referred to as the missing moments and denoted by $\{\mu_r | 0 \leq r \leq m\}$. The rational polynomial structure of the coefficient functions in equation (13) allows the operator to be transformed into MER form (the details are provided in the specific examples in section 3–5). The generating form of the MER relation is given by:
\[ \mu(p) = \sum_{\ell=0}^{m} M_{\ell}(p, \epsilon) \mu_{\ell}, \]  

(16)

for nonnegative integers, \( p \geq 0 \). The \( M_{\ell}(p, \epsilon) \) coefficients can be generated exactly and involve known algebraic functions of \( E \) (i.e. rational polynomials in \( E \), etc.). They can be generated in closed form up to any arbitrary expansion order, \( p \leq P \). That is, the \( M_{\ell}(p, \epsilon) \) will satisfy the same finite difference equation as the moments (relative to the \( p \) index), and are generated based on their initialization conditions: \( M_{\ell}(\epsilon, \epsilon) = \delta_{\ell,\epsilon} \). Also, the normalization on the physical solution is now defined in terms of the missing moments:

\[ C_{\text{Norm}}(\mu_{p_1}, \ldots, \mu_{m}) = 1. \]  

(17)

One can adopt the unit-missing moment vector normalization, \( \sum_{\ell=0}^{m} |\mu_{\ell}|^2 = 1 \), or any other nonlinear or linear normalization. Thus, if we know that the desired physical solution satisfies \( \mu_0 \neq 0 \), we can simply choose the normalization \( \mu_0 = 1 \). Once the OPPQ-BM quantization conditions are imposed, all the other missing moments will be determined.

For multidimensional problems, as the expansion order increases, the number of missing moments increases; therefore, the only consistent normalization across all expansion orders is for a restricted normalization in which a fixed number of missing moments are normalized, regardless of the expansion order. For the multidimensional quadratic Zeeman effect considered in section 5, we will simply work with the multidimensional counterpart to \( \mu_0 \).

From section 1, the OPPQ-BM formalism requires the selection of an appropriate weight, \( R(x) \geq 0 \). Through asymptotic analysis, such as WKB, we can determine the asymptotic form of the physical and unphysical solutions. The desired weights are those that satisfy the following, positive, integral conditions/

\[ \mathcal{T}[\Psi; R] \equiv \int_{\mathcal{D}} dx |\Psi(x)|^2 \frac{R(x)}{R(x)} = \left\{ \begin{array}{ll}
\text{finite} & \iff \Psi = \Psi_{\text{phys}}, \\
\infty & \iff \Psi = \Psi_{\text{unphys}},
\end{array} \right. \]  

(18)

where \( \mathcal{D} = \mathbb{R} \). The convergent/divergent nature of the above integral expression is determined by the asymptotic properties of the physical and unphysical solutions relative to that of the weight. On compact domains, \( \mathcal{D} \), if the boundary is denoted by \( \partial \mathcal{D} \), then the physical boundary conditions will usually correspond to \( \Psi(\partial \mathcal{D}) = 0 \). The weight must become zero, \( \lim_{x \to \partial \mathcal{D}} R(x) = 0 \), in a manner that validates equation (18). For unphysical solutions (with non-zero boundary conditions), having the weight become zero, sufficiently fast, will make the corresponding integral infinite, as suggested by equation (18). In the appendix we consider the infinite square well problem, and generate eigenvalue bounds based on Eq.18.

For the case \( \mathcal{D} = \mathbb{R} \), the chosen weight will generally satisfy equation (18) if it is asymptotic to the physical configuration at infinity: \( R(x) \sim \Psi_{\text{phys}}(x) \). A more general statement is that the weight must be chosen so that it asymptotically decreases no faster than the asymptotic form of the physical solution [37, 38]:

\[ \lim_{x \to \pm \infty} \frac{|\Psi(x)|}{R(x)} = \left\{ \begin{array}{ll}
C_{\pm} & \iff \Psi = \Psi_{\text{phys}}, \\
\infty & \iff \Psi = \Psi_{\text{unphys}} \text{ for either or both } x \to \pm \infty,
\end{array} \right. \]  

(19)

where \( 0 \leq C_{\pm} < \infty \). One can relax this condition, and allow \( R(x) \) to decay faster than the physical solutions, so long as equation (18) is satisfied; however, the restriction in equation (19) has the added importance that it emphasizes that the weights can be chosen to emulate the physical solution, when convenient. That is, we only use weights modeled after the asymptotic form of the physical solution, so long as the power moments of \( R \) are straightforward to compute to high accuracy; whereby allowing for the generation of the associated orthonormal polynomials, as required by the OPPQ-BM formalism (this is further elaborated upon in the following discussion). If this is not the case, we then determine a suitable \( R(x) \) that captures as much of the asymptotic behavior of the physical states, as possible, while permitting computable power moments.

We also want \( R^{-1}(x) \geq \text{Const}_{R} = \{ 0, \infty \} \), so that \( 0 < \int_{\mathcal{R}} dx |\Psi(x)|^2 \leq \frac{\mathcal{T}[\Psi, R]}{\text{Const}_{R}} \). Thus, since the physical solutions to equation (13) are uniquely \( L^2 \) integrable (i.e. unphysical solutions are not \( L^2 \) integrable on unbounded domains), they are identified through the condition in equation (18). That is, if \( \Psi \) is any solution to equation (13), then the condition in equation (18) will determine if its physical or not (i.e. \( L^2 \) integrable or not).

In general, we will utilize Freud type weights, \( R(x) = \mathcal{N} \exp(-|x|^q) \), for some \( q \). This will generate a complete (weighted polynomial) basis [51] in the uniform norm (if \( q \geq 1 \)) of the form \( \{ \mathcal{B}_n(x) \equiv P_n(x)R(x) \mid n \geq 0 \} \), involving the polynomials
\[ P_n(x) = \sum_{j=0}^{n} \Xi_j^{(n)} x^j, \]  

which are orthonormal with respect to the weight

\[ \int_{\mathbb{R}} dx \ P_n(x) R(x) P_n(x) = \langle P_n | R | P_n \rangle = \delta_{m,n}. \]  

The bra-ket notation is used symbolically. The basis is non-orthogonal, since

\[ \langle B_m | B_n \rangle = \epsilon_{m,n} \text{ if } m \neq n. \]  

In this work, the problems considered (both in one and two space dimensions) will correspond to \( q = 1 \) and \( q = 2 \), associated with the Laguerre and Hermite polynomials, respectively.

If the weight is not one of the classic weights with known orthonormal polynomials, then they must be generated. This can be done through a Cholesky decomposition of the positive definite, Hankel moment matrix, for the weight. Denote the power moments of the weight by

\[ \rho = \int_{\mathbb{R}} x^j w(x) dx, \]  

then the corresponding Hankel moment matrix is given by

\[\begin{bmatrix} \rho_{0,0} & \rho_{0,1} & \cdots & \rho_{0,m} \\ \rho_{1,0} & \rho_{1,1} & \cdots & \rho_{1,m} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{m,0} & \rho_{m,1} & \cdots & \rho_{m,m} \end{bmatrix}.\]  

The Cholesky decomposition for generating the orthonormal polynomials is described in the following sections, in the context of the specific SL systems considered. One does not have to numerically generate all the power moments \( \{w(i)\} \). Usually, the chosen weight will have power moments that also satisfy a corresponding MER relation; thus only the lower order moments need to be determined to high accuracy, so that the other moments can be determined, and the orthonormal polynomials generated.

2.2. The Christoffel-Darboux Expansion
Consider the decomposition of the physical, \( L^2 \) integrable, solution \( \Psi \), in terms of a particular, weighted-orthonormal polynomial, basis:

\[ \Psi(x) = \sum_{n=0}^{\infty} c_n \ P_n(x) R(x). \]  

As noted in section 1, we refer to this as the Christoffel-Darboux Expansion/Representation (CDE/R) due to the orthonormal nature of the polynomials relative to the weight \( R \) (and not \( R^2 \)). The theory of Christoffel-Darboux Kernels [47] depends on such orthonormal polynomials, and motivates our use of the phrase.

The projection coefficients are given by (note the symbolic use of the bra-ket notation)

\[ c_n = \int_{\mathbb{R}} dx \ P_n(x) \Psi(x) \equiv \langle P_n | \Psi \rangle, \]  

involving the power moments, \( \mu(j) = \int_{\mathbb{R}} x^j \Psi(x) dx. \)

Substituting the MER relation in equation (16) into equation (25) we obtain

\[ c_n(E, \mu) \equiv \sum_{\ell=0}^{m_i} \Lambda^0_{\ell} \mu_\ell \equiv \Lambda^0_E \cdot \mu, \]  

where

\[ \Lambda^0_E \equiv \sum_{j=0}^{n} \Xi_j^{(n)} M_{E} (j, \ell), \]  

for \( n \geq 0 \) and \( 0 \leq \ell \leq m_i \); with missing moment vector :

\[ \mu \equiv (\mu_1, \ldots, \mu_{m_i}). \]  

Since the \( M_{E}(j, \ell) \) can be generated in closed form exactly, the \( c_n(E, \mu) \) are known rational polynomials of the energy, \( E \), and linearly dependent on the missing moments.

2.3. The orthonormal polynomial projection quantization-approximation method
The Orthonormal Polynomial Projection Quantization—Approximation Method (OPPQ-AM) was described in the context of equation (12). We can now better appreciate its actual structure through the explicit form given for the CDE expansion coefficients in equation (26). The OPPQ-AM quantization condition corresponds to implementing equation (12) through a truncation analysis:

\[ c_{N-\ell}(E, \mu_\ell) = \Lambda^{(N-\ell)}_E \cdot \mu_\ell = 0, \]  

for \( \ell \geq 0 \).
\[ 0 \leq \ell \leq m_x \text{ for fixed } N \to \infty. \] This becomes an \( m_x + 1 \) dimensional secular equation approximating the eigenenergy:

\[ \det(A^{(N-\ell)}_\ell(E)) = 0. \] (30)

The OPPQ-AM was used to generate high accuracy eigenenergies for both hermitian and non-hermitian systems, including the potentials: \( V(x) = i x^2, V(x) = x^4 + iax, \) and \( V(x,y) = x^2 + y^2 + i 2x y \) [37].

The importance of the OPPQ-AM formalism is its introduction of the CDE/R representation in equation (23), and the convenient, closed form for the corresponding projection coefficients, \( c_n \). Additionally, the OPPQ-AM formalism established the importance of choosing weights whose asymptotic form matches, as best as possible, the asymptotic form for the physical states, since this results in faster converging eigenenergy estimates, within OPPQ-AM, and faster converging eigenenergy bounds within OPPQ-BM.

2.4. Transforming OPPQ-AM into a bounding theory: OPPQ-BM

The OPPQ-AM formalism overlooks the full import of equation (11), particularly in the context of the CDE representation with regard to the unphysical solutions:

\[ \langle \Psi | \frac{1}{R} | \Psi \rangle = \sum_{n=0}^{\infty} |c_n(E, \vec{\mu})|^2 = \begin{cases} \text{finite } & E = E_{\text{phys}} \text{ and } \vec{\mu} = \vec{\mu}_{\text{phys}} \\ \infty & E \neq E_{\text{phys}} \text{ or } \vec{\mu} \neq \vec{\mu}_{\text{phys}} \end{cases} \] (31)

where some normalization condition is implicitly assumed, \( C_{\text{Norm}}(\vec{\mu}) = 1 \). This relation is suggestive of a shooting method in the energy-missing moment parameter space. Our objective is to eliminate the explicit dependence on the missing moments, resulting in an eigenenergy bounding procedure.

Define the positive partial sums of moduli-squared of the CDE coefficients,

\[ S_l(E, \vec{\mu}) = \sum_{n=0}^{l} |c_n(E, \vec{\mu})|^2. \] (32)

From equation (26) we obtain

\[ S_l(E, \vec{\mu}) = \langle \vec{\mu} | P_l(E) | \vec{\mu} \rangle, \]

where

\[ P_l(E) = \sum_{n=0}^{l} \Lambda_n^E \Lambda_n^E, \] \hspace{1cm} (34)

defines a dyad. It will be positive definite if \( l \geq m_x \), since there will then be \( I + 1 \geq m_x + 1 \), independent vectors, and the \( 1 + m_x \) dimensional, missing moment vector cannot be orthogonal to all of them.

These partial sums form an (essentially) increasing sequence (trivially, by definition)

\[ S_l(E, \vec{\mu}) < S_{l+1}(E, \vec{\mu}) < \ldots < S_{\infty}(E, \vec{\mu}) \],

and becomes infinite for unphysical \( E \) and/or \( \mu \) values; or finite, for the exact physical values. This is the OPPQ-BM quantization condition:

\[ \langle \Psi | \frac{1}{R} | \Psi \rangle = S_{\infty}(E, \vec{\mu}) = \begin{cases} \text{finite } & E = E_{\text{phys}} \text{ and } \vec{\mu} = \vec{\mu}_{\text{phys}} \\ \infty & E \neq E_{\text{phys}} \text{ or } \vec{\mu} \neq \vec{\mu}_{\text{phys}} \end{cases} \] (36)

where we implicitly assume that some normalization prescription on the missing moments has been adopted, \( C_{\text{Norm}}(\mu_1, \ldots, \mu_m) = 1 \).

One can interpret this OPPQ-BM quantization condition as the basis for a shooting method within the \( E \times (\mu_1, \ldots, \mu_m) \) parameter space (i.e. one generates the sequence \( \{S_l(E, \vec{\mu})\} \) attempting to observe behaviors consistent with equation (36)). Clearly this is inefficient (since the missing moment order, \( m_x \), can be large, although finite); fortunately, the OPPQ-BM formalism will allow us to remove the explicit missing moment dependence.

A different interpretation of equation (36) is that

\[ S_{\infty}(E_{\text{phys}}, \vec{\mu}_{\text{phys}}) = \text{Local Minimum}_{\vec{\mu}}(\text{Global Minimum}_{\vec{\mu}} S_{\infty}(E, \vec{\mu})), \] \hspace{1cm} (37)

constrained by \( C_{\text{Norm}}(\mu_1, \ldots, \mu_m) = 1 \).

The above is a qualitative relation that will guide the more exact parts of the ansatz, as given below. Thus, from equation (36) we know that \( S_{\infty}(E_{\text{phys}}, \vec{\mu}) \) will be infinite everywhere except for the physical missing moments. Thus the physical missing moments corresponds to the global minimum of \( S_{\infty}(E_{\text{phys}}, \vec{\mu}) \) in the missing moment space. If \( E \neq E_{\text{phys}} \) then the Global Minimum\( \vec{\mu} \)\( S_{\infty}(E, \vec{\mu}) = \infty \). It will only be finite (hence a local minimum in the energy parameter variable) at the next physical energy value.
This in turn motivates that one work with the global minimum of $S_l(E, \mu)$, with respect to the missing moment dependence constrained by the adopted missing moment normalization, and arbitrary $E$. This then transforms the OPPQ-BM quantization condition into a Constrained Quadratic Form Minimization (CQFM) problem (due to the positive definite quadratic form in equation (33)):

$$\mathcal{L}_I(E) \equiv \inf \{ \mathcal{S}_l(E, \mu) | C_{\text{Norm}}(\mu) = 1 \},$$

and examine its local minima in $E$ as $I \to \infty$.

Two important properties are satisfied by these energy parameter dependent functions. The first is that they define an increasing, positive sequence:

$$0 < \mathcal{L}_I(E) < \mathcal{L}_{I+1}(E) \cdots < \mathcal{L}_\infty(E). \quad (39)$$

The proof of this is given in the appendix.

The other important property is that for a given physical energy, $E_{\text{phys}}$, the physical missing moments correspond to the global minimum in the missing moment space:

$$\mathcal{L}_\infty(E_{\text{phys}}) = S_{\infty}(E_{\text{phys}}, \mu_{\text{phys}}). \quad (40)$$

The (simple) proof of this is also given in the appendix.

2.4.1. The unit missing moment normalization case: $\|\mu\|^2 = 1$

It is instructive to examine the implications of equations (38)-(40) for the missing moment—unit normalization case, where $C_{\text{Norm}}(\mu) \equiv \|\mu\|^2 = 1$. This is the adopted normalization for the examples discussed in section 3 (the harmonic oscillator) and section 4 (the quartic anharmonic double well oscillator). For this normalization choice, the $\mathcal{L}_I(E)$ become the smallest eigenvalue for the $\mathcal{P}_I(E)$ dyad matrix:

$$\mathcal{L}_I(E) = \lambda_I(E) \equiv \text{Smallest Eigenvalue of } \mathcal{P}_I(E), \text{ if } \|\mu\|^2 = 1. \quad (41)$$

One dimensional problems will have a fixed missing moment order. Furthermore, the positive definite matrices, $\mathcal{P}_I(E)$, are of fixed dimension, $1 + m_0$, regardless of the expansion order, $I$. It is also easy to see from the definition of these dyad matrices in equation (34) that

$$\mathcal{P}_{I+1}(E) = \mathcal{P}_I(E) + \mathcal{D}_I(E), \quad (42)$$

where $\mathcal{D}_I(E)$ is the semidefinite dyad matrix, $\frac{N_{E}}{E} \Lambda_I \Lambda_I^\dagger$. Since all three matrices in equation (42) have the same dimension, $1 + m_0$, it is then straightforward to argue that with respect to the smallest eigenvalue we have $0 < \lambda_I(E) < \lambda_{I+1}(E)$; or more generally:

$$0 < \lambda_1(E) < \lambda_{I+1}(E) < \lambda_{I+2}(E) \cdots < \lambda_\infty(E). \quad (43)$$

This is an example of equation (39).

These relations do not apply in the multidimensional case, since the corresponding $\mathcal{P}_I(E)$ matrices will be of varying dimensions. That is, the unit missing moment normalization is inapplicable in the multidimensional case, to all orders. In the multidimensional case, as discussed in section 5, only a fixed (but arbitrary) number of missing moments can be normalized to all orders.

The counterpart to equation (40), for the unit missing moment normalization case, is

$$\mu_{\text{phys}} = \text{Eigenvector of } \mathcal{P}_\infty(E_{\text{phys}}) \text{ with eigenvalue } \lambda_\infty(E_{\text{phys}}), \text{ if } \|\mu\|^2 = 1, \quad (44)$$

as argued in section 4.

2.4.2. Case: $m_0 = 0$

For the zero-missing moment order case, $m_0 = 0$, there is no missing moment vector dependence for $S_l(E)$. In this case, we have

$$\lambda_I(E) = S_l(E) \iff m_0 = 0, \text{ and } \mu_0 \equiv 1, \quad (45)$$

as used in the quantum harmonic oscillator problem.

2.5. OPPQ-BM: Generating the converging, eigenenergy, bounds

The increasing positive sequence in equation (39), together with equation (38), equation (36), and equation (40), lead to an alternate, and more efficient, reformulation of the OPPQ-BM quantization condition (as given in equation (36)).
Clearly, this is telling us that the physical solutions are the local minima of $\mathcal{L}_\infty(E)$. Although the remaining analysis also applies for the case of non-hermitian systems with complex eigenenergies (and $L^2$ integrable on the real axis), we will now assume that the system is hermitian. Accordingly, we can express the local minima of the positive $\mathcal{L}_\infty(E)$ functions in equation (46) as:

$$\frac{\partial}{\partial E} \mathcal{L}_\infty(E_{\text{phys}}) = 0;$$

therefore, one should focus on the local minima of the $I$-th order function, $\mathcal{L}_I(E)$, since these should approximate the physical energies to $I$-th order.

Within a large neighborhood of the physical energy, $E_{\text{phys}}$, the $\mathcal{L}_I(E)$ will have well defined local minima, defined by:

$$\frac{\partial}{\partial E} \mathcal{L}_I(E_{\text{min}}^{(I)}) = 0.$$

From the definition of the local minima, at $I$-th order, we have: $\mathcal{L}_I(E_{I-1}^{(I)}) < \mathcal{L}_I(E_{I+1}^{(I)})$; however, from the increasing sequence in equation (39), we have $\mathcal{L}_I(E_{I-1}^{(I)}) < \mathcal{L}_I(E_{I+1}^{(I)})$. It then follows that $\mathcal{L}_I(E_{I-1}^{(I)}) < \mathcal{L}_{I+1}(E_{I-1}^{(I)})$, or more generally:

$$0 < \mathcal{L}_I(E_{I-1}^{(I)}) < \mathcal{L}_{I+1}(E_{I-1}^{(I)}) < \cdots < \mathcal{L}_{\infty}(E_{\text{phys}}) = \text{finite}.$$

That is, as the order increases, $I \rightarrow \infty$, from equation (39) we see that the $\mathcal{L}_I(E)$ will become a nested sequence of functions, concave upwards, becoming tighter around the local minima, and becoming infinite everywhere except at the physical energies. This behavior is depicted in figures 1–3 for the harmonic oscillator problem.

From equation (49), the sequence of local extrema will converge to the physical energies:

$$\lim_{I \rightarrow \infty} E_{I-1}^{(I)} = E_{\text{phys}}.$$

Let $B_U$ be any (coarse) upper bound to the bounded sequence in equation (49)

$$\mathcal{L}_I(E_{I-1}^{(I)}) < \mathcal{L}_{I+1}(E_{I-1}^{(I)}) < \mathcal{L}_{I+2}(E_{I-1}^{(I)}) < \cdots < \mathcal{L}_{\infty}(E_{\text{phys}}) < B_U.$$

We repeat this important point. The generation of tight bounds is dependent only on determining any coarse upper bound to the sequence, which will also be an upper bound to the limit of the sequence:

$$B_U > \mathcal{L}_{\infty}(E_{\text{phys}}) = \text{finite}.$$

Solve for the roots:

$$\mathcal{L}_I(E_{I-1}^{(I)}) = \mathcal{L}_I(E_{I-1}^{(I)}) = B_U,$$
which will always have a solution, due to equation (46). These roots will then define lower and upper bounds to the physical energies:

\[ E_I^{(L)} < E_{phys} < E_I^{(U)}, \]

with

\[ \lim_{I \to \infty} (E_I^{(U)} - E_I^{(L)}) = 0^+. \]  

3. The quantum harmonic oscillator

The OPPQ-BM formalism is built around two types of functions. The first are the expressions \{S_I(E, \mu)\}, as defined in equation (33), which depend on the energy and missing moment vector. The second are the purely energy dependent expressions \{L_I(E)\}, as defined in equation (38). Both types of functions assume the same missing moment normalization. The bounding capabilities of OPPQ-BM are built around the behavior of the \{L_I(E)\} functions. If the missing moment normalization is that of a unit vector, \(|\mu| = 1\), then \(L_I(E) = \lambda_I(E)\), the smallest eigenvalue of the \(P_I(E)\) positive matrix in equation (34). If a problem corresponds to \(m_s = 0\), then the \(S_I\) have no missing moment dependence and \(\lambda_I(E) \equiv S_I(E)\).
The quantum harmonic oscillator problem has physical solutions that are either symmetric (even) or antisymmetric (odd). We can transform the Hamburger moment MER representation (i.e. involving the $\mu(p)$ moments defined over $\mathbb{R}$) into a Stieltjes MER representation for the even states, and another one for the odd states. The Stieltjes MER representation involves power moments for a related configuration defined on the nonnegative real axis. They are denoted by $\{u(p)\}$. Within the Stieltjes representations, for the even or odd harmonic oscillator states, the missing moment order is $m_s = 0$. Instead of working with the corresponding $\lambda(E)$ expressions, we will work with the identical expressions corresponding to $S_f(E)$. The behavior of these functions, for the harmonic oscillator case, are identical to how either the $\lambda(E)$ or $L_f(E)$ functions will behave, for problems in which $m_s \neq 0$.

### 3.1. The moment equation representation (MER)

Consider the harmonic oscillator,

$$-\partial_x^2 \Psi(x) + x^2 \Psi(x) = E \Psi(x). \quad (56)$$

To transform it into MER form multiply both sides by $x^p$, and integrate by parts, assuming that $\Psi$ is a discrete state ($L^2$ integrable) configuration. We obtain the Hamburger moment equation representation:

$$\mu(p + 2) = E\mu(p) + p(p - 1)\mu(p - 2), \quad (57)$$

for $p \geq 0$. This is, effectively, a finite difference equation of order 2, in which the initialization moments $\{\mu(0), \mu(1)\}$ must be specified before all the other moments can be generated, for any energy parameter value, $E$. We refer to these initialization moments as the missing moments. For the full harmonic oscillator (working with the even and odd states simultaneously), the missing moment order is $m_s = 1$. We also note that the order of the finite difference equation does not change if the kinetic energy term (i.e. $p(p - 1)\mu(p - 2)$) is removed. This suggests that within a moments representation, or equivalently, a Fourier space representation, singular-perturbation expansions in configuration space become (more) regular perturbation expansions.

The MER relation can be rewritten as

$$\mu(p) = \sum_{\ell = 0}^{m_s - 1} \bar{M}_E(p, \ell) \mu_\ell, \quad (58)$$

for $p \geq 0$, $\mu_\ell \equiv \mu(\ell)$, and $\bar{M}_E(\ell_1, \ell_2) = \delta_{\ell_1, \ell_2}$. The energy dependent coefficients $\bar{M}_E(p, \ell)$ (polynomials in $E$) also satisfy the same MER relation in equation (57) with respect to the $p$-index, subject to the indicated initialization conditions.

Restricting our analysis to the symmetric states, for simplicity, the odd order Hamburger moments become zero, $\mu(odd) = 0$. The even order Hamburger moments become Stieltjes moments of a configuration restricted to the nonnegative real axis (i.e. $\xi \equiv x^2$). Thus, let $u(p) \equiv \mu(2p) = \int_0^\infty d\xi \xi^p \Phi(\xi)$ where $\Phi(\xi) \equiv \Psi(\sqrt{\xi})/\sqrt{\xi}$. The new MER relation is

$$u(p + 1) = E \, u(p) + 2p(2p - 1) \, u(p - 1), \quad (59)$$

$p \geq 0$. This is an $m_s = 0$ problem since only one missing moment is required, $u(0) \equiv u_0$. We then have the relation (expressed in the standard form)

$$u(p) = \sum_{\ell = 0}^{m_s - 0} M_E(p, \ell) u_\ell, \quad (60)$$

for $p \geq 0$, and $M_E(0, 0) = 1$. The $M_E(p, \ell)$ energy dependent coefficients satisfy equation (59) with respect to the $p$-index.

### 3.2. The christoffel-darboux expansion

Since the Stieltjes moments, $u(p)$, are the power moments of a function on the nonnegative real axis, $\Phi(\xi)$, $\xi \geq 0$, we can expand the physical solutions in terms of the orthonormal polynomials of an appropriate weight, $R(\xi)$.

Given that the asymptotic form for $\Psi(x)$ is governed by $R(x) = \exp\left(-\frac{x^2}{2}\right)$, whose orthogonal polynomials are the Hermite polynomials $H_{nm}(x)$ satisfying $(H_{nm}R(x))|H_{nm} = N_{n,m} \delta_{n,m}$, the transformation $x \to \xi = x^2$ will involve the weight $R(\xi) \equiv \exp\left(-\frac{\xi^2}{2}\right)/\sqrt{\xi}$. The corresponding orthogonal polynomials would be $H_{2\eta}(\xi^{1/2})$ which become polynomials of degree $\eta$ in the $\xi$ variable. Let us represent their orthonormal counterparts by

$$P_\eta(\xi) = \sum_{j=0}^{\eta} \Xi_j(\eta) \xi^j, \quad (61)$$
where
\[ \langle P_\eta|\mathcal{R}|P_\eta \rangle = \xi_{\eta;\eta} \xi_\eta. \] (62)

The Christoffel-Darboux expansion (CDE) decomposes the physical configuration in terms of the basis \{\(P_\eta(\xi)\mathcal{R}(\xi)|\eta \geq 0\)\}:
\[ \Phi(\xi) = \sum_{\eta=0}^{\infty} c_\eta P_\eta(\xi) \mathcal{R}(\xi). \] (63)

We emphasize that although the polynomials are orthonormal relative to the chosen weight, the basis functions \(P_\eta(\xi)\mathcal{R}(\xi)\) are non-orthogonal relative to each other.

The projection coefficients are generated in closed form from the associated MER relation:
\[ c_\eta(E) = \langle P_\eta|\Phi \rangle = \sum_{j=0}^{\infty} \Xi^{(\eta)}(j), \]
\[ = \sum_{j=0}^{\infty} \Xi^{(\eta)}(\sum_{\zeta=0}^{\infty} M_{\eta \zeta}(j, \zeta) u_\zeta), \]
\[ = \sum_{\zeta=0}^{\infty} \Lambda^{(\eta)}_{\zeta, \xi}, \]
\[ = \Lambda^{(\eta)}_{\xi}, \] (64)

where we have overspecified the notation in anticipation of the more general case, and taken \(u_0 \equiv 1\). The \(\Lambda\)-coefficients are given by
\[ \Lambda^{(\eta)}_{\xi} = \sum_{j=0}^{\infty} \Xi^{(\eta)}(M_{\chi}(j, \xi)). \] (65)

For the chosen weight, the orthonormal polynomials are given through closed form expressions:
\[ P_\eta(\xi) = \left( \frac{-1}{2} \right)^{\eta} \frac{(2\eta)!}{(2\pi)^{\eta}} \sum_{j=0}^{\infty} \frac{(-2)^j}{(\eta - j)! (2j)!} \xi^j. \] (66)

3.3. Orthonormal polynomial projection quantization—approximation method (OPP-Q-AM)

The OPPQ-AM eigenenergy (estimation) condition in equation (29), is the result of the requirement that
\[ \lim_{\xi \to -\infty} \frac{\Phi^2_{\text{phys}}(\xi)}{\mathcal{R}(\xi)} \to 0, \]
fast enough, so that we have
\[ \langle \Phi_{\text{phys}} | \mathcal{R} | \Phi_{\text{phys}} \rangle = \sum_{\eta=0}^{\infty} c_\eta^2(E_{\text{phys}}) < \infty, \] (67)
leading to the quantization condition in equation (29):
\[ \lim_{\eta \to -\infty} c_\eta(E_{\text{phys}}) = 0. \] (68)

However, this is an exact condition for the harmonic oscillator, since the CDE coefficients assume the form
\[ c_\eta(E) = \begin{cases} \frac{1}{(2\pi)^{\eta}}, & \text{for } \eta = 0, \\ \Lambda^{(\eta)}_{\xi} \Pi_{j=1}^{\eta}(E - (1 + 4(j - 1))), & \text{for } \eta \geq 1. \end{cases} \] (69)
the roots being the exact even parity state energy values, \(E_{2N} = 1 + 4N\), for \(N = 0, 1, \ldots\).

3.4. The OPPQ-BM quantization condition

From equation (32), we consider the partial sums:
\[ S_l(E) \equiv \sum_{\eta=0}^{l} c_\eta^2(E), \] (70)
which define a positive, increasing, sequence
\[ 0 < S_l(E) < S_{l+1}(E) \ldots < S_{\infty}(E), \] (71)
becoming finite in the asymptotic limit, for physical states; and unbounded for unphysical energies. This defines the OPPQ-BM quantization condition in equation (36):
\[ \lim_{\eta \to -\infty} S_l(E) = \begin{cases} \text{finite}, & \iff E = E_{\text{phys}}, \\ \infty, & \iff E \neq E_{\text{phys}}. \end{cases} \] (72)

In figures 1–3 we illustrate the validity of equations (71), (72) over different energy intervals.
From equations (71), (72) an eigenenergy bounding ansatz emerges, as outlined in section 2. Clearly, the essence of equation (72), in the \( I \to \infty \) limit, is that the local minima of \( S_\infty(E) \), correspond to the physical energies:

\[
\partial_E (S_\infty(E_{\text{phys}})) = 0. \tag{73}
\]

This suggest that to finite order, the corresponding local minima approximate the physical energies.

Define the local minima:

\[
\partial_E (S_I(E^{(\text{min})})) = 0. \tag{74}
\]

Then using the same reasoning associated with equation (49), it follows that

\[
S_I(E_{I+1}^{(\text{min})}) < S_I(E_I^{(\text{min})}) < S_{I+1}(E_{I+1}^{(\text{min})}),
\]

or

\[
0 < S_I(E_I^{(\text{min})}) < S_{I+1}(E_{I+1}^{(\text{min})}) < \ldots < S_\infty(E_{\text{phys}}) < \infty.
\]

In particular, the local minima converge to the physical energies:

\[
\lim_{I \to \infty} E_{I}^{(\text{min})} = E_{\text{phys}}.
\]

### 3.5. OPPQ-BM: The eigenenergy bounding process

Let \( B_U \) be any coarse upper bound to the local minima sequence in equation (76):

\[
B_U > \{S_I(E_I^{(\text{min})}) | I \geq 0 \}. \tag{78}
\]

Usually, the increasing positive sequence, \( S_I(E_I^{(\text{min})}) \), converges fast enough, allowing for a quick estimate of the coarse upper bound, \( B_U \).

From equations (71)–(72) it follows that at expansion order \( I \), there will be roots to the equations

\[
S_I(E_I^{(L)}) = S_I(E_I^{(U)}) = B_U.
\]

The interval \([E_I^{(L)}, E_I^{(U)}]\) must contain the physical energy; thereby generating bounds:

\[
E_I^{(L)} < E_{\text{phys}} < E_I^{(U)}.
\]

Furthermore, in the infinite expansion limit, these lower and upper bounds must converge to each other:

\[
\lim_{I \to \infty} (E_I^{(U)} - E_I^{(L)}) = 0.
\]

### 3.6. OPPQ-BM numerical results for the harmonic oscillator

In figure 1, we plot \( \log_{10}(S_I(E)) \) over the interval \( 0 \leq E \leq 20 \). The nesting of the \( S_I(E) \) curves is readily apparent, consistent with equation (71) and equation (76). Although these functions are nested within each other, their local minima do not necessarily coincide (i.e. as clearly shown in figure 3 for the second excited state).

In figure 2 we show the progression of localized concavity around the ground state energy \( (E_{gr} = 1) \) for the lower order partial sums, \( \{S_I(E) | 3 \leq I \leq 12 \} \). Indeed, the \( S_I(1) \) sequence is \( S_0(1) = S_1(1) = \ldots = 1 = \sqrt{1/2\pi} = 0.398942 \); thereby concluding, within our OPPQ-BM formulation, that the ground state energy is precisely 1.
Things are more interesting for the second excited state, as given in figure 3 and table 1. We determine the local minima $\partial_E S_l(E_i^{(\text{min})}) = 0$, and generate the sequence $\{ S_l(E_i^{(\text{min})}) \}$ whose convergence defines $S_\infty(E_2) = 3.5904805$. Inspection of the sequence in the third column leads us to conclude that convergence is already setting in at the fourth decimal place. A coarse upper bound $B_u(E) = 3.6 > S_\infty(E_2)$ then allows us to generate converging bounds to the excited state by taking $S_l(E_i^{(1)}) = S_l(E_i^{(0)}) = B_u$, for $I \rightarrow \infty$. Note that the coarseness of the upper bound estimate for $B_u$ does not determine the tightness of the eigenenergy bounds (which depend only on the expansion order $I$).

4. The double well, quartic, anharmonic, oscillator

The quartic anharmonic (double well) potential corresponds to an $m_i = 1$ problem, within each parity symmetry class; and is representative of the most general type of problem amenable to OPPQ-BM analysis. For this system, the $S_l(E, \overline{u})$ functions in equation (35) retain their missing moment dependence. We then introduce the purely energy dependent $\lambda_d(E)$ functions (i.e. equation (41)). These will allow us to implement the OPPQ-BM eigenenergy bounding formalism. A more general class of purely energy dependent functions, $L_l(E)$ (i.e. equation (38)), involving different normalization constraints on the missing moment vectors, can also be introduced. This process is more relevant for multidimensional problems, as discussed in section 5. Both the $\lambda_d(E)$ and $L_l(E)$ functions will have the same properties as the $S_l(E)$ functions for the harmonic oscillator case discussed in the previous section. We prove these properties, here, for the $\lambda_d(E)$. The proofs for the $L_l(E)$ functions is deferred to the appendix; although the structure is similar to that for the $\lambda_d(E)$.

4.1. OPPQ-BM: MER and CDE representations

For simplicity, we solely focus on the symmetric states of the quartic anharmonic, double well, potential, $V(x) = x^4 - 5x^2$. We implement the same analysis as that of the harmonic oscillator. The (Stieltjes) moments satisfy the MER representation:

$$u(p + 2) = 5u(p + 1) + Eu(p) + 2p(2p - 1)u(p - 1), \quad p \geq 0.$$  

We note that $\{ u(0) \equiv u_0, u(1) \equiv u_1 \}$ are the two independent initialization, or missing, moments.

The moment equation can be expressed as

$$u(p) = \sum_{\ell = 0}^{m_p = 1} M_E(p, \ell) u_\ell,$$  

where

$$M_E(p + 2, \ell) = 5M_E(p + 1, \ell) + EM_E(p, \ell) + 2p(2p - 1)M_E(p - 1, \ell),$$  

$p \geq 0$, and

$$M_E(\ell_1, \ell_2) = \delta_{\ell_1, \ell_2}, \quad 0 \leq \ell_1, \ell_2 \leq m_p = 1.$$  

Using the same CDE representation (and weight) as in the harmonic oscillator case we have (i.e. the Stieltjes representation, for the symmetric states, involves the configuration $\Phi$)

$$c_q(E, u_0, u_1) = \langle P_q|\Phi \rangle,$$  

$$c_q(E, u_0, u_1) = \sum_{j = 0}^{q} \Xi_j^{(q)} u(j),$$  

$$c_q(E, u_0, u_1) = \sum_{\ell = 0}^{q} \bar{N}_q^{(q)} u_\ell = \bar{N}_q^{(q)} \cdot \bar{u},$$  

where $\bar{u} \equiv (u_0, u_1)$, and

$$\bar{N}_q^{(q)} = \sum_{j = 0}^{q} \Xi_j^{(q)} M_E(j, \ell).$$

4.2. The General Form for the OPPQ-BM Quantization Condition

The following discussion retraces how the formalism in section 2 was developed. The reader should forget section 2 and go through the process, given below, of rediscovering the bounding formalism in section 2.

The partial sums correspond to

$$S_l(E, \bar{u}) = \sum_{\eta = 0}^{l} c_q^2(E, \bar{u}),$$

$$\lambda_d(E_i^{(n)}) = \sum_{\ell = 0}^{n} \Xi_{\ell}^{(n)} M_E(\ell, \ell).$$
or

\[ S_i(E, \vec{u}) = \sum_{\eta=0}^{i} \left( \vec{A}_E^{(\eta)} \cdot \vec{u} \right)^2, \]

\[ \equiv \langle \vec{u} | \mathcal{P}_i(E) | \vec{u} \rangle. \]  

(89)

The matrix in equation (89) can be argued to be positive if \( i \geq 1 \):

\[ \mathcal{P}_i(E) = \sum_{\eta=0}^{i} \Lambda_E^{(\eta)} \Lambda_E^{(\eta)*} > 0. \]  

(90)

This symmetric matrix is of dimension \( 1 + m_i = 2 \). It is positive definite if \( i \geq 1 \), since it should involve at least two linearly independent \( \vec{A} \) vectors, and the missing moment vector cannot be orthogonal to both.

From the definition of the \( \mathcal{P}_i(E) \) matrices, it follows that:

\[ \mathcal{P}_{i+1}(E) = \mathcal{P}_i(E) + \Lambda_E^{(i+1)} \Lambda_E^{(i+1)*}, \]  

(91)

where \( \mathcal{P}_i(E) \) is positive definite (if \( i \geq 1 \)) and the dyad matrix is semidefinite. More importantly, all the matrices have the same dimension \( 1 + m_i = 2 \).

Define the smallest eigenvalue for the \( \mathcal{P}_i(E) \) matrix:

\[ \lambda_i(E) \equiv \text{Smallest Eigenvalue of } \mathcal{P}_i(E). \]  

(92)

Since the dimension of the matrices in equation (91) are all the same, it follows that

\[ 0 < \lambda_i(E) < \lambda_{i+1}(E) < \ldots < \lambda_\infty(E). \]  

(93)

Forgetting section 2, at this point in the developing formalism (i.e. ‘rediscovering section 2’), we have not concluded that the \( \lambda_i(E) \)’s are relevant for OPPQ-BM quantization (i.e. equation (11)).

The energy and missing moment partial sums define a positive, increasing sequence:

\[ 0 < S_i(E, \vec{u}) < S_{i+1}(E, \vec{u}) < \ldots < S_\infty(E, \vec{u}). \]  

(94)

The asymptotic limit, \( S_\infty(E, \vec{u}) \), corresponds to the expression \( \langle \Phi | \frac{1}{R} | \Phi \rangle \) which, from equation (36), must be finite for physical states, and infinite, for unphysical values for the energy and/or missing moments. This becomes the OPPQ-BM quantization condition:

\[ \text{Lim}_{i \to \infty} S_i(E, \vec{u}) = \begin{cases} \text{finite}, & \iff E = E_{\text{phys}} \text{ and } \vec{u} = \vec{u}_{\text{phys}} \\ \infty, & \iff E \neq E_{\text{phys}} \text{ or } \vec{u} \neq \vec{u}_{\text{phys}} \end{cases} \]  

(95)

This is the general type of expression for both one dimensional and multidimensional problems.

4.3. Solving the OPPQ-BM quantization conditions, equation (95)

The challenge is to develop a procedure for solving equation (95). This was outlined in section 2; however, we repeat the reasoning within this specific example.

Given the strictly increasing nature of the smallest eigenvalue sequence in equation (93), one may suspect that these expressions, involving no explicit missing moment dependence, should be relevant for, effectively, implementing equation (95). We first prove certain additional properties of the eigenvalue sequence. We note that for the one dimensional case, if the focus is on the \( \lambda_i(E) \) expressions, then the missing moment vector must be normalized to unity: \( \vec{u} \to \hat{u} \).

Adapting equation (95) to the one dimensional case, involving unit missing moment vectors, we have:

\[ \text{Lim}_{i \to \infty} S_i(E, \hat{u}) = \begin{cases} \text{finite}, & \iff E = E_{\text{phys}} \text{ and } \hat{u} = \hat{u}_{\text{phys}} \\ \infty, & \iff E \neq E_{\text{phys}} \text{ or } \hat{u} \neq \hat{u}_{\text{phys}} \end{cases} \]  

(96)

The question is: what must be the physical missing moment unit vector, at infinite order, satisfying equation (96), or:

\[ S_\infty(E_{\text{phys}}, \hat{u}_{\text{phys}}) = \text{finite}. \]  

(97)

The answer is, it must correspond to the eigenvector with smallest eigenvalue for the \( \mathcal{P}_\infty(E_{\text{phys}}) \) positive definite matrix defining \( S_\infty(E, \hat{u}) = \langle \hat{u} | \mathcal{P}_\infty(E) | \hat{u} \rangle \).

The proof of this simple, but important, result is by reductio ad absurdum. Denote by \( \hat{u}_\sigma \) the missing moment eigenvector with the smallest eigenvalue, for the \( \mathcal{P}_\infty(E_{\text{phys}}) \) matrix:

\[ S_\infty(E_{\text{phys}}, \hat{u}_\sigma) \equiv \lambda_\infty(E_{\text{phys}}) \equiv \inf_{\hat{u}} [S_\infty(E_{\text{phys}}, \vec{u})] \text{ where } |\vec{u}|^2 = 1. \]  

(98)
Then if we assume that both unit vectors, \( \hat{u}_{\text{phys}} \) and \( \hat{u}_e \), are different, we obtain a contradiction:

\[
\hat{u}_{\text{phys}} \neq \hat{u}_e \implies \text{Contradiction.}
\] (99)

The simple reason is that the smallest eigenvalue is smaller than the expectation value with respect to any other unit vector. However, since the smallest eigenvalue corresponds to an unphysical (by assumption) missing moment unit vector, it must be in finite, based on the OPPQ-BM quantization condition:

\[
\sum_{\text{finite}} E_{\text{phys}} = \sum_{\text{finite}} (E_{\text{phys}}, \hat{u}_{\text{phys}}) = \text{finite}.
\] (100)

This is the contradiction that validates:

\[
\lambda_{\infty}(E_{\text{phys}}) = \text{finite},
\] (101)

or \( \hat{u}_{\text{phys}} = \hat{u}_e \).

It is the conclusion summarized in Eq.101 that underscores the relevance of the smallest eigenvalue (i.e. Equation (93)) in solving the OPPQ-BM quantization condition in equation (96). Thus, we can replace Eq.96 with a similar result solely involving the eigenvalue functions:

\[
\lim_{I \to \infty} \lambda_I(E) = \begin{cases} 
\text{finite,} & E = E_{\text{phys}} \\
\infty, & E = E_{\text{phys}}.
\end{cases}
\] (102)

Given Eq.101, it is now clear that for one dimensional systems, the smallest eigenvalue functions, \( \lambda_I(E) \), will have exactly the same properties as the \( S(E) \) functions for the quantum harmonic oscillator. All the properties identified for the harmonic oscillator problem repeat themselves. The most important are given below.

The local minima of \( \lambda_I(E) \) or \( \lambda_I(E_{I}^{(\text{min})}) \), where

\[
\partial_E \lambda_I(E_{I}^{(\text{min})}) = 0,
\] (103)
generate the positive, increasing, bounded sequence:

\[
0 < \lambda_I(E_{I}^{(\text{min})}) < \lambda_{I+1}(E_{I+1}^{(\text{min})}) < \ldots < \lambda_{\infty}(E_{\text{phys}}) < \infty;
\] (104)

which in turn yield high accuracy estimates for the eigenenergies:

\[
\lim_{I \to \infty} E_{I}^{(\text{min})} = E_{\text{phys}}.
\] (105)

Any coarse upper bound \( B_U \) to the sequence in equation (104), will generate converging bounds to the physical energies. In particular, the roots of \( \lambda_I(E_{I}^{(L)}) = \lambda_I(E_{I}^{(U)}) = B_U \) define converging lower and upper bounds to the physical energy,

\[
E_{I}^{(L)} < E_{\text{phys}} < E_{I}^{(U)},
\] (106)

and

\[
\lim_{I \to \infty} (E_{I}^{(U)} - E_{I}^{(L)}) = 0^+.
\] (107)

### 4.4. Numerical results

In tables 2 and 3 we give the OPPQ-BM energy estimates for our problem, and bounds for the fifth even parity state, \( E_5 \). In table 3, already at \( I = 100 \) we are confident of a coarse upper bound (i.e. .7) to the \( S(E) \) limit of approximately .64. Despite a 9% coarseness in the \( B_U \) estimate (i.e. \( \frac{.7}{.64} = 9\% \)), we can continue to bound the energy up to \( I = 250 \), achieving a bounding accuracy of \( 10^{-15} \).

The following brief discussion assumes the notation defined for the harmonic oscillator problem.

| \( I \) | \( E_0 \) | \( E_5 \) | \( E_4 \) | \( E_6 \) | \( E_8 \) |
|---|---|---|---|---|---|
| 10 | -3.28719572670 | 1.199 863 176 56 | 9.039 422 794 37 |
| 20 | -3.40545088630 | .6975276413 | 6.124 399 208 46 | 13.850 882 804 3 |
| 30 | -3.41010392876 | .6393679163 | 5.892 068 980 15 | 13.567 599 854 1 |
| 40 | -3.41014379139 | .63892839165 | 5.885 342 897 05 | 13.548 320 327 0 |
| 50 | -3.41014273834 | .63892037926 | 5.885 296 198 78 | 13.547 579 045 5 |
| 60 | -3.41014275904 | .63891958477 | 5.885 294 050 95 | 13.547 570 784 3 |
| 70 | -3.41014276214 | .63891956388 | 5.885 293 859 55 | 13.547 570 844 9 |
| 80 | -3.41014276214 | .63891956381 | 5.885 293 858 89 | 13.547 570 848 2 |
| 90 | -3.41014276214 | .63891956378 | 5.885 293 858 79 | 13.547 570 848 6 |
| 100 | -3.41014276214 | .63891956378 | 5.885 293 858 78 | 13.547 570 848 6 |
Faster converging results than those exhibited in tables 2 and 3 can be obtained if we modify the chosen weight. In the case of the harmonic oscillator, the asymptotic form of the physical solutions led to the adopted weight,

\[ \psi = \frac{1}{2} R x x \exp \left( -\frac{R}{2} \right), \]

resulting in the transformed weight

\[ \psi = \frac{1}{2} \xi \exp \left( -\frac{\xi^2}{2} \right), \]

within the even parity symmetry class. This is the weight also used for the quartic anharmonic oscillator. Alternatively, for the quartic anharmonic potential, the physical solutions have a different asymptotic form. This suggests that we could use

\[ \psi = \frac{1}{2} R x x \exp \left( -\frac{R}{2} \right), \]

which transforms into

\[ \psi = \frac{1}{2} \xi \exp \left( -\frac{\xi^2}{2} \right), \]

for \( \xi > 0 \); yielding faster converging results, although not pursued here.

4.5. Closed form expression for \( \partial_E \lambda(E) \)

In determining the roots of \( \partial_E \lambda(E) = 0 \), we can exploit the fact that these expressions can be generated in closed form, if the smallest (missing moment) unit eigenvector is generated.

In terms of its eigenvector, \( \lambda(E) = \langle \tilde{u}(E) | \mathcal{P}(E) | \tilde{u}(E) \rangle \), we have:

\[ \partial_E \lambda(E) = \langle \tilde{u}(E) | \partial_E \mathcal{P}(E) | \tilde{u}(E) \rangle = 0. \]  

The expression \( \partial_E \mathcal{P}(E) \) can be calculated as follows:

\[ \partial_E \mathcal{P}(E) = \partial_E \left( \sum_{j=0}^{\infty} \frac{N_E^{(0)}}{E^j} \right) = \sum_{j=0}^{\infty} \frac{\partial_E N_E^{(0)}}{E^j} \]

(109)

and

\[ \frac{\partial_E N_E^{(0)}}{E} = \frac{\partial_E \left( N_E^{(0)} E^{(0)} \right)}{E^{j+1}} = \sum_{j=0}^{\infty} \frac{\partial_E \left( N_E^{(0)} E^{(0)} \right)}{E^{j+1}}; \]

(110)

assuming the orthonormal polynomial coefficients are independent of the energy parameter, \( E \). Exceptions to this can arise. The expression \( \partial_E \mathcal{M}(j, \ell) \) can be obtained from the moment equation directly, as follows.

Table 3. OPPQ-BM Bounds for \( E_8: V(x) = x^4 - 5x^2, R = \xi \frac{1}{2} \).

| \( I \) | \( \partial_E \lambda(E) \text{ [mm]} \) | \( \lambda(E) \) | \( E_{I,1} \) | \( E_{I,2} \) |
|---|---|---|---|---|
| 30 | 22.677 422 284 0 | .64106446 | 21.4017 | 23.8979 |
| 40 | 22.634 760 748 7 | .64116603 | 22.3932 | 22.9076 |
| 50 | 22.635 974 362 5 | .64117354 | 22.5408 | 22.7332 |
| 60 | 22.636 324 763 1 | .64117452 | 22.6215 | 22.6512 |
| 70 | 22.636 336 021 8 | .64117456 | 22.6339 | 22.6387 |
| 80 | 22.636 336 357 4 | .64117456 | 22.6355 | 22.6372 |
| 90 | 22.636 336 380 3 | .64117456 | 22.636 248 | 22.636 368 |
| 100 | 22.636 336 380 9 | .64117456 | 22.636 304 | 22.636 368 |
| 110 | 22.636 336 380 8 | .64117456 | 22.636 341 8 | 22.636 368 |
| 120 | 22.636 336 333 2 | .64117456 | 22.636 333 5 | 22.636 368 |
| 130 | 22.636 336 360 0 | .64117456 | 22.636 336 7 | 22.636 368 |
| 140 | 22.636 336 333 9 | .64117456 | 22.636 336 43 | 22.636 368 |
| 150 | 22.636 336 336 0 | .64117456 | 22.636 336 97 | 22.636 368 |
| 160 | 22.636 336 338 9 | .64117456 | 22.636 336 18 | 22.636 368 |
| 170 | 22.636 336 338 0 | .64117456 | 22.636 336 84 | 22.636 368 |
| 180 | 22.636 336 338 8 | .64117456 | 22.636 336 88 9 | 22.636 368 |
| 190 | 22.636 336 336 0 | .64117456 | 22.636 336 88 9 | 22.636 368 |
| 200 | 22.636 336 336 3 | .64117456 | 22.636 336 88 9 | 22.636 368 |

\[ .64117456 < R_E = .7 \]
From equation (84) it follows that
\[
\partial_{E}\mathcal{M}_{E}(p + 2, \ell) = 5\partial_{E}\mathcal{M}_{E}(p + 1, \ell) + E\partial_{E}\mathcal{M}_{E}(p, \ell) + \mathcal{M}_{E}(p, \ell) + 2p(2p - 1)\partial_{E}\mathcal{M}_{E}(p - 1, \ell), \ p \geq 0,
\]
(112)
where
\[
\partial_{E}\mathcal{M}_{E}(s, \ell_{2}) = 0, \ 0 \leq \ell_{1,2} \leq m,
\]
(113)
Thus, assuming the \(\mathcal{M}_{E}(p, \ell)\) have been generated then the partial derivative with respects to the energy can be also generated.

5. The quadratic zeeman problem

In this problem we show the inadequacy of using the \(\lambda_{\ell}(E)\) functions for implementing OPPQ-BM in multidimensions. Instead, by using different missing moment constraint relations within an \(L_{\ell}(E)\) formulation (i.e. Equation (58)), we can implement OPPQ-BM and generate tight bounds, over a broad range of magnetic fields. The necessary proofs that these new energy dependent functions satisfy the basic OPPQ-BM structure (i.e. equation (39)) is found in the appendix. This in turn leads to all the other OPPQ-BM bounding relations given in equations (46)–(55).

5.1. The MER representation

For simplicity, we examine the even parity, zero azimuthal angular momentum states, for the quadratic Zeeman (QZM) problem corresponding to:
\[
\left( -\frac{1}{2}\Delta + \frac{B^{2}}{8}(x^{2} + y^{2}) - \frac{1}{r} - E \right)\Psi = 0.
\]
(114)
We adopt the parabolic coordinate representation formalism used by Handy et al [14], transforming the three dimensional QZM problem (atomic units adopted), into a parabolic coordinate representation defined by \(\xi = r - z \geq 0, \eta = r + z \geq 0\). Additionally, from EMM we know that a more efficient missing moment structure (i.e. a reduction in the order of the finite difference equation) is obtained if we transform the wavefunction according to
\[
\Phi(\xi, \eta) \equiv \Psi(\xi, \eta)\exp(-B\xi\eta/4).
\]
(115)
The transformed parabolic partial differential equation becomes
\[
\partial_{\xi}(\xi\partial_{\xi}\Phi) + \partial_{\eta}(\eta\partial_{\eta}\Phi) + \frac{1}{2}B\xi\eta(\partial_{\xi}\Phi + \partial_{\eta}\Phi)
\]
\[
+ \left[\frac{1}{2}(E + \frac{1}{2}B)(\xi + \eta) + 1\right] \Phi = 0.
\]
(116)
The asymptotic form of the transformed configuration is given by
\[
\Phi(\xi, \eta) \to \exp\left[-\frac{1}{2}B\xi\eta - \left(\frac{\epsilon}{2}\right)^{2}\frac{1}{2} |\eta - \xi| \right],
\]
(117)
where the binding energy is given by \(\epsilon = B/2 - E\).

The two dimensional Stieltjes moments for \(\Phi\) are defined by
\[
u(m, n) = \int_{0}^{\infty} d\xi \int_{0}^{\infty} d\eta \ \xi^{m}\eta^{n}\Phi(\xi, \eta),
\]
(118)
with moment equation
\[
m^{2}u(m - 1, n) + n^{2}u(m, n - 1) - \frac{1}{2}[Bm + \epsilon]u(m, n + 1) + u(m, n)\]
\[
- \frac{1}{2}[Bn + \epsilon]u(m + 1, n) + u(m, n) = 0,
\]
(119)
with even parity invariance \((z \leftrightarrow -z\) or \(\xi \leftrightarrow \eta\) reflected in the moment reflection symmetry \(u(m, n) = u(n, m)\).

The moment equation defines a ‘nearest neighbor’ pattern in which the \(u(m, n)\) moment is linked to the \{\(u(m + 1, n), u(m - 1, n), u(m, n + 1), u(m, n - 1)\}\} moments, so long as the reflection symmetry is exploited, and the moment indices limited to the nonnegative integers \(m, n \geq 0\). The missing moments correspond to \{\(u(\ell, \ell)/\ell \geq 0\)\}. For \(0 \leq \ell \leq m\), the \(1 + m\) missing moments, \(u(\ell, \ell) \equiv u_{\ell}\), generate all the moments defined through their antidiagonal index: \{\(u(m, n)/m + n \leq 2m_{i} + 1\)\}. In this manner we generate the moment—missing moment relation:
\[ u(m, n) = \sum_{\ell=0}^{m} M_{\ell}(m, n, \ell) u_{\ell}, \text{ where } 0 \leq m + n \leq 2m + 1, \]  
\[ u_{\ell} \equiv u(\ell, \ell) \text{ and } M_{\ell}(\ell, \ell, \ell_{2}) = \delta_{\ell,\ell_{2}}. \]

Given the first \( 1 + m \) missing moments, \( \{ u_{\ell}; 0 \leq \ell \leq m \} \), a finite number of moments are generated, defining the \( U_{m} \) subspace. These subspaces form a nested hierarchy, \( U_{m} \subset U_{m+1} \subset \cdots \subset U_{\infty} \). The MER relation is an exact projection of the Schrödinger equation into each of these subspaces.

The binding energy matrix coefficients, \( M_{\ell}(m, n, \ell) \), satisfy the moment equation with respect to the \((m,n)\) indices and the given initialization conditions:

\[ m^{2}M_{\ell}(m - 1, n, \ell) + n^{2}M_{\ell}(m, n - 1, \ell) = \frac{1}{2}[Bn + \epsilon]M_{\ell}(m, n + 1, \ell) \]
\[ - \frac{1}{2}[Bn + \epsilon]M_{\ell}(m + 1, n, \ell) + M_{\ell}(m, n, \ell) = 0, \]

where \( M_{\ell}(\ell, \ell, \ell_{2}) = \delta_{\ell,\ell_{2}}. \)

### 5.2. Generating the orthonormal polynomials

The preferred reference function—weight is any expression which takes on the asymptotic form of the physical solutions. Alternatively, this can be relaxed so long as the integral in equation (10) is finite: \( \int \Psi_{\text{phys}} R \, \mathrm{d} \xi < \infty \). Instead of using the expression in equation (117), an easier expression to use (with respect to generating the required power moments of the weight, and in turn the coefficients of the orthonormal polynomials) is

\[ R_{\text{QZM}}(\xi, \eta) = \exp\left( -\frac{1}{2}B\xi\eta - \left( \frac{\epsilon}{2} \right)^{2}(\xi + \eta) \right), \]

with power moments

\[ w_{\text{QZM}}(m, n) = \int_{0}^{\infty} d\xi \int_{0}^{\infty} d\eta \, \xi^{m}\eta^{n} \exp(-\beta\xi\eta - \alpha(\xi + \eta)), \]

\[ \equiv \frac{n!}{\alpha^{m+n+2}}\Omega(m, n + 1, g) \]

where \( \alpha = \left( \frac{\epsilon}{2} \right)^{1/2} \), \( \beta = \frac{1}{2}B \), and \( g = \frac{\beta}{\alpha^2} = \frac{B}{\epsilon} \). The \( \Omega \) functions are recursively generated as follows. First, \( \Omega(0, 1, g) < 1 \) is numerically determined to high accuracy. This then allows us to generate

\[ \Omega(0, n + 1, g) = \sum_{j=1}^{n} \frac{(-1)^{j+1}(n-j)!}{g^{j}} + \frac{(-1)^{n}}{g^{n}} \Omega(0, 1, g), \]

for \( n \leq N \). For each such ‘\( n \)’, we can generate

\[ \Omega(m + 1, n + 1, g) = \frac{1}{g} \delta_{m,0} + \frac{m}{g^{m}}\Omega(m - 1, n + 1, g) + [m - n - g^{-1}]\Omega(m, n + 1, g), \]

for \( 0 \leq m \leq M \).

One can allow the reference function to incorporate the binding energy parameter, as given above. This makes the generation of the orthonormal polynomials more time consuming. We do this to low order to obtain an estimate of the physical binding energy (i.e. \( \epsilon_{0} \approx \epsilon_{\text{phys}} \)). Once this is determined, we then keep \( \epsilon_{0} \) fixed within \( R_{\text{QZM}} \) and keep \( \epsilon \) as a variable within the moment equation. So long as \( \epsilon > \epsilon_{0} \), we preserve the asymptotic requirements of the OPPQ formalism. A more precise analysis is given below. Implementing the above process for \( \epsilon_{0} \), we find that it corresponds to the first significant figure for the (eventual) physical energy. The data in tables 4 are generated on this basis.

We repeat the above important point. Let the asymptotic form of the physical solutions correspond to the expression in equation (117), and let the adopted weight function be \( R_{\text{QZM}}(\xi, \eta; \epsilon_{0}) \), as given in equation (122), making explicit its \( \epsilon_{0} \) dependence. Then the expression

\[ \Psi_{\text{phys}}^{R} \sim \exp\left[-\frac{1}{2}B\xi\eta - (2\epsilon)\frac{1}{2}\xi\eta - \frac{1}{4}(\epsilon_{0})^{2}(\xi + \eta)\right]. \]

This expression is integrable, particularly because along the \( \eta \), or \( \xi \), axes (i.e. \( \eta \rightarrow \infty \) and \( \xi = \text{fixed} \), and vice versa) the expression decays exponentially, provided \( \epsilon > \frac{\epsilon_{0}}{4} \).

The orthonormal polynomials will take on the form

\[ P_{l}(\xi, \eta) \equiv \sum_{j=0}^{l} \Xi_{l}^{(j)}\xi^{m}\eta^{n}, \]

(127)
for some appropriate coordinate pair sequence ordering, \(\{(m_j, n_j) : j = 0, 1, 2, \ldots\}\). This sequence ordering must map into the set of nonnegative coordinate integer pairs in a one-to-one and onto manner. Given that the missing moments generate the previously identified moment subspaces, \(\bigcup \mathcal{M}_s\), the most efficient sequence ordering must emulate this as well. The most natural choice is in a progression based on their antidiagonal sum:

\[
(0, 0) \quad 0, \quad (1, 0) \quad 1, \quad (0, 1) \quad 2, \quad (2, 0) \quad 3, \quad (1, 1) \quad 4, \quad (0, 2) \quad 5, \ldots
\]

The orthonormal polynomials must satisfy the orthonormal relations relative to the chosen weight, \(\langle \xi | \psi \rangle \rangle = \delta_{ij}\), where the positive Hankel moment matrix is given by \(W_{ij} = w_{QZM}(m_i + m_j, n_i + n_j)\). The coefficients are then obtained through the Cholesky decomposition \(W = \mathcal{C}^\dagger\mathcal{C}\), resulting in \(\Xi^{(l)} = (\mathcal{C})^{-1}\hat{e}_l\), where \(\hat{e}_l\) is the unit coordinate vector in the \(I\)-th direction.

5.3. The CDE representation

Assembling all the OPPQ-BM components we have the following. The CDE expansion takes on the form

\[
\Phi(\xi, \eta) = \sum_{l=0}^{\infty} c_l P_l(\xi, \eta) R_{QZM}(\xi, \eta),
\]

(128)
and the projection coefficients become (i.e. \( c_I = \langle P_I | \Phi \rangle \))

\[
c_I = \sum_{j=0}^{I} \Xi_j^{(I)} u(m_j, n_j),
\]

or

\[
c_I = \sum_{\ell=0}^{m(I)} \Lambda_{\ell,\ell}^{(I)} u_\ell,
\]

where \( m(I) \) is the missing moment order required to generate \( c_I \), and

\[
\Lambda_{\ell,\ell}^{(I)} = \sum_{j=0}^{I} \Xi_j^{(I)} M_{\ell}(m_j, n_j, \ell).
\]

An alternative way to use the above relations is to say that the dimensionality of the positive definite dyadic matrices changes. We make this explicit:

\[
S_I(\epsilon, u_\ell) = \sum_{j=0}^{I} (c_j(\epsilon, u_\ell))^2 \equiv \langle \vec{u}^{I}| P_I(\epsilon)| \vec{u}^{I} \rangle,
\]

where \( \vec{u}^{I} \) is a missing moment vector of dimension \( 1 + m(I) \), corresponding to the number of missing moments required to generate the \( I \)-th order expansion. Additionally

\[
S_I(\epsilon, u_\ell) = \sum_{\ell'=0}^{m(I)} u_{\ell'} \cdot P_{I,\ell',\ell}(\epsilon) u_\ell,
\]

\[
P_{I,\ell',\ell}(\epsilon) \equiv \sum_{i=0}^{I} \Lambda_{\ell',\ell}^{(I)} \Lambda_{i,i}^{(I)}
\]

\[
P_{I}(\epsilon),
\]

a symmetric positive definite matrix made up of individual semidefinite dyadic matrices. This matrix, \( P_{I}(\epsilon) \), is positive definite because \( T \) is much larger than the dimension \( (1 + m_s) \) of the \( \Lambda \)-vectors. It is relative to this positive definite matrix that the constrained quadratic form minimization (CQFM) formalism is implemented, as discussed below.

It is important to note that all the orthonormal polynomials with index \( I \) satisfying \( I \leq I_{m_s} \) as defined previously, will depend on the first \( 1 + m_s \) missing moments. Those with index greater than this, \( I_{m_s} + 1 \leq I \leq I_{m_s + 1} \), will depend on the first \( 2 + m_s \) missing moments. It is at the transition point \( I = I_{m_s} \to I = I_{m_s + 1} \) that the dimensionality of the positive definite matrices changes. We make this explicit:

\[
P_{I_{m_s}+1}(\epsilon) = P_{I_{m_s}}(\epsilon) + \frac{\Lambda_{I_{m_s}+1}^{(I)}}{\Lambda_{I_{m_s}+1}^{(I)}} P_{I_{m_s}}(\epsilon) \frac{\Lambda_{I_{m_s}+1}^{(I)}}{\Lambda_{I_{m_s}+1}^{(I)}},
\]

involving two positive definite matrices and one semidefinite (dyadic) matrix. The dimensions of all three satisfy

\[
\text{Dim}(P_{I_{m_s}}) = \text{Dim}(\Lambda_{I_{m_s}+1}) \text{ and Dim}(P_{I_{m_s}+1}) = \text{Dim}(P_{I_{m_s}}) + 1.
\]

Due to this change in dimensionality, the more general CQFM analysis is required. That is, the standard normalization \( \sum_{\ell'=0}^{m(I)} u_{\ell'}^2 = 1 \) cannot be applied consistently across all \( \mathcal{U}_{m_s} \) for \( m_s = 0, 1, \ldots \), subspaces generated by the missing moments.

5.4. Implementation of the constrained quadratic form minimization

We will be adopting the normalization condition

\[
u_0 \equiv 1,
\]

which is expected to be valid (i.e. not interfere with any symmetry conditions) for the even parity states. Such a normalization is possible from the physics perspective; and is mathematically valid within our OPFQ framework.

The uniform normalization, \( u_0 = 1 \), leads to a constrained quadratic form (i.e. \( S_I \) is a positive definite quadratic form in the missing moments, as given in equation (132)).
\[
S_i(E, \mathbf{u}) \equiv S_i(\epsilon, u_0 = 1, u_1, \ldots, u_m),
\]
whose global minimum value over the unconstrained missing moment variables defines the energy dependent function, \( \mathcal{L}_i(\epsilon) \), as discussed in section 2.

\[
\begin{align*}
S_i(\epsilon, \mathbf{u}) &= \sum_{\ell_1=0}^{\infty} \cdots \sum_{\ell_m=0}^{\infty} u_{\ell_1,\ell_2,\ldots,\ell_m} \mathcal{P}_{1,0,0}(\epsilon) u_{\ell_1}, \\
S_i(\epsilon, (1, u_1, \ldots, u_m)) &= \mathcal{P}_{1,0,0}(\epsilon) + 2 \sum_{\ell_1=1}^{\infty} \mathcal{P}_{1,0,0}(\epsilon) u_{\ell_1} + \sum_{\ell_1=1}^{\infty} \sum_{\ell_2=1}^{\infty} \cdots \sum_{\ell_m=1}^{\infty} u_{\ell_1,\ell_2,\ldots,\ell_m} \mathcal{P}_{1,\ell_1,\ell_2,\ldots,\ell_m}(\epsilon) u_{\ell_2}, \\
&= G_i(\epsilon) + 2 \mathbf{B}_i(\epsilon) \cdot \mathbf{u} + \langle \mathbf{u} | \mathbf{A}_i(\epsilon) | \mathbf{u} \rangle.
\end{align*}
\]

The definitions for the \( C_i, \mathbf{B}_i \), and \( \mathbf{A}_i \) are self-evident by association.

The global minimum, for fixed \( \epsilon \),

\[
\mathcal{L}_i(\epsilon) = \inf_{\mathbf{u}} \{ S_i(\epsilon, \mathbf{u}) | u_0 = 1 \},
\]

corresponds to the solution

\[
\mathbf{u}_{\epsilon,\text{opt}} = -(\mathbf{A}_i(\epsilon))^{-1} \mathbf{B}_i(\epsilon),
\]

yielding

\[
\mathcal{L}_i(\epsilon) = C_i(\epsilon) - \langle \mathbf{B}_i(\epsilon) | \mathbf{A}_i^{-1}(\epsilon) | \mathbf{B}_i(\epsilon) \rangle.
\]

Clearly, \( \mathbf{u}_{\epsilon,\text{opt}} \), a non-unit vector, is the counterpart to the ‘eigenvector of smallest eigenvalue’ within the one dimensional formulation; whereas \( \mathcal{L}_i(\epsilon) \) is the counterpart to \( \lambda_i(\epsilon) \) within the one dimensional formulation, as well.

As outlined in the appendix, \( \mathcal{L}_i(\epsilon) \) has all the properties associated with \( \lambda_i(E) \) in the one dimensional case, the most important of which is the positive, increasing, sequence form in equation (39); and from this, eigenenergy estimates and bounds produced, in the exact manner as in the harmonic oscillator and quartic anharmonic oscillator examples.

### 5.5. QZM Numerical Results

Table 4 summarizes the OPPQ-BM results for QZM, including the energy estimates (column three), \( \epsilon_{\text{opt}}^{(\text{min})} \), defined by the local minima relations \( \partial_i \mathcal{L}_i(\epsilon_{\text{opt}}^{(\text{min})}) = 0 \); and the energy bounds (columns four and five), based on a constrained minimization analysis of the quadratic form given in equations ((135)–(140)). The ground and first excited states within the even parity, zero azimuthal angular momentum, symmetry class correspond to \( \epsilon_{\text{gr}} \) and \( \epsilon_1 \), respectively. That is, the subscript index (i.e. ‘gr’ or ‘1’) associated with the data in column 3 refers to the ground state or first excited state, respectively. The sixth column is the \( \epsilon_{\text{opt}} \) parameter value used for the reference function weight, as explained earlier. We emphasize that the bounds are true bounds for the physical energies. The actual positive sequences, and their convergence behavior, are not given here due to space limitations.

For comparative purposes, we quote the energy estimates reported by Kravchenko et al [35] which appear to be the more accurate estimates in the literature, yielding twelve-thirteen significant figures for the ground state binding energy, \( \epsilon_{\text{gr}} \), for magnetic field values \( B \leq 400 \). Their results for the first excited state, \( \epsilon_1 \), vary from twelve significant figures to six, for magnetic field strengths \( B \leq 1000 \), with no energies reported for higher magnetic fields. The OPPQ-BM estimates in table 4 exceed or match their reported \( \epsilon_{\text{gr}} \) values provided \( B \leq 200 \). For \( B = 2000 \), the OPPQ-BM results for \( \epsilon_{\text{gr}} \) generate approximately nine of the thirteen significant figures. The only limitation of OPPQ-BM is the computational speed of our computing platform (i.e. MacBook Pro 2.2 GHz/1333MHz).

For the first excited state, \( \epsilon_1 \), OPPQ-BM matches or surpasses the reported accuracy of Kravchenko et al’s [35] results for \( B \leq \mathcal{O}(200) \). For \( B = 2000 \), the OPPQ-BM results for \( \epsilon_1 \) are compared to those of Schimerczek and Wunner [36]; while for \( B = 10^4 \) we also compare both states to their B-spline analysis results. The ground state results manifest faster convergence than the first excited state. The generated OPPQ-BM bounds are modest, at these higher magnetic field strengths, given the higher expansion orders required for implementing OPPQ-BM. Tighter bounds would be generated on a faster computer platform, or through an alternate choice to the MER representation chosen here. These possibilities are currently under investigation.

For large magnetic fields, the expansion order required to obtain results comparable to those in the literature increases. Results corresponding to \( I_{\text{opt}} > \mathcal{O}(40) \) requires considerable time (i.e. several hours), with available computing resources.

### 6. Conclusion

We have shown that for a broad class of low dimension, homogeneous, LPDE, eigen-parameter problems, hermitian or non-hermitian, transformable into MER form, the Christoffel-Darboux expansion involving the
orthonormal polynomials of an appropriate weight, can generate tight eigen-parameter (i.e. eigenvalue/eigenenergy) bounds, through a straightforward algebraic procedure. We have demonstrated its capabilities through several one and two dimensional Sturm-Liouville (Schrodinger equation) problems, including the important quadratic Zeeman interaction. This method, the Orthonormal Polynomial Projection Quantization-Bounding Method (OPPQ-BM), can be applied to both bosonic and fermionic systems, and expands the computational tools available to researchers, particularly for strong coupling—singular perturbation type systems. Given that there are many important physical systems admitting MER representations, the approach presented should be of great interest to many, where accuracy is important in estimating physical quantities.

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Appendix: Additional Comments and proofs for the OPPQ-BM Formalism

All the main elements of the OPPQ-BM formalism have been presented and argued, except for several. The more important of these is to show that the constrained quadratic form minimization (CQFM) formalism in equation (38) yields energy dependent functions, \( L_i(E) \), that generate a positive, increasing, sequence, as given in equation (39), both for one dimensional problems (where \( m_i \) is fixed) and multidimensional problems (where \( m_i \) increases, with the order of the expansion).

A.1. Proof of equation (39)

Consider the functions

\[
L_i(E) \equiv \inf_{\mu} \{ S_i(E, \mu) | C(\mu) = 1 \},
\]

where the constraint is arbitrary. Clearly, for \( C(\mu) = [\mu]^2 = 1 \), then \( L_i(E) = \lambda_i(E) \), corresponding to the smallest eigenvalue of the positive definite \( P_i \) matrix associated with \( S_i \), as given in equation (33) and equation (132), for the one dimensional and multi-dimensional cases, respectively.

For one dimensional problems, the missing moment vector, \( \mu = (\mu_0, \ldots, \mu_m) \) is of fixed dimension, \( 1 + m \).

Given that the \( S_i(E, \mu) \) functions (trivially) form an increasing sequence, as given in equation (35), it follows that \( L_i(E) < L_{i+1}(E) \), for any choice of missing moment constraint, as indicated in equation (39).

The same follows for the multidimensional case, provided the constraint relation applies to the same missing moments.

For multidimensional systems the following symbolic relation is true for some appropriate choice of the expansion order index, \( I \), and the associated missing moment order, \( m_i \);

\[
S_{I_k}(E, \mu_0, \ldots, \mu_m) < S_{I_k}(E, \mu_0, \ldots, \mu_{m_1}) \ldots \mu_{m_2}),
\]

where \( I_1 < I_2 \) and \( m_1 < m_2 \). This inequality is a consequence of how the partial sums are defined for multidimensional systems. Both expressions involve at least the same missing moments \{ \( \mu_\ell \mid 0 \leq \ell \leq m_i \} \). If the missing moment constraint used for \( L_{I_k}(E) \) is the same as that for \( L_{I_k}(E) \) (i.e. they involve the same \( \mu_\ell \) missing moments, where \( \ell \in I \), then it follows from equation (38) that

\[
L_{I_k}(E) = \inf_{\mu_0, \ldots, \mu_m} \{ S_{I_k}(E, \mu_0, \ldots, \mu_m) | C_{\text{Norm}}(\mu_0, \ldots, \mu_m) = 1 \}
\]

\[
< L_{I_k}(E) = \inf_{\mu_0, \ldots, \mu_m} \{ S_{I_k}(E, \mu_0, \ldots, \mu_m) | C_{\text{Norm}}(\mu_0, \ldots, \mu_m) = 1 \}.
\]

This then proves that the increasing sequence nature of the \( L_i(E) \), in equation (39), applies in the multidimensional case, provided the sequence starts at the expansion order that includes all the missing moments that define the constraint. Accordingly, taking \( u_0 = 1 \) in equation (135) is adequate for QZM. Other, nonlinear choices, are possible, but not considered here.

A.2. Proof of equation (40)

We must prove that:

\[
L_\infty(E_{\text{phys}}) = S_\infty(E_{\text{phys}}, \mu_{\text{phys}}).
\]
In other words, the physical missing moment vector (at \( I = \infty \)) is the one that corresponds to the global minimum for \( S_{\infty}(E_{\text{phys}}, \mu) \), with respect to the missing moment variables, subject to the adopted normalization.

The proof is also by reductio ad absurdum and similar to that used for the quartic anharmonic oscillator example in which \( L(E) \equiv \lambda(E) \) (i.e. equations (97) through (101)).

Define \( \mu_{\text{phys}} \) as the optimal solution to the constrained quadratic form minimization problem at infinite order, for the physical energy:

\[
S_{\infty}(E_{\text{phys}}, \mu_{\text{phys}}) \equiv L_{\infty}(E_{\text{phys}}) = \inf_{\mu} (S_{\infty}(E_{\text{phys}}, \mu)|C(\mu) = 1);
\]

whereas the missing moment vector \( \mu_{\text{phys}} \) satisfies

\[
S_{\infty}(E_{\text{phys}}, \mu_{\text{phys}}) = \text{finite}.
\]

We now argue that if \( \mu_{\text{phys}} = \mu_{\infty} \Rightarrow \) Contradiction.

(Proof) From the infimum property: \( L_{\infty}(E_{\text{phys}}) = S_{\infty}(E_{\text{phys}}, \mu_{\infty}) \leq S_{\infty}(E_{\text{phys}}, \mu_{\text{phys}}) = \text{finite} \).

A.3. Infinite Square Well

On unbounded domains, \( D \subset \Re^3 \), one can find positive weights, \( R > 0 \), whose asymptotic properties satisfy the important integral condition in equation (10). However, on compact domains, if the physical boundary conditions are that \( \Psi_{\text{phys}}(0, \infty) = 0 \), then the weight must be zero on the boundary as well, \( R \geq 0 \), otherwise the finiteness (i.e. \( L^2 \) integrability) of unphysical solutions will violate equation (10). To emphasize this, we consider the infinite square well problem:

\[
-\partial^2_{xx} \Psi(x) = E \Psi(x),
\]

on the interval \([-a, a]\), subject to the condition, \( \Psi_{\text{phys}}(\pm a) = 0 \). The eigenenergies are \( E_n = \left( \frac{(N + 1) \pi}{2a} \right)^2 \), \( N = 0, 1, 2, 3, \ldots \). The physical solutions will correspond to symmetric (even) and antisymmetric (odd) configurations.

Clearly, we cannot take the OPPQ-BM weight to be unity, \( R(x) \equiv 1 \), since then the integral

\[
\int_{-a}^{a} dx \, \Psi^2(x)/R(x) = \text{finite} \quad \text{for both physical and unphysical solutions.}
\]

Assume that near the boundaries we have: \( \Psi_{\text{phys even}}(x) \sim N(a^2 - x^2) \), for \( x \rightarrow a^+ \); whereas \( \Psi_{\text{phys odd}}(x) \sim N(x^2 - a^2) \). Then \( R(x) = (a^2 - x^2) > 0 \), is a possible weight. Furthermore, from equation (10), we will satisfy

\[
\int_{-a}^{a} dx \, \Psi^2(x)/R(x) = \text{finite/infinite},
\]

where the unphysical solutions do not satisfy the zero-boundary condition. That is, since the unphysical solutions are not zero at \( x = \pm a \), these integrals become infinite.

If we multiply both sides of equation (147) by \( x^2(a^2 - x^2) \) and integrate by parts, using the zero boundary condition for the physical states, we obtain:

\[
E_{\text{phys}}(p + 1) = a^2 p(p - 1) + (Ea^2 - (p + 2)(p + 1)) \mu(p),
\]

for \( p \geq 0 \), where \( \mu(p) = \int_{-a}^{a} dx \, x^p \Psi(x) \). Note, no boundary terms The moment equation incorporates the physical boundary value condition. The moments of the weight satisfy

\[
w(p) = \int_{-a}^{a} dx \, x^p(a^2 - x^2) = \frac{4a^{p+3}}{(p + 1)(p + 3)}, \quad \text{if } p = \text{even}; \quad 0, \text{if } p = \text{odd}.
\]

The above is an \( m \) = 0 order problem. As in the harmonic oscillator case in section 3, we can treat separately the even and odd states, through a Stieltjes moment formulation. We do the same for the symmetric states, for simplicity. This results in the Stieltjes moment equation:

\[
E_{\text{phys}}(p + 1) = a^2 p(p - 1) + (Ea^2 - (p + 2)(p + 1)) u_{\text{phys}}(p),
\]

for \( p \geq 0 \), setting \( u_{\text{phys}}(0) \equiv 1 \). This is an \( m_n = 0 \) problem. The associated weight is (i.e. \( \xi = a^2 \))

\[
\mathcal{R}(\xi) = \frac{1}{\sqrt{\xi}}, \quad \text{with Stieltjes moments } \omega(p) = \frac{4a^{p+3}}{(2p + 1)(2p + 3)}, \quad \text{if } p \geq 0.
\]

It is generally possible to obtain MER relations, for problems on compact domains, that do not include boundary terms. Just as in the present case, the EMM analysis of the infinite quantum dot, involved two dimensional moment equations with no boundary terms.[52]

Implementing a similar OPPQ-BM formulation as was done for the harmonic oscillator case in section 3, we generate the CDE representation: \( \Phi(\xi) = \sum_{n=0}^{\infty} a_n B_n(\xi) \mathcal{R}(\xi) \). We choose to generate the orthonormal polynomials through a Cholesky decomposition of the \( \omega(i + j) \) Hankel matrix: \( \omega(i + j) = CC^t \);
solving for $C_{\Xi}^{(n)} = \tilde{c}_n$, vector coefficients of the relevant orthonormal polynomials, $P_n(\xi) = \sum_j^n = 0 \Xi_j^{(n)} \xi^j$. We generate $c_n(E) = \sum_j^n = 0 \Xi_j^{(n)} \vartheta_j (j)$, and the partial sums $S_j(E) = \sum_n = 0 c_j^{(n)}(E)$.

Implementation of OPPQ-BM generates bounds on the discrete states. We take $a = 1$, then using $S_j(E)$, we obtain $2.4673 < E_{gf} < 2.4675$, where $E_{gf} = 2.4674$. Using $S_j(E)$, we obtain $22.205 < E_{gf} < 22.208$, where $E_{2nd} = 22.20661$, etc. These rough bounds were estimated from the plots. Examining the partial sums $S_2(E) < S_3(E) < S_4(E) < \ldots < S_n(E)$, the generated bounds are very tight, as in all the previous examples. We do not give the details, here. The important point is that the weight must take on the zero boundary conditions for the physical solutions, in order for equation (10), or its one dimensional equivalent, equation (18), to hold.

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**References**

[1] Ritz W 1909 J. für die Reine Angewandte Math 1-61
[2] MacDonald J K L 1933 Phys. Rev. 43 830
[3] Temple G 1928 Proc. B. Soc. A Math. Phys. Eng. Sci 119 276
[4] Hill R N 1980 J. of Math. Phys 21 2182
[5] Martinazzo R and Pollak E 2020 Proc. of the Natl. Acad. Sc. of the United States of America 117 16181–86
[6] Schrodinger E 1926 Phys. Rev. 28 1049
[7] Bender C M and Boettcher S 1998 Phys. Rev. Lett. 80 5243
[8] Dorey P, Dunning C and Tateo R 2001 J. Phys. A: Math. Gen 34 L391
[9] Bender C M 2007 Rep. Prog. Phys. 70 947
[10] Handy C R 2001 J. Phys. A 34 5065
[11] Handy C R, Khan D, Wang X-Q and Tymczak C J 2001 J. Phys. A: Math. Gen. 34 5593
[12] Delabare E and Trinh D T 2000 J. Phys. A: Math. Gen 33 8771
[13] Handy C R and Bessis D 1985 Phys. Rev. Lett. 55 931
[14] Handy C R, Bessis D, Sigismondi G and Morley T D 1988 Phys. Rev. Lett. 60 253
[15] Shohat J A and Tamarkin J D 1963 The Problem of Moments (Providence, Rhode Island: American Mathematical Society,)
[16] Baker G A Jr+ 1975 Essentials of Pade Approximants (New York: Academic)
[17] Bender C M and Wu T T 1971 Phys. Rev. Lett. 27 461
[18] Bender C M and Dunne G V 1999 J. of Math. Phys 40 4616
[19] Beals R and Wong R 2016 Special Functions and Orthogonal Polynomials (UK: Cambridge Studies in Advanced Mathematics, Cambridge University Press)
[20] Ushveridze A G 1988 Sov. Phys. -Lebedev Inst. Rep. 2 50 54
[21] Nikiforov A F and Uvarov V B 1988 Special functions of Mathematical Physics (Boston: Birkhauser)
[22] Cooper F, Khare A and Sukhatme U 1995 Phys. Report: Supersymmetry and Quantum Mechanics 251 267
[23] Bender C M and Dunne G V 1996 J. of Math. Phys 37 6
[24] Boyd S and Vandenberghe L 2004 Convex Optimization (New York: Cambridge University Press)
[25] Vasseur J H 2009 Moments, Positive Polynomials and Their Applications (London: Imperial College Press)
[26] Handy C R, Bessis D, Sigismondi G and Morley T D 1988 Phys. Rev. A 37 4557
[27] Chvatal V 1983 Linear Programming (New York: Freeman)
[28] Handy C R and Lee P 1991 J. Phys. A: Math. Gen 24 1565
[29] Bessis D and Handy C R 1986 Systematic Construction of Upper and Lower Bounds to the Ground State Energy of the Schrodinger Equation Int. J. of Quantum Chem: Quantum Chem. Symp. 30 (New York, New York: John Wiley & Sons, Inc.) 21-32
[30] Handy C R 2001 J. Phys. A 34 L271
[31] Yan Z and Handy C R 2001 J. Phys. A: Math. Gen 34 9907
[32] Handy C R and Xiao-Qian Wang 2001 J. Phys. A: Math. Gen 34 8297
[33] Rosner W, Wunner G, Herold H and Ruher H 1984 J. Phys. B 17 29
[34] Le Guillou J C and Zinn-Justin J 1983 Ann. Phys. (N.Y.) 147 57
[35] Kravchenko Y P, Liberman M A and Johansson B 1996 Phys. Rev. A 54 287
[36] Schimerczek C and Wunner G 2014 Comp. Phys. Comm 185 614
[37] Handy C R and Vrinceanu D 2013 J. Phys. A: Math. Theor 46 135202
[38] Handy C R and Vrinceanu D 2013 J. Phys. B: At. Mol. Opt. Phys 46 115002
[39] Bender C M and Orszag S A 1999 Advanced Mathematical Methods for Scientists and Engineers (New York: Springer)
[40] Handy C R 1981 Phys. Rev. D 24 378
[41] Grossmann A and Morlet J 1984 SIAM J. Math. Anal 15 723
[42] Muzy J F, Bacity E and Arneodo A 1991 Phys. Rev. Lett. 67 3515
[43] Handy C R and Murzena R 1998 Phys. Lett. A 248 7
[44] Agmon S 1983 Lectures on the Exponential Decay of Solutions of Second Order Elliptic Equations, Math. Notes Ser: No. 29(Princeton: Princeton Univ, Press)
[45] Glazman I M 1965 Direct Methods of Qualitative Spectral Analysis of Singular Differential Operators (Jerusalem, Israel: Israel Program for Scientific Translation)
[46] Mhaskar H N 1996 Introduction to the Theory of Weighted Polynomial Approximation (Singapore: World Scientific Pub Co, Inc)
[47] Simon B 2008 Proc. Symp. Pure Math. Amer. Math. Soc 314 (Providence, R I)
[48] Hall B C 2013 Quantum Theory for Mathematicians, Graduate Texts in Mathematics 267 (Berlin: Springer)
[49] Reed M and Simon B 1978 Methods of Modern Mathematical Physics (New York: Academic)
[50] Handy C R, Appiah K and Bessis D 1994 Phys. Rev. A 50 988
[51] Koosis P 1988 The Logarithmic Integral I (Cambridge, UK: Cambridge Univ. Press) Refer to discussion in Chapter VI pg. 170.
[52] Handy C R, Trallero-Giner C and Rodriguez A H 2001 J. Phys A: Math. Gen 34 10991