Mathematics **2015**, *3*, 1045-1068; doi:10.3390/math3041045

OPEN ACCESS

mathematics

ISSN 2227-7390

www.mdpi.com/journal/mathematics

Article

Pointwise Reconstruction of Wave Functions from Their Moments through Weighted Polynomial Expansions: An Alternative Global-Local Quantization Procedure

Carlos R. Handy [1,†,*], Daniel Vrinceanu [1,†], Carl B. Marth [2,†] and Harold A. Brooks [1,†]

[1] Department of Physics, Texas Southern University, Houston, TX 77004, USA;
E-Mails: vrinceanud@tsu.edu (D.V.); hbrooks123@comcast.net (H.A.B.)

[2] Dulles High School, Sugar Land, TX 77459, USA; E-Mail: carlbmarth@gmail.com

[†] These authors contributed equally to this work.

* Author to whom correspondence should be addressed; E-Mail: handycr@tsu.edu;
Tel.: +1-713-313-1850.

Academic Editor: Zhongqiang Zhang

Received: 15 July 2015 / Accepted: 26 October 2015 / Published: 5 November 2015

Abstract: Many quantum systems admit an explicit analytic Fourier space expansion, besides the usual analytic Schrödinger configuration space representation. We argue that the use of weighted orthonormal polynomial expansions for the physical states (generated through the power moments) can define an L^2 convergent, non-orthonormal, basis expansion with sufficient pointwise convergent behaviors, enabling the direct coupling of the global (power moments) and local (Taylor series) expansions in configuration space. Our formulation is elaborated within the orthogonal polynomial projection quantization (OPPQ) configuration space representation previously developed The quantization approach pursued here defines an alternative strategy emphasizing the relevance of OPPQ to the reconstruction of the local structure of the physical states.

Keywords: weighted polynomial expansions; moment representations; Hill determinant method; algebraic quantization

PACS classifications: 03.65.Ge; 02.30.Hq; 03.65.Fd

---

1. Introduction

1.1. Preliminaries

Many quantum systems are defined by analytic solutions, which in turn compel us to generate them through (approximate) analytic methods. Although one is generally more interested in the hierarchical large-scale structure leading to quantization (*i.e.*, determining the discrete state energies and L^2 convergent approximations to the wave function configurations), recovering the local structure is also important and the principal focus of this work. Our methods have the important advantage that they are essentially algebraic in nature, allowing for high precision calculations through multiple precision algorithms and symbolic calculations facilitated by computer algebraic systems, such as *Mathematica*. Recent works also adopt a similar computational philosophy as developed in the context of supersymmetric quantum mechanics [1,2], group theory [3] and Hermite distributed approximating functionals [4]. These emphasize an algebra-based analysis for addressing the global (discrete state) structure of appropriate physical systems.

The emphasis on developing high precision, algebraic methods for addressing analytical problems is particularly important. What is desired are algebraic methods that originate from the analysis of purely algebraic quantum systems for which all discrete states are known in closed form. These are referred to as exactly-solvable (ES) systems. One can then attempt to extend the methods developed for ES systems to more general Hamiltonians, in a manner that preserves the basic algebraic structure of such methods in the numerical computation of physical properties. In this regard, supersymmetric and group theory formulations have played a prominent role [1–3]. Two other approaches, of direct relevance to this work, are highlighted in the ensuing discussion: the Hill determinant (HD) method and the orthogonal polynomial projection quantization (OPPQ) method. The latter has important advantages over the former (*i.e.*, L^2 and pointwise convergence, greater numerical stability, *etc.*) in facilitating our "global-local" quantization interests, as identified in Subsection 1.2. Before discussing these, we define particular structures of importance to this work. Although our methods are applicable to multidimensional systems, for simplicity all of our analysis is developed for one-dimensional problems.

We are interested in the large and important class of problems for which the Schrödinger equation can be Fourier transformed into the momentum space representation, $\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int dx\, e^{-ikx} \Psi(x)$, and a power series analysis implemented therein, $\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \sum_p \frac{\mu_p}{p!} (-ik)^p$, generating a recursive, linear, finite difference equation for the power moments $\mu_p = \int dx\, x^p \Psi(x)$. This recursive relation will be referred to as a moment equation, of order $1 + m_s$ (problem dependent). The recursion coefficients involve the energy variable. In reality, the generation of such moment equations is independent of the ability to perform a Fourier transform. Many Schrödinger systems, after a coordinate transformation if necessary, can be directly transformed into such moment equation representations.

We also assume that within the original configuration space representation, the physical discrete state solutions are analytic, $\Psi(x) = \sum_n c_n x^n$, and the power series coefficients can be generated through a linear, second order recursion relation involving energy-dependent coefficients. Directly coupling such local expansions to the asymptotic properties of the physical solutions is not straightforward. Numerically, the "shooting method" attempts to do this [5]. This is also the objective of JWKBmethods,

particularly in their analysis around turning points [6]. Neither approach is algebraic or capable of high accuracy.

The Hill determinant (HD) method [7], of relevance to this work, does define a quantization ansatz connecting the behavior of the c_n-coefficients for discrete states to the boundedness criteria for such states: $\lim_{|x|\to\infty} \Psi(x) = 0$. It does so by representing the wavefunction as $\Psi(x) = A(x)\mathcal{R}(x)$, involving an appropriate (arbitrary) positive, analytic, exponentially-bounded reference function, $\mathcal{R}(x) > 0$. It investigates the power series expansion coefficients generated through $A(x) = \sum_n a_n x^n = \frac{\Psi(x)}{\mathcal{R}(x)}$; achieving quantization through the imposition of truncation relations corresponding to $a_N = 0$, $a_{N+1} = 0$ (for second order differential systems) and taking $N \to \infty$. Since these expressions involve energy-dependent coefficients, this leads to a 2×2 determinantal expression for the energy. The energy roots of this expression converge to the physical energies, when HD works.

Despite its simplicity, and widespread popularity, it is well known that the HD method can lead to anomalous results yielding incorrect energies or becoming otherwise unstable. This was dramatized by Tater and Turbiner [8] in their study of the double well sextic anharmonic oscillator. Since their work does not clearly reveal these difficulties, we have repeated the calculations as demonstrated in Figure 1. These anomalous behaviors were anticipated by Hautot [9], who proposed non-trivial strategies for circumventing these difficulties. If one can avoid these anomalous cases, HD can produce high precision results, since it is readily implementable, to unlimited precision, through Mathematica. However, the anomalous cases appear to correspond [8,9] to using reference functions that imitate the physical asymptotic form of the physical solution. Intuitively, one expects the best convergence when the reference function is allowed to assume this form. Indeed, this is one of the strengths of the alternative approach, OPPQ, to be discussed shortly. OPPQ allows one a wide choice of reference functions. When compared to HD, OPPQ manifests convergence at much higher rates, when the appropriate reference function is used. Furthermore, OPPQ has a stronger theoretical foundation than HD, for reasons given shortly. Despite all of these issues, HD was rediscovered by Tymczak *et al.* [10,11], who also applied it in a new way within momentum space. It continues to be the subject of much interest, as amply demonstrated in the recent works by Killingbeck and Grosjean [12].

The HD method does not define for us a rigorous, high precision, algebraic quantization method that is robust (numerically stable), efficient (producing rapidly converging results) and effective. The principal reason is that the underlying formalism does not readily impose on the a_n's constraints due to the L^2 boundedness criteria $\int dx\ |\Psi(x)|^2 < \infty$. That is, there is no way to impose, or ensure, the latter condition on the behavior of the a_n's. We believe that this is the primary reason for HD's anomalous behaviors, particularly when the reference function assumes the asymptotic form of the physical states, as suggested by Tater and Turbiner's investigations. As previously indicated, the results in Figure 1 reveal the potential instability and slow convergence properties of HD, particularly when the reference function assumes the physical asymptotic form. In summary, we are interested in algebraic, arbitrary precision, quantization methods tied to representations that imitate, as much as possible, the true asymptotic form of the physical solutions. Despite all of its successful implementations, HD does not fall into this class of quantization schemes.

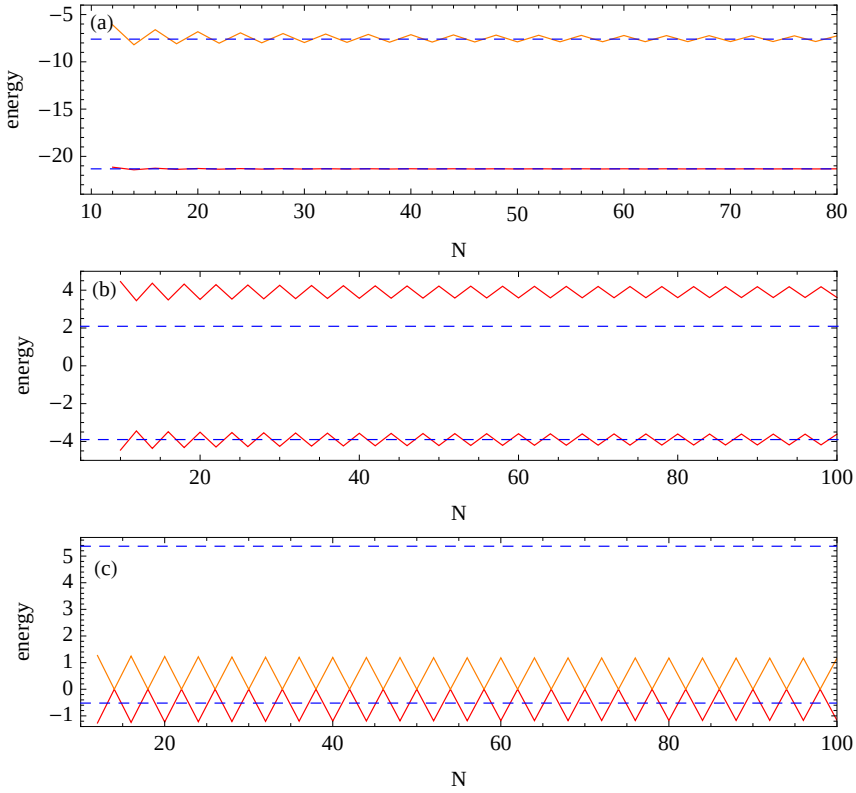

Figure 1. Convergence of the Hill determinant calculation of the first two energy eigenvalues for anomalous cases of the sextic anharmonic oscillator $V(x) = mx^2 + bx^4 + x^6$. Parameter values are: (**a**) ($m = -18$, $b = 0$); (**b**) ($m = -8$, $b = 0$); and (**c**) ($m = -4$, $b = 0$). The dashed lines show the exact energy values. Case (a) show convergences to the correct values, although extremely slowly. Case (b) shows convergence for both energies, but only the ground state converges to the correct value, while the excited state converges to the wrong value. Case (c) shows complete lack of convergence for both energies.

Despite the fact that the power moments are global, and therefore natural objects to study for determining the discrete states, until two years ago, with the discovery of the OPPQ method [13,14], of relevance to this work, there were very few, easily implementable moment methods for quantizing all of the discrete states of multidimensional physical systems. The only exception to this might be the momentum space application of HD, referred to as the multiscale reference function (MRF) method, as discussed in [10,11]. It does appear that MRF is (significantly) faster at converging than configuration space-HD, as demonstrated in [13] (Figure 1). However, it is not clear if the HD theoretical problems specified above also apply to the MRF case. The irony is that OPPQ, despite its basis formulation in configuration space, depends on the power moments for its generation. All of this is discussed below. Thus, OPPQ combines the best features of a configuration space analysis (*i.e.*, in easily identifying the physical asymptotic form for the required weight or reference function) with the effectiveness of moment representation quantization.

The earliest attempts in using moments for solving linear systems were by Blankenbeckler *et al.* [15] and Killinbgeck *et al.* [16]. Another work attempted the same for strongly-coupled, singular perturbation, nonlinear systems ("kink" solutions) [17].

In 1984, Handy achieved a significant theoretical and computational advance by demonstrating that the classic moment problem theorems [18] (*i.e.*, the moment-dependent positivity constraints required for nonnegative measures) could be used to constrain the moment equation solutions corresponding to positive wavefunction configurations; the most important of these being the multidimensional bosonic ground state, $\Psi_{gr} > 0$. This led to a new spectral bounding method that could generate tight (converging) lower and upper bounds to the discrete state energies associated with positive configurations. This is referred to as the eigenvalue moment method (EMM). Handy's original discovery was by way of the nesting property for Padé approximants generated from positive Stieltjes measures [19]. This philosophy was further refined, making it more amenable to multidimensional systems, through the use of the well-known positivity Hankel Hadamard (nonlinear) determinantal inequality constraints [20].

This seminal work by Handy and Bessis [20] is one of the first to use semidefinite programming (SDP) analysis [21,22] to solve quantum operators. Since SDP algorithms were not available, Handy developed a cutting algorithm, within the context of a linear convex optimization analysis [23], that allowed the extension of these methods to multidimensional systems. The most famous of these was the notoriously difficult, strong coupling, singular perturbation problem corresponding to determining the ground state binding energy of the quadratic Zeeman effect for super-strong magnetic fields (of the type encountered in neutron stars). Handy *et al.* [24,25] were able to extend the EMM analysis to such problems confirming, through tight bounds, the results of Le Guillou and Zinn-Justin [26] derived through more sophisticated, analytical methods.

The EMM analysis can also be used for bounding the excited discrete state energies of one-dimensional problems, since the probability density, $\Psi^2(x)$, for Sturm–Liouville problems with a real potential function, must satisfy a third order linear differential equation for which a moment equation can also be generated, for the types of systems considered here [27,28]. The same applies to Sturm–Liouville problems with complex potentials (*i.e.*, pseudo-Hermitian systems), since the Herglotz extension into the complex plane for the probability density $|\Psi(x)|^2$ leads to a fourth order linear differential equation, for which a moment equation also ensues [29,30]. The application of EMM to the case $V(x) = iax + ix^3$ led to the generation of tight bounds for the real and imaginary parts of the discrete state complex eigenenergies. This led to the first computational prediction for the onset of spontaneous PT-symmetry breaking (predicting the a-parameter regions where the discrete spectrum changed from being real to complex) for this important system [30,31], the subject of much current research.

1.2. Defining Global-Local Quantization

Despite its limitations, the HD formalism exploits the local analytic structure of the wavefunction, in configuration space, in order to solve for the physical solutions. Similarly, through methods, such as OPPQ, further elaborated upon below, we can quantize by exploiting the momentum space power series structure, as embodied in the power moments, as constrained through the moment equation. It would seem that any method that can combine both into one effective quantization procedure should be the ideal procedure. This work makes one attempt at identifying such a procedure.

1.3. OPPQ and HD: General Quantization Strategies Motivated by Exactly Solvable and Quasi-Exactly Solvable Quantum Systems

Exactly solvable (ES) systems are those for which the discrete states can be determined in closed form: energies and wavefunctions. In one dimension, they can be characterized as corresponding to wavefunctions of the form $\Psi_j(x) = Q_j(x)\mathcal{R}(x)$, where $Q_j(x)$ is an orthogonal polynomial of degree "j", with respects to a particular positive weight $\mathcal{W}(x) > 0$ [32]. The function factor $\mathcal{R}(x) > 0$ corresponds to a positive, exponentially-bounded configuration that embodies the controlling form of the asymptotic behavior of the physical solution.

It follows that if $\{P_n(x)|n \geq 0\}$ denotes the orthonormal polynomials of $\mathcal{R}(x)$ (*i.e.*, where "n" is the degree), then we must have $\Omega_n \equiv \int dx\ P_n(x)\Psi_j(x) = 0$, for $n \geq j+1$. This ensues from the orthogonality properties of the P_n polynomials and the fact that the polynomial Q_j can be represented in terms of the first "$j+1$", P_n polynomials (where $0 \leq n \leq j$). These integral expressions depend on the power moments of the physical solution, $\mu_p = \int dx x^p \Psi(x)$. We can thus characterize ES systems as those for which the Ω_n's truncate exactly.

The same applies to the case of quasi-exactly solvable (QES) systems [33–37]. In this case, only a subset of the discrete states can be calculated in closed form. The corresponding wavefunctions take on the form $\Psi_j(x) = O_{n_{*,j}}(x)\mathcal{R}(x)$, where $O_{n_{*,j}}$ is a polynomial of fixed degree, n_* (but with j-dependent coefficients). In this case, we also have $\Omega_n = 0$, for $n \geq n_* + 1$. That is, there is also exact truncation in the behavior of the Ω_n's.

The OPPQ generalization of the above to arbitrary Hamiltonians (provided they admit a moment equation representation) assumes that the wavefunction can be represented as:

$$\Psi(x) = \sum_n \Omega_n P_n(x)\mathcal{R}(x),$$

for an arbitrary, positive, exponentially-bounded (not necessarily analytic) weight $\mathcal{R}(x) > 0$ and its family of orthonormal polynomials, $\int dx\ P_{n_1}(x)P_{n_2}(x)\mathcal{R}(x) = \delta_{n_1,n_2}$.

The expansion coefficients project out exactly, $\Omega_n = \int dx P_n(x)\Psi(x)$, and involve all of the first $n+1$ power moments, which are assumed to be generated through their corresponding moment equation.

If we choose the weight to satisfy $\int dx \frac{|\Psi(x)|^2}{\mathcal{R}(x)} < \infty$, then because $\int dx \frac{|\Psi(x)|^2}{\mathcal{R}(x)} = \sum_n |\Omega_n|^2$, it follows that the projection coefficients must satisfy the asymptotic condition: $\lim_{n\to\infty} \Omega_n = 0$. We can use this to define a truncation approximation quantization analysis involving $\Omega_{N+\ell} = 0$, for $0 \leq \ell \leq m_s$, and $N \to \infty$. Here, we assume that $1 + m_s$ denotes the order of the associated linear moment equation. To order N, these relations define a purely energy-dependent function (an $(m_s+1)\times(m_s+1)$ determinant) whose zeroes converge (exponentially) to the physical energies.

One expects, as confirmed empirically, that the best convergence is when the weight $\mathcal{R}(x)$ mimics the asymptotic form of the physical states. The admissible weight can be arbitrary, provided $\int dx \frac{|\Psi(x)|^2}{\mathcal{R}(x)} < \infty$, which allows for the weight to imitate the physical asymptotic form (assuming Ψ is also L^1).

In the Appendix (Table A1), we reproduce the results communicated in [13], for the quartic and sextic anharmonic oscillators. The reader will note that when the weight (reference function) imitates the physical, asymptotic form, improved convergence is obtained. We also show that slower convergence can

be obtained even when the above condition is not satisfied (*i.e.*, the last entry for the quartic anharmonic oscillator). What is not shown is the impressive fact that the non-analytic reference function, $e^{-\frac{|x|^3}{3}}$, also yields good converging results for the quartic case. Unlike the HD case, the OPPQ reference function does not have to be analytic, if one only wants to compute the energies.

The OPPQ wavefunction representation is usually referred to as a weighted polynomial expansions. It is well known that such expansions, particularly for Freudian weights, $\mathcal{R}(x) = e^{-|x|^q}$, $q > 1$, can exhibit pointwise convergence, in addition to L^2 convergence [38]. We stress that the expressions $\{P_n(x)\mathcal{R}(x)\}$ represent a non-orthogonal basis, which is an essential component to the flexibility of the above representation as used here. Despite the extensive mathematical literature on the importance of weighted polynomial expansions, or orthogonal polynomial expansions (as referenced throughout this work), its relevance for quantizing physical systems (by incorporating the moment equation structure) had not been appreciated until its exploitation by Handy and Vrinceanu [13,14].

One example of the flexibility of the OPPQ representation is that one can take the weight to be as complicated as one wants, provided the corresponding orthonormal polynomials can be generated. Thus, instead of the non-analytic reference function $e^{-\frac{|x|^3}{3}}$, for the quartic anharmonic potential, one can consider working with the analytic counterpart $\mathcal{R}(x) = \left(e^{\frac{x^3}{3}} + e^{-\frac{x^3}{3}}\right)^{-1}$. Regardless of what weight is chosen, the moment equations stay unchanged.

Another aspect of OPPQ's flexibility is that one does not need the explicit functional form for the weight, in order to generate the discrete state energies. If one knows the moments for the weight, then its orthonormal polynomials can still be generated, leading to the generation of the discrete state energies. This is possible through the well-known three-term recursion relation for the monic orthogonal polynomials [19]. An alternative approach (for multidimensional systems) is to use LUdecomposition methods on the (multidimensional) Hankel moment matrix (for the weight), in order to generate the same orthogonal polynomials [39]. One interesting application of this is to use EMM [20,24,25] to determine the power moments of the physical (positive) bosonic ground state (through tight bounds), for a given system. These can then be incorporated within OPPQ to generate the discrete state energies for all of the desired discrete states. The advantage of using EMM is that the generated moments will have automatically satisfied the necessary Hankel–Hadamard positivity constraints essential for ensuring that one is generating the orthonormal polynomials of a positive configuration (up to the order of the EMM analysis).

Returning to the previous ES/QES discussion, one can see that such states can also be characterized as corresponding to $\Psi_j(x) = A_j(x)\mathcal{R}(x)$, where the analytic (polynomial) factor $A_j(x) = \sum_n a_n x^n$, truncates exactly: $a_n = 0$, if $n \geq j + 1$. One might consider this as a motivational factor for the development of the Hill determinant (HD) method, as previously discussed.

We have already noted that HD can manifest anomalous behavior (*i.e.*, convergence to the wrong energies, non-convergent or slow convergence behavior, *etc.*), particularly when the reference function, $\mathcal{R}$, assumes the physical asymptotic form (refer to Figure 1); whereas OPPQ converges fastest precisely in such cases. To underscore the importance of this, we can consider the problem of varying the potential function parameters in order to determine the existence of ES/QES states. Within an HD framework, one cannot do this, reliably, since this type of variational analysis requires explicitly working with a weight, or reference function, that specifically incorporates the physical asymptotic form. Instead, by

working with the OPPQ representation, where $\mathcal{R}$ incorporates the physical asymptotic form, one can reliably determine the parameter regimes corresponding to ES/QES states.

Consider the sextic anharmonic problem $-\Psi''(x) + (mx^2 + x^6)\Psi(x) = E\Psi(x)$. The ground state is of QES form for $m = -3$, with lowest energy state $E_{gr} = 0$ [20,36]. The HD analysis will recover the QES states; however, if we slightly perturb things, $m \to m + \delta m$, the resulting HD energies do not suggest the existence of QES states. This is summarized in the Appendix (Table A2, extracted from a forthcoming article on ES and QES states). Whereas the OPPQ results appear to vary continuously for $m = -3 + \delta m$, where $\delta m = -0.1, 0, +0.1$, the same is not true for the HD results. Besides the fact that HD yields erroneous, or slowly converging, results for all of the states (*i.e.*, with the exception of $E_{gr} \equiv E_0$ for $m = -3$) both in the QES regime ($m = -3$) and non-QES regimes ($m = -2.9, -3.1$), HD does not appear to demonstrate continuity in its generated energies, for this case. Thus, $E_1 = 0$ for $\delta m = 0.1$ and then shoots to $E_1 = 0.354478$ for $\delta m = -0.1$. The same is true for the ground state energy. However, the true energies (obtained by OPPQ and confirmed through EMM) show a smooth variation in all of the energies for $\delta m = \pm 0.1$.

Of greater importance to us is that the OPPQ representation is numerically stable and converges rapidly for the appropriate weight. Furthermore, the OPPQ representation is both L^2 and pointwise convergent, globally. The latter property allows us to implement the global-local quantization analysis identified at the outset. These properties cannot be easily claimed by HD.

1.4. Connecting the Power Moments to the Local Behavior of the Physical Solutions: Scaling Transform Reconstruction

There is another related result derived from the scaling transform formalism underlying continuous wavelet analysis [40,41]. It also couples the power moments to the local structure of the wave function.

Consider the scaling transform of the physical wave function, for some appropriate, exponentially-bounded, analytic scaling function, $\mathcal{S}(x) \equiv \sum_n \sigma_n x^n$, satisfying the normalization $\mathcal{N}_a \int dx \mathcal{S}(\frac{x}{a}) = 1$:

$$\underline{S\Psi}(a,b) = \mathcal{N}_a \int dx\, \mathcal{S}(\frac{x-b}{a})\Psi(x). \tag{1}$$

Depending on the asymptotic decay of the scaling function relative to the physical solution, the scaling transform will be analytic (even entire) in the inverse scale variable, $\frac{1}{a}$, as generated from the power moments:

$$\underline{S\Psi}(a,b) = \mathcal{N}_a \sum_n \frac{\sigma_n}{a^n}\mu_n(b), \tag{2}$$

where $\mu_n(b) = \int dx x^n \Psi(x+b)$, involving a linear combination of the power moments for $b = 0$.

Thus, the power moments control the large-scale structure of the scaling transform. Recovery of the local properties for the wavefunction then requires implementing an effective analytic continuation/re-summation strategy for Equation (2), combined with the small-scale asymptotic limits:

$$\begin{aligned} \underline{S\Psi}(a,b) &= a\mathcal{N}_a \int dx \mathcal{S}(x)\Psi(ax+b) \\ \lim_{a\to 0} \underline{S\Psi}(a,b) &\approx \frac{1}{\nu_0}\sum_n a^n \frac{\Psi^{(n)}(b)\nu_n}{n!}, \end{aligned} \tag{3}$$

where $\nu_n = \int dx x^n \mathcal{S}(x)$. That is, the analytic continuation, or re-summation, of Equation (2), combined with asymptotic matching at some intermediary scale, can be used to generate the $\Psi^{(n)}(b) = \partial_b^n \Psi(b)$ derivates at an arbitrary point b.

For one-dimensional systems admitting a moment equation representation, we can generate an exact, closed set, of autonomous, coupled, first order differential equations (in the inverse scale variable) for scaling transform related expression. These can be integrated in order to generate an effective analytic continuation of Equation (1) into a sufficiently small-scale regime within which asymptotic matching with Equation (3) is used to recover the local properties of the physical solution at an arbitrary point b. This approach works very well for the various examples considered in [42,43].

For two-dimensional systems, there are no such closed coupled differential equations; however, we believe that through OPPQ, one can generate a hierarchy of such autonomous differential equations, with increasing accuracy as the order of the hierarchy is increased. Alternatively, for appropriate scaling functions, for which Equation (2) defines a convergent series in $1/a$, we can achieve the same, through appropriate re-summation methods, and then use asymptotic matching to recover the physical, configuration space, solution.

All of the above assumes that the (infinite scale) moments, $\mu_n(0)$, for each discrete state, are known. That is, knowledge of the physical power moments (derived through OPPQ, momentum space HD, EMM, *etc.*) coupled with the appropriate analytic continuation strategy, proves very effective in recovering the local solution. However, it proves to be difficult to use the above scaling transform relations to couple the power moments to the local structure (*i.e.*, the local power series expansion of $\Psi(b)$), in order to determine the physical energies. It is this type of global-local analysis that we are trying to implement through the pointwise convergent properties of the OPPQ expansion.

As shown in this work, the OPPQ representation does allow for this type of "global-local" analysis.

The following sections provide the technical details for our global-local quantization analysis based on the OPPQ expansion. The energies will be determined by constraining the OPPQ expansion to generate the exact local structure of the wavefunction at a particular point b, based on the actual local configuration space power series expansion.

Section 2 gives the technical details for OPPQ. This includes generating the moment equation. We also motivate its L^2 properties, as well as its global pointwise convergence to the configuration space function, along the real axis. Some of the earlier discussion is presented in greater detail.

Section 3 specifies the relations essential for our "global-local" quantization formalism. Two problems are considered: the general sextic anharmonic potential for parameter values where the HD method fails, or becomes ineffective, as depicted in Figure 1; and a rational fraction potential problem with a ground state solution that is meromorphic. For the latter, we demonstrate the nonuniform, global, pointwise convergence (along an infinite strip in the complex-x plane) for the OPPQ expansion of the solution, as determined by our "global-local" quantization analysis. We also provide numerical data on the error in the pointwise convergence.

2. Implementing OPPQ and Motivating Its L^2 and Pointwise Convergence Properties

In order to make more precise the above claims, consider the one-dimensional Fourier transform, assumed to be analytic (usually entire), with a corresponding k-space power series:

$$\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int dx\, e^{-ikx} \Psi(x) \tag{4}$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{p=0}^{\infty} \frac{\mu_p}{p!} (-ik)^p, \tag{5}$$

involving the power moments $\mu_p = \int x^p \Psi(x)\, dx$.

We limit our analysis to quantum systems for which the moments can be generated through a linear recursive relation of order $1 + m_s$, referred to as the moment equation. This equation is obtained by multiplying the Schrödinger's equation by x^p and integrating over its whole range (implicitly assuming that Ψ is an exponentially-bounded discrete state):

$$\int \left(-\frac{d^2\Psi}{dx^2} + (V(x) - E)\Psi(x) \right) x^p\, dx = 0.$$

After integrating by parts, one obtains a linear dependence among a number of consecutive moments. For example, the harmonic oscillator $V(x) = x^2$ provides a moment equation:

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

that has $m_s = 1$ because the whole moment sequence ($\{\mu_p | p \geq 0\}$) can be generated recursively from μ_0 and μ_1 or $1 + m_s = 2$ linear initialization, or missing moment, variables.

In many cases, a coordinate transformation may be necessary to obtain a moment equation. Its structure will take on the general form:

$$\mu_p = \sum_{\ell=0}^{m_s} M_{p,\ell}(E) \mu_\ell, \tag{6}$$

where m_s is problem dependent. The $M_{p,\ell}(E)$'s are known functions of the energy. The unconstrained moments $\{\mu_0, \ldots, \mu_{m_s}\}$ are referred to as the missing moments. Extensions of moment equations to multidimensional systems is possible.

The configuration space wavefunction is assumed to be analytic and can be represented as:

$$\Psi(x) = \Big(\sum_{n=0}^{\infty} a_n x^n \Big) R(x), \tag{7}$$

for some positive, analytic weight function, $R(x) > 0$. Under these assumptions, the a_n coefficients satisfy a three-term recursion relation to give:

$$a_n = T_{n,0}(E) a_0 + T_{n,1}(E) a_1, \tag{8}$$

due to the second order nature of the Schödinger equation.

Given that the global power moments, μ_p, and the local c_n coefficients, satisfy known energy-dependent constraints, how can we quantize by constraining both sets of variables? This is what we refer to as "global-local" quantization.

2.1. OPPQ

In this section, we summarize the main points that lead to the formulation of the OPPQ method. For a more detailed discussion, the reader is encouraged to refer to the original paper in [13], although the emphasis on orthonormal polynomials is not as explicit as it should have been. This is partly because the well-known three-term recursion relation for orthogonal polynomials [19] assumes that they are of monic form (and therefore, not normalized). Explicitly insisting on the use of orthonormal polynomials, from the outset, makes OPPQ less cumbersome in its derivation.

In order to develop a "global-local" quantization strategy that can couple the power moments to the local structure of the corresponding solution, one needs a robust wave function representation capable of recovering (in a stable manner) the local structure of the wave function from the global power moments. Weighted polynomial expansions [38], as implemented within the OPPQ representation, can provide this. Specifically, we will work with:

$$\Psi(x) = \sum_{j=0}^{\infty} \Omega_j P_j(x) \mathcal{R}(x), \tag{9}$$

where the orthonormal polynomials, $P_j(x) \equiv \sum_{i=0}^{j} \Xi_i^{(j)} x^i$, satisfy:

$$\int P_{j_1}(x) P_{j_2}(x) \mathcal{R}(x)\, dx = \delta_{j_1,j_2}. \tag{10}$$

The projection coefficients are easily generated:

$$\Omega_j = \int dx\ \Psi(x) P_j(x), \tag{11}$$

$$= \sum_{i=0}^{j} \Xi_i^{(j)} \mu_i, \tag{12}$$

or:

$$\Omega_j(\mu_0, \ldots, \mu_{m_s}) = \sum_{\ell=0}^{m_s} \Big(\sum_{i=0}^{j} \Xi_i^{(j)} M_{i,\ell}(E) \Big) \mu_\ell. \tag{13}$$

If the weight $\mathcal{R}(x)$ satisfies the condition that $\int dx\ \frac{\Psi^2(x)}{\mathcal{R}(x)} < \infty$, then one can argue that [13]:

$$\lim_{j \to \infty} \Omega_j = 0. \tag{14}$$

This analysis is repeated, in a more complete manner, in Section 2.3. These conditions hold, in particular, if the weight decays, asymptotically, no faster than the physical solutions: $\lim_{|x| \to \infty} \frac{|\Psi(x)|}{\mathcal{R}(x)} < \infty$.

Within the OPPQ quantization analysis, we approximate this asymptotic limit by taking $\Omega_n = 0$ for $N \leq n \leq N + m_s$, $N \to \infty$. This leads to an $(m_s + 1) \times (m_s + 1)$ determinant constraint on the energy, yielding rapidly converging approximations to the physical energies.

This approach allows for great flexibility in how the weight, or reference function, is chosen. In particular, one can allow the weight to mimic the asymptotic form of the physical solution or to take on the form of any positive physical solution (*i.e.*, the bosonic ground state, if known, even approximately).

In general, within the OPPQ ansatz, the better the reference function mimics the asymptotic form of the solution, the faster the convergence to the physical energies. Other redeeming features of the OPPQ procedure are that the reference function need not be analytic. Thus, for the quartic anharmonic potential, $V(x) = x^4 + mx^2$, converging results are obtained if $\mathcal{R}(x) = e^{-\frac{|x|^3}{3}}$. In principle, for this case, a differentiable form of the reference function would be $\mathcal{R}(x) = \frac{1}{exp(\frac{x^3}{3}) + exp(-\frac{x^3}{3})}$.

Furthermore, for generating the energies, one does not need the explicit configuration space representation for the reference function. Thus, one could use the (unknown) bosonic ground state (which must be positive), provided its power moments can be generated to high accuracy, enabling the generation of its corresponding orthonormal polynomials. In principle, the Eigenvalue Moment Method (EMM) could be used for such cases (generating high precision values for the power moments of the ground state, as well as the energy, through converging bounds) [20,24,25].

We note that the OPPQ basis $\{P_n(x)\mathcal{R}(x)|n \geq 0\}$ is not orthogonal. A more conventional analysis involving expanding $\Psi(x)$ in terms of an orthonormal basis $\mathcal{P}_n(x)\mathcal{R}^{\frac{1}{2}}(x)$, or $\Psi(x) = \sum_n \gamma_n \mathcal{P}_n(x)\mathcal{R}^{\frac{1}{2}}(x)$, does not provide the flexibility of OPPQ, since the generation of the projection coefficients involves the integrals $\gamma_n = \int dx\ \mathcal{P}_n(x)\mathcal{R}^{\frac{1}{2}}(x)\Psi(x)$, which cannot be expressed, generally, as a known (*i.e.*, in closed form) linear combination of the power moments of $\mathcal{R}^{\frac{1}{2}}(x)\Psi(x)$, except for special weights.

A better example of the flexibility offered by the OPPQ formalism, in contrast to a more conventional, ortho-normal basis expansion, is the aforementioned observation that OPPQ allows the use of the (accurately determined) power moments of the (bosonic) ground state, for quantizing the excited states. This type of analysis is not possible within the more conventional, ortho-normal basis (Rayleigh–Ritz) formalism.

2.2. Deficiencies of the Hill Determinant Method

The flexibility in the choice of the reference function within the OPPQ method is in sharp contrast to the popular Hill determinant approach corresponding to taking $a_N = 0, a_{N+1} = 0$ in Equation (8) and letting $N \to \infty$. Within the Hill determinant approach, truncating the a-power series is relevant if the system is exactly, or quasi-exactly, solvable (and the $R(x)$ in Equation (7) assumes the exact asymptotic form for these solutions). One might then believe that this works as an approximation in the general case. Initial studies of the Hill determinant approach confirmed this, for weights that did not mimic the physical asymptotic form of the solution, as argued in Section 1.

One simple observation that suggests potential problems with the Hill determinant approach is that the asymptotic behavior of the a's cannot be directly related to the normalizable, or non-normalizable, behavior of the physical or unphysical states, respectively. Indeed, it was pointed out by Tater and Turbiner [8] that the Hill determinant fails to converge, or converges to the wrong energy levels, in cases where the reference function is chosen to mimic the physical asymptotic form.

They used the sextic anharmonic potential as an example: $V(x) = mx^2 + bx^4 + x^6$. The asymptotic form of the wavefunction is $\mathcal{R}(x) = e^{-(x^4+bx^2)/4}$. The corresponding recursion relation for the a's is:

$$a_{n+2} = \frac{(m + 2n - 1 - b^2/4)a_{n-2} + (b(n + 1/2) - E)\, a_n}{(n + 1)(n + 2)}. \tag{15}$$

Consistent with the results of Tater and Turbiner [8], Hautot [9] had argued that such finite difference relations, coupled with the Hill determinant conditions ($a_N = 0$, $N = even$, $N \to \infty$, for parity invariant systems) can fail to take into account certain dominant solutions essential to quantization. He proposed a complicated procedure for fixing this problem. We believe that OPPQ is a more transparent solution that achieves the same result.

For illustrative purposes, we note that in Figure 1a–c, we give the convergence of the first two even energy levels for three parameter cases: ($m = -18$, $b = 0$), ($m = -8$, $b = 0$) and ($m = -4$, $b = 0$). In the first case, both energy levels appear to converge to the correct limit, albeit at a very slow rate. For the second case, only the ground state shows correct convergence, while the first excited state converges to the wrong limit. In the third situation, the Hill determinant method fails for all energy levels; there is no convergence; and in some cases, there are no real solutions, represented by a value of "0" in Figure 1c.

All three cases in Figure 1 are correctly recovered by either the original OPPQ formulation [13] or the global-local OPPQ variant developed in this paper (described in Section 3.1), as given in Table 1. The indicated limits in Table 1, are in keeping with a pure OPPQ analysis as published elsewhere [13]. For the $m = -4$ case, Table A1 in the Appendix allows the reader to compare the results of the original OPPQ formulation (for the R_{TT} physical weight) with those of a global-local analysis. Both results are consistent.

Table 1. Convergence properties for $V(x) = mx^2 + bx^4 + x^6$ using $R(x) = e^{-x^4/4}$ by using the global-local quantization.

N	E_0	E_1	E_2	E_3
		$m = -18$, $b = 0$		
10	−23.943914597	−17.917277160	−11.400078722	−8.480104521
20	−21.324952739	−21.322438503	−7.599903464	−7.359503437
30	−21.323394711	−21.321841616	−7.599035456	−7.360657993
40	−21.323394694	−21.321841620	−7.599035461	−7.360657990
		$m = -8$, $b = 0$		
10	−5.477684656	−3.531662882	1.811585056	6.570677286
20	−3.900838586	−3.534341976	2.086375864	6.054510025
30	−3.900635158	−3.534354171	2.086528016	6.055405087
40	−3.900635159	−3.534354170	2.086528012	6.055405205
		$m = -4$, $b = 0$		
10	−0.625342803	1.038625070	5.801273017	8.725547624
20	−0.523263742	1.005832318	5.374951631	10.5614373902
30	−0.523268623	1.005768335	5.374969926	10.572585458
40	−0.523268622	1.005768340	5.374970009	10.572585045

In the same reference [13], it is also demonstrated that even though the Hill determinant fails for the exact asymptotic reference function $R(x) = e^{-x^4/4}$, it can provide converging results when the reference

function is taken as the much more slowly decaying $R(x) = e^{-x^2}$ (Fig. in [13]). In this case, the Hill determinant results manifest a very poor convergence rate diminishing its practical value. Table A1 confirms for the reader (*i.e.*, the top entry results for R_G) that OPPQ is much faster than HD when using physical weights.

2.3. General Considerations: Motivating OPPQ's L^2 and Pointwise Convergence

Traditional orthonormal basis expansion methods in quantum mechanics, $\Psi(x) = \sum_n d_n \mathcal{B}_n(x)$ (*i.e.*, $\langle \mathcal{B}_m | \mathcal{B}_n \rangle = \delta_{m,n}$) are not designed to recover the pointwise structure of the approximated solution, since they emphasize an L^2 convergence. That is, the N-th partial sum, $\Psi_N(x) = \sum_{n=0}^{N} d_n \mathcal{B}_n(x)$, converges to the physical solution according to $\lim_{N\to\infty} \int dx \, |\Psi(x) - \Psi_N(x)|^2 = 0$. This does not imply pointwise convergence, since in the infinite limit, one could have $\Psi(x_j) - \Psi_\infty(x_j) \neq 0$ on a subset of measure zero. The OPPQ representation has a greater chance of pointwise convergence, because its underlying structure mimics the usual power series expansion.

As previously noted, the OPPQ basis functions $P_n(x)\mathcal{R}(x)$ are non-orthonormal. The advantage of this representation is that the Ω_j projection coefficients are easily determined for the types of (multidimensional) systems of interest to us, although the present work is limited to one-dimensional problems.

We note that $P_n(x)\sqrt{\mathcal{R}(x)}$ is expected to correspond to a complete orthonormal basis; however, the expansion $\Psi(x) = \sum_n \gamma_n P_n(x)\sqrt{\mathcal{R}(x)}$ does not lead to an easy, algebraic (closed form) generation of the projection coefficients, $\gamma_n = \langle P_n(x)\sqrt{\mathcal{R}} | \Psi \rangle$, for arbitrary $\mathcal{R}$, as pursued here.

Despite this, $\frac{\Psi}{\sqrt{\mathcal{R}}} = \sum_{n=0}^{\infty} \Omega_n P_n(x)\sqrt{\mathcal{R}(x)}$ will correspond to a conventional orthonormal basis expansion, with expected L^2 convergence:

$$Lim_{N\to\infty} \int dx \, |\frac{\Psi(x)}{\sqrt{\mathcal{R}(x)}} - \sum_{n=0}^{N} \Omega_n P_n(x)\sqrt{\mathcal{R}(x)}|^2 = 0. \tag{16}$$

Given that $Min_x \frac{1}{\mathcal{R}(x)} > 0$ (a positive global minimum), we then also have:

$$Lim_{N\to\infty} \int dx \, |\Psi(x) - \Psi_N(x)|^2 = 0, \tag{17}$$

where the OPPQ N-th partial sum is defined by:

$$\Psi_N(x) = \sum_{n=0}^{N} \Omega_n P_n(x)\mathcal{R}(x). \tag{18}$$

That is, the OPPQ representation will also be L^2 convergent.

The relation in Equation (18), upon squaring and taking the corresponding integrals, gives the important result:

$$Lim_{N\to\infty} \sum_{n=0}^{N} \Omega_n^2 = \int dx \, \frac{\Psi^2}{\mathcal{R}} < \infty \; (i.e., \; condition \; on \; \mathcal{R}), \tag{19}$$

or:

$$Lim_{n\to\infty} \Omega_n = 0. \tag{20}$$

That is, if the basis $\{P_n(x)\sqrt{\mathcal{R}(x)}\}$ is complete, then the limit in Equation (20) holds.

An alternative representation for the orthonormality relations of the P_n's is:

$$\int dx\ x^p P_n(x)\mathcal{R}(x) = 0, \tag{21}$$

for $p < n$, leading to:

$$\mu_p = \int dx\ x^p \Psi_N(x),\ 0 \leq p \leq N. \tag{22}$$

Thus, the N-th OPPQ partial sum has its first $1 + N$ moments identical to that of the physical state. This is the more general interpretation of the equality in Equation (9). Thus, the $\Psi_N(x)$ contain physical information.

Let us assume that the physical Fourier transform, $\hat{\Psi}(k)$, and the Fourier transform of the N-th OPPQ partial sum, $\hat{\Psi}_N(k)$, are entire functions in the complex k plane. This is easily the case if the $\mathcal{R}(x)$ and $|\Psi(x)|$ decay, along the asymptotic real axis, much faster than $e^{-\kappa|x|}$, for any $\kappa > 0$. Many quantum systems satisfy this. Therefore, since both $\hat{\Psi}_N(k)$ and $\hat{\Psi}(k)$ have identical power series expansions, to order $O(k^N)$, we can expect $|\hat{\Psi}(k) - \hat{\Psi}_N(k)| < \epsilon_N$ over some interval on the real k axis, $|k| < \kappa_N$, where $Lim_{N\to\infty}\epsilon_N = 0$ and $Lim_{N\to\infty}\kappa_N = \infty$. Indeed, $\hat{\Psi}_N(k)$ uniformly converges to $\hat{\Psi}(k)$ over any compact domain. Therefore, the error in local approximation is controlled by $|\Psi(x) - \Psi_N(x)| < \frac{1}{\sqrt{2\pi}}|\int dk\ e^{ixk}(\hat{\Psi}(k) - \hat{\Psi}_N(k))| < \frac{1}{\sqrt{2\pi}}\Big(2\epsilon_N\kappa_N + \int_{|k|>\kappa_N} dk\ |\hat{\Psi}(k) - \hat{\Psi}_N(k)|\Big)$. If $Lim_{N\to\infty}\epsilon_N\kappa_N = 0$, combined with $Lim_{N\to\infty}\kappa_N = \infty$, and the boundedness assumption for both $\hat{\Psi}(k)$ and $\hat{\Psi}_N(k)$ would result in (uniform) pointwise convergence in x. This is further enhanced if the chosen reference function mimics the true physical asymptotic form in x-space, as well as in k-space, since it would greatly diminish the contribution of the integral expression "$\int_{|k|>\kappa_N} dk(\cdots)$" given above, implying a faster pointwise convergence at x.

In other words, how the reference function is chosen will lead to enhanced convergence rates to the local properties of the wavefunction in configuration space. More generally, it is to be expected that the OPPQ representation will generally converge, pointwise, to the physical solution. This is in keeping with available theorems [38].

3. Global-Local Quantization

3.1. The Global-Local Quantization Conditions and Application to the Sextic Anharmonic Oscillator

The OPPQ expansion in Equation (9) was originally developed in the spirit of a (non-orthonormal) basis expansion where the expansion coefficients are given by Equation (11) and the following integral expression is required to be finite: $\int dx\ \frac{\Psi^2(x)}{\mathcal{R}(x)} = \sum_j \Omega_j^2 < \infty$. There was no demand for pointwise convergence. However, there are good mathematical reasons for expecting the OPPQ representation to be (non-uniformly) convergent in a pointwise manner. As previously noted, this representation is a specific case of the more general problem of representing analytic functions by weighted families of polynomials. For Freudian weights of the form $\mathcal{R}(x) = e^{-|x|^q}$, $q > 1$, it is known [38] that the representation in Equation (9) converges within an infinite strip in the complex-x plane whose width is determined by the closest singularity (of the physical solution) to the real axis.

If we assume this, in general, for the types of physical systems of interest, then the natural question is to test the pointwise convergence of such representations at the origin (among other possibilities):

$$\frac{\Psi(x)}{\mathcal{R}(x)} = \sum_{j=0}^{\infty} \Omega_j P_j(x) = \Big(\sum_{n=0}^{\infty} a_n x^n \Big), \tag{23}$$

where:

$$\sum_{j=n}^{\infty} \Xi_n^{(j)} \Omega_j = a_n = T_{n,0}(E) a_0 + T_{n,1}(E) a_1. \tag{24}$$

We approximate this through the truncation:

$$\sum_{j=n}^{N} \Xi_n^{(j)} \Omega_j(\mu_0, \ldots, \mu_{m_s}) \ = a_n = T_{n,0}(E) a_0 + T_{n,1}(E) a_1, \tag{25}$$

where we make explicit Ω's linear dependence on the missing moments.

Since there are $m_s + 3$ linear variables $\{a_0, a_1, \mu_0, \ldots, \mu_{m_s}\}$, we must take $n = 0, \ldots, m_s + 2$, in Equation (25), although $N \to \infty$. An energy-dependent, $(m_s + 3) \times (m_s + 3)$ determinantal equation ensues, yielding converging results for the physical energies, as $N \to \infty$.

The above analysis was implemented on the anomalous parameter values for the sextic anharmonic oscillator, as calculated through the Hill determinant approach given in Figure 1. Table 1 shows the exceptional stability of the above "global-local" quantization procedure. These results agree with a pure OPPQ analysis as given in [13], thereby strongly affirming the reliability of the OPPQ representation in capturing the local behavior of the physical solutions. A second example is given in the next section.

3.2. Global-Local Quantization for a Rational Anharmonic Oscillator

In order to further evaluate the convergence properties of the local-global OPPQ method, we chose a non-trivial problem that has a solution that is known exactly. To the best of our knowledge this potential function has not been previously studied.

We consider the rational anharmonic oscillator potential:

$$V(x) = x^2 - \frac{48}{(3 + 2x^2)^2}, \tag{26}$$

for which the ground state is exactly known:

$$\Psi_{gr}(x) \equiv \frac{e^{-x^2/2}}{(1 + \frac{2}{3}x^2)} \ .$$

This potential and the ground state associated with eigen-energy $E = -3$ are represented in Figure 2, together with the underlying harmonic oscillator potential (represented with a dashed line). The advantage of knowing the ground state exactly is that the claimed pointwise convergence of global-local method can be easily verified.

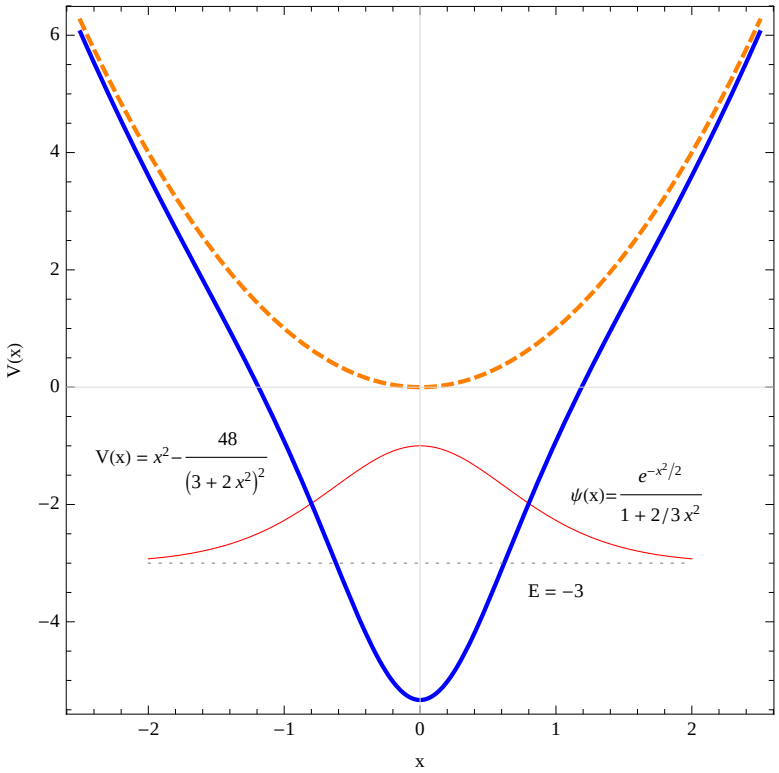

Figure 2. The anharmonic potential (solid line), the unperturbed harmonic potential energy curves and the ground state wave function corresponding to ground state energy $E = -3$.

The corresponding moment equation for this system is:

$$\begin{aligned}\mu_{p+6} = \quad & (E-3)\mu_{p+4} + \Big(p(p+7) + 3E + \tfrac{39}{4}\Big)\mu_{p+2} \\ & + \Big(3p(p+3) + \tfrac{9}{4}E + 18\Big)\mu_p + \tfrac{9}{4}p(p-1)\mu_{p-2},\end{aligned} \tag{27}$$

with $m_s = 5$. The corresponding recursion relation for Taylor's coefficients is:

$$a_{n+2} = \frac{4(2n-E-7)a_{n-4} + 4(n(11-n) - 3E - 15)a_{n-2} - 3(13 + 3E + 2n(3n-5))a_n}{9(n+1)(n+2)}. \tag{28}$$

Three representative calculations are given in Table 2. The first is OPPQ using the weight $\mathcal{R}(x) = e^{-x^2/2}$, the asymptotic form for the bound states. The second is obtained by implementing the global-local ansatz given in Equation (25), ensuring not only accurate and fast converging energy eigenvalues, but also faithful representation of the wave function that has implicitly both the correct local ($x \approx 0$) and global behavior. The third set of results illustrates the freedom of choice of the reference function within the OPPQ method, by taking it to be the exactly known ground state.

Figure 3 demonstrates the pointwise convergence properties for the wave function calculated using the global-local quantization. The results presented are obtained by using Equations (9) and (18) with truncation order $N = 80$. It is also instructive to compare the power expansion of the reconstructed ground state wave function, scaled by the reference function $\mathcal{R}(x) = e^{-x^2/2}$, which is given by:

$$\Psi_{\text{rec}}(x)/e^{-\frac{x^2}{2}} = 1 - 0.662562x^2 + 0.420992x^4 - 0.237655x^6 + \mathcal{O}(x^8),$$

with the corresponding exact expansion of the ground state:

$$\frac{1}{(1+\frac{2}{3}x^2)} = 1 - 0.666666x^2 + 0.444444x^4 - 0.296296x^6 + \mathcal{O}(x^8).$$

This shows that the solution provided by the global-local quantization has the claimed pointwise convergence properties of the wave function together with the fast convergence of energy levels.

It is instructive to compare the global convergence (on the real line) of the OPPQ representation with the local Taylor series expansion. Specifically, the wave function representation in terms of orthogonal polynomials as in Equation (18) has global convergence properties, as opposed to the local convergence of Taylor's power expansion, which is always restricted to a disk. This point is illustrated in Figure 4, where the convergence domain in the complex x-plane of Ψ_{gr} covers an increasing horizontal strip, as the OPPQ truncation order in Equation (18) increases from $N = 20$ to $N = 140$. The strip is determined by the $\pm i\sqrt{\frac{3}{2}}$ singularities. On the other hand, the convergence of Taylor's expansion of the ground state is always local, limited by a disk around the expansion center (chosen in Figure 4 to be centered at 1.4) and bordered by the singularities.

Table 2. Convergence for energy levels of the rational anharmonic potential for various methods as a function of truncation order. OPPQ, orthogonal polynomial projection quantization.

N	E_0	E_1	E_2	E_3
Direct OPPQ method with reference function $e^{-x^2/2}$				
20	−2.919286247	0.910167637	3.603889662	5.913948003
40	−2.996045597	0.799435213	3.437942536	5.720225364
60	−2.999705662	0.792968365	3.426931961	5.705551770
80	−2.999970901	0.792460681	3.426034090	5.704282111
100	−2.999996463	0.792409589	3.425942480	5.704148274
Matching local and global behavior through Equation (25)				
20	−3.192388811	−0.534923547	3.546551239	5.743802129
40	−3.008483327	0.735594478	3.407202508	5.604497284
60	−3.000567710	0.789212601	3.424198982	5.696740280
80	−3.000052234	0.792139749	3.425751715	5.703466230
100	−3.000006028	0.792374246	3.425907672	5.704054764
Ground state wave function as the reference function				
10	−3.000000000	0.757672016	3.265699150	5.407722347
20	−3.000000000	0.790563451	3.418884509	5.691130493
30	−3.000000000	0.792220915	3.425272253	5.702879442
40	−3.000000000	0.792377300	3.425841380	5.703957354
50	−3.000000000	0.792398005	3.425914514	5.704099238
60	−3.000000000	0.792401433	3.425926384	5.704122686

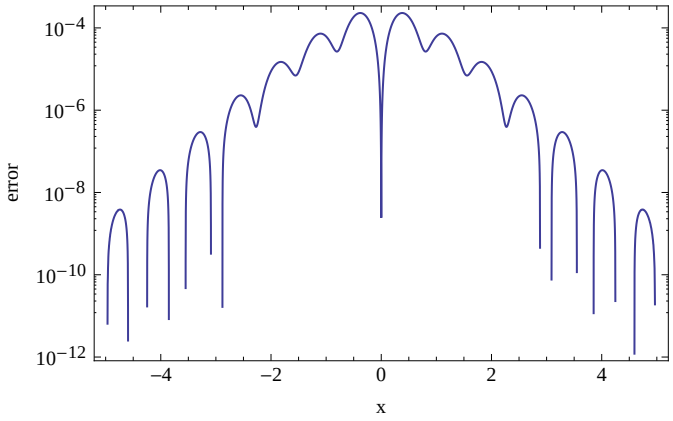

Figure 3. The difference between the ground state wave function calculated by using the local-global OPPQ method and the exact wave function $\Psi_{\rm gr}$.

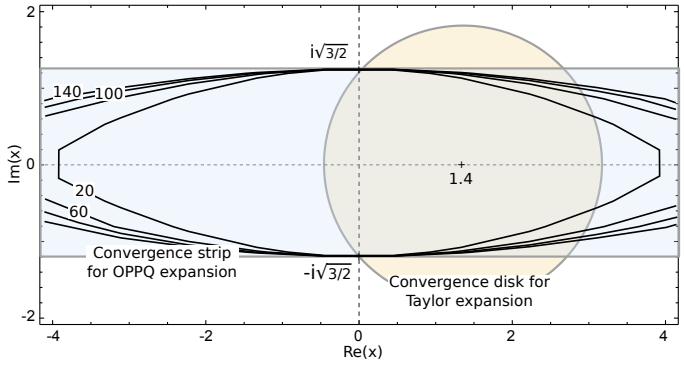

Figure 4. Converge domains in the complex plane for Taylor's expansion and OPPQ expansion for the ground state wave function scaled by the reference function ($\Psi_{gr}/\mathcal{R}$) of the rational anharmonic oscillator in Equation (26). The OPPQ expansion is carried out for the sequence of truncation orders $N = 20, 60, 100$ and 140, showing that in the $N \to \infty$ limit, its convergence domain is a horizontal strip bordered by the singular point of the wave function. In contrast, Taylor's expansion does not converge outside the disk centered at the chosen expansion center, in the calculated case $x_0 = 1.4$.

The process of the analytic continuation of a function, $f(x)$, results in power series expansions for the local expression $f(\tau + \chi) = \sum_j c_j(\tau)\chi^j$, involving non-global expansion coefficients (*i.e.*, the $c_j(\tau)$ are τ dependent). The orthonormal polynomial expansion in Equation (19) transcends this into a global statement, particularly close to the real axis. Of course, one advantage of the conventional analytic continuation process is that one can control the uniformity of the convergence of the analytic continuation to the target function. For our purposes, the non-uniform nature of the pointwise convergence of the OPPQ expansion is not a problem, since we are using the local information (*i.e.*, the derivatives, *etc.*) at a chosen point.

4. Conclusions

The importance of moment representations in the context of algebraic quantization problems is often overlooked. The importance, and flexibility, of weighted orthonormal polynomial representations has

been amply demonstrated here and in previous works with regards to their ability to generate the discrete energies to arbitrary precision. The relevance of such representations for reconstructing the wavefunctions is strongly suggested by the present work, including our ability to quantize by imposing global-local constraints on the OPPQ, weighted polynomial expansion.

Acknowledgments

Discussions with Daniel Bessis, Donald Kouri and Walter Gautschi are greatly appreciated. Additional correspondences with Hrushikesh Narhar Mhaskar and Doron Lubinsky are also appreciated. One of the authors (Daniel Vrinceanu) is grateful for the support received from the National Science Foundation through grants for the Center for Research on Complex Networks (HRD-1137732) and Research Infrastructure for Science and Engineering (RISE) (HRD-1345173).

Author Contributions

Carlos R. Handy provided the mathematical framework and wrote sections 1.1, 1.2, 1.3, 2.1, 2.3, 3.1 and 4. Daniel Vrinceanu wrote implemented the algorithms described in the paper and wrote sections 2.2 and 3.2. Carl B. Marth wrote, run and processed the computer codes required to obtained the results in this paper. Carlos R. Handy and H. A. Brooks wrote Section 1.4, Harold A. Brooks provided expertise regarding systems of weighted polynomials.

Conflicts of Interest

The authors declare no conflict of interest.

Appendix

In this section, we give two sets of data demonstrating the effectiveness of OPPQ *versus* HD, as discussed in Section 1.

Table A1. Convergence for the four lowest energy levels using the OPPQ method for sextic and quartic anharmonic potentials and two choices of reference functions from [13].

N	E_0	E_1	E_2	E_3
sextic anharmonic potential $V_S(x) = x^6 - 4x^2$, $R_G = e^{-x^2/2}$				
20	−0.537657110	0.921572505	5.339158198	9.811119432
40	−0.523594783	1.004743974	5.370894371	10.564676143
60	−0.523274535	1.005763660	5.374907198	10.572468833
80	−0.523268715	1.005768392	5.374969108	10.572583491
100	−0.523268624	1.005768348	5.374969994	10.572585099
120	−0.523268622	1.005768341	5.374970009	10.572585052

Table A1. *Cont.*

N	E_0	E_1	E_2	E_3
sextic anharmonic potential $V_S(x) = x^6 - 4x^2$, $R_{TT} = e^{-x^4/4}$				
10	−0.515914799	1.045574144	5.804384109	17.182737481
20	−0.523268924	1.005781188	5.374994734	10.569841387
30	−0.523268622	1.005768339	5.374969977	10.572585105
40	−0.523268622	1.005768340	5.374970009	10.572585045
quartic anharmonic potential $V_Q(x) = x^4 - 5x^2$, $R_G = e^{-x^2/2}$				
20	−3.408037638	−3.245130319	0.639251525	2.658824906
40	−3.410143687	−3.250676404	0.638914360	2.581226627
60	−3.410142761	−3.250675363	0.638919564	2.581216254
80	−3.410142761	−3.250675362	0.638919564	2.581216271
100	−3.410142761	−3.250675362	0.638919564	2.581216271
quartic anharmonic potential $V_Q(x) = x^4 - 5x^2$, $R_{TT} = e^{-x^4/4}$				
20	−4.744467615	−1.478468321	0.650460871	7.285067700
40	−3.455553264	−3.216259804	0.563362433	4.499199879
60	−3.408827067	−3.250616350	0.644873375	2.554622225
80	−3.410171198	−3.250696184	0.638737424	2.581302222
100	−3.410142290	−3.250674625	0.638923526	2.581226358
120	−3.410142766	−3.250675380	0.638919503	2.581215858
140	−3.410142761	−3.250675362	0.638919564	2.581216281

Table A2. Convergence for the four lowest energy levels using OPPQ and Hill determinant (HD) methods for $V(x) = mx^2 + x^6$, using physical reference function $\mathcal{R}(x) = e^{-x^4/4}$. Results are part of a recently-completed study to be submitted for publication elsewhere.

N	E_0	E_1	E_2	E_3
$m = -3$ with OPPQ				
10	0	2.054436575	9.958184097	19.819537375
18	0	1.935440477	6.293869877	11.675087668
26	0	1.935482012	6.298503667	11.680999150
30	0	1.935482098	6.298495775	11.680971308
$m = -3$ with HD				
10	0	0	0	0
20	0	0	0	0
30	0	0	-5.78622×10^{-12}	-5.78622×10^{-12}
40	0	0	-1.38145×10^{-11}	-1.38145×10^{-11}

Table A2. *Cont.*

N	E_0	E_1	E_2	E_3
		$m = -2.9$ with OPPQ		
10	0.047242645	2.153684719	10.159896054	20.084855463
18	0.047391597	2.024490454	6.386902706	11.785825578
26	0.047388401	2.024539898	6.391623098	11.791298393
30	0.047388406	2.024539984	6.391614829	11.791270104
		$m = -2.9$ with HD		
10	0	0	0	0
20	-6.24163×10^{-14}	-6.24163×10^{-14}	-3.59906×10^{-16}	-3.59906×10^{-16}
30	-1.62247×10^{-12}	-1.62247×10^{-12}	-6.76293×10^{-13}	-6.76293×10^{-13}
40	-5.44154×10^{-10}	-5.44154×10^{-10}	-1.01764×10^{-10}	-1.01764×10^{-10}
50	-2.56717×10^{-10}	-2.56717×10^{-10}	-4.57929×10^{-11}	-4.57929×10^{-11}
		$m = -3.1$ with OPPQ		
10	−0.047793552	1.954915616	9.757023047	19.554492101
18	−0.048220094	1.845699719	6.200934698	11.564288882
26	−0.048216730	1.845733983	6.205472766	11.570595945
30	−0.048216736	1.845734070	6.205465245	11.570568579
		$m = -3.1$ with HD		
20	−0.367955	0.367955	-8.28907×10^{-14}	-8.28907×10^{-14}
40	−0.359878	0.359878	-3.92834×10^{-10}	-3.92834×10^{-10}
60	−0.356466	0.356466	-4.00409×10^{-8}	-4.00409×10^{-8}
80	−0.354478	0.354478	0	0

References

1. Cooper, F.; Khare, A.; Sukhatme, U. *Supersymmetry in Quantum Mechanics*; World Scientific: Singapore, Singapore, 2001.
2. Chou, C.C.; Biamonte, M.T.; Bodmann, B.G.; Kouri, D.J. *New System-Specific Coherent States by Supersymmetric Quantum Mechanics for Bound State Calculations*; INTECH Open Access Publisher: Rijeka, Croatia, 2013.
3. Levai, G.; Cannata, F.; Ventura, A. Algebraic and scattering aspects of a $\mathcal{PT}$-symmetric solvable potential. *J. Phys. A Math. Gen.* **2001**, *34*, 839–846.
4. Bodmann, B.G.; Hoffman, D.K.; Kouri, D.J.; Papadakis, M. Hermite distributed approximating functionals as almost-ideal low-pass filters. *Sampl. Theory Signal Image Process.* **2008**, *7*, 15–39.
5. Press, W.H.; Teukolsky, S.A.; Vetterling, W.T.; Flannery, B.P. *Numerical Recipes: The Art of Scientific Computing*, 3rd ed.; Cambridge University Press: New York, NY, USA, 2007.

6. Bender, C.M.; Orszag, S.A. *Advanced Mathematical Methods for Scientists and Engineers*; McGraw Hill: New York, NY, USA, 1978.
7. Banerjee, K. Rescaling the Perturbation Series. *Proc. R. Soc. Lond. A* **1979**, *368*, 155–162.
8. Tater, M.; Turbiner, A.V. Failure of the Hill determinant method for the sextic anharmonic oscillator. *J. Phys. A Math. Gen.* **1993** , *26*, 697-714.
9. Hautot, A. On the Hill-determinant method. *Phys. Rev. D* **1986**, *33*, 437–443.
10. Tymczak, C.J.; Japaridze, G.S.; Handy, C.R.; Wang, X.-Q. New Perspective on Inner Product Quantization. *Phys. Rev. Lett.* **1998**, *80*, 3673-3677.
11. Tymczak, C.J.; Japaridze, G.S.; Handy, C.R.; Wang, X.-Q. Iterative solutions to quantum-mechanical problems. *Phys. Rev. A* **1998**, *58*, 2708–2720.
12. Killingbeck, J.P.; Grosjean, A. A simple Hill-series approach to the linear potential. *J. Math. Chem.* **2012**, *50*, 2648–2658.
13. Handy, C.R.; Vrinceanu, D. Orthogonal polynomial projection quantization: A new Hill determinant method. *J. Phys. A Math. Theor.* **2013**, *46*, doi:135202.10.1088/1751-8113/46/13/135202.
14. Handy, C.R.; Vrinceanu, D. Rapidly Converging Bound State Eigenenergies for the Two Dimensional Quantum Dipole. *J. Phys. B Atom. Mol. Opt. Phys.* **2013**, *46*, 115002, doi:10.1088/0953-4075/46/11/115002.
15. Blankenbeckler, R.; de Grand, T.; Sugar, R.L. Moment method for eigenvalues and expectation values. *Phys. Rev. D* **1980**, *21*, 1055–1061.
16. Killingbeck, J.; Jones, M.N.; Thompson, M.J. Inner product methods for eigenvalue calculations. *J. Phys. A* **1985**, *18*, 793–814.
17. Handy, C.R. Strong Coupling Singular Perturbation Theory and the Moments Problem. *Phys. Rev. D* **1981**, *24*, 378–383.
18. Shohat, J.A.; Tamarkin, J.D. *The Problem of Moments*; American Mathematical Society: Providence, RI, USA, 1963.
19. Baker, G.A., Jr. *Essentials of Pade Approximants*; Academic: New York, NY, USA, 1975.
20. Handy, C.R.; Bessis, D. Rapidly Convergent Lower Bounds for the Schrödinger-Equation Ground-State Energy. *Phys. Rev. Lett.* **1985**, *55*, 931–934.
21. Lasserre, J.-B. *Moments, Positive Polynomials and Their Applications*; Imperial College Press: London, UK, 2009.
22. Boyd, S.; Vandenberghe, L. *Convex Optimization*; Cambridge University Press: New York, NY, USA, 2004.
23. Chvatal, V. *Linear Programming*; W. H. Freeman and Co.: New York, NY, USA, 1983.
24. Handy, C.R.; Bessis, D.; Sigismondi, G.; Morley, T.D. Generating quantum energy bounds by the moment method: A linear-programming approach. *Phys. Rev. A* **1988**, *37*, 4557–4569.
25. Handy, C.R.; Bessis, D.; Sigismondi, G.; Morley, T.D. Rapidly Converging Bounds for the Ground-State Energy of Hydrogenic Atoms in Superstrong Magnetic Fields. *Phys. Rev. Lett.* **1988**, *60*, 253–256.
26. Le Guillou, J.C.; Zinn-Justin, J. New hybrid non-linear transformations of divergent perturbation series for quadratic Zeeman effects. *J. Phys. A Gen. Phys.* **1983**, *147*, 57–66.

27. Handy, C.R. Moment-method quantization of a linear differential eigenvalue equation for $||\Psi||^2$. *Phys. Rev. A* **1987**, *36*, 4411–4416.
28. Handy, C.R. Nonnegativity and moment quantization for $|\Psi|^2$. *Phys. Lett.* **1987**, *124*, 308–312.
29. Handy, C.R. Generating converging eigenenergy bounds for the discrete states of the $-ix^3$ non-Hermitian potential. *J. Phys. A* **2001**, *34*, L271–L275, doi:10.1088/0305-4470/34/19/102.
30. Handy, C.R. Generating converging bounds to the (complex) discrete states of the $P^2+iX^3+i\alpha X$ Hamiltonian. *J. Phys. A* **2001**, *34*, 5065–5074.
31. Handy, C.R.; Khan, D.; Wang, X.Q.; Tymczak, C.J. Multiscale reference function analysis of the $\mathcal{PT}$ symmetry breaking solutions for the $P^2+iX^3+i\alpha X$ Hamiltonian. *Phys. A Math. Gen.* **2001**, *34*, 5593–5602.
32. Nikiforov, A.F.; Uvarov, V.B. *Special Functions of Mathematical Physics*; Birkhauser Verlag: Basel, Switzerland, 1988.
33. Turbiner, A. Quantum mechanics: Problems intermediate between exactly solvable and completely unsolvable. *Sov. Phys. JETP* **1988**, *67*, 230–236.
34. Turbiner, A. Quasi-exactly-solvable problems and $sl(2)$ algebra. *Commun. Math. Phys.* **1988**, *118*, 467–474.
35. Morozov, A.; Perelomov, A.; Roslyi, A.; Shifman, M.; Turbiner, A. Quasi-Exactly-Solvable Quantal Problems: One-Dimensional Analogue Of Rational Conformal Field Theories. *Int. J. Mod. Phys.* **1990**, *A5*, 803–832.
36. Handy, C.R.; Vrinceanu, D.; Gupta, R. A moments's analysis of quasi-exactly solvable systems: A new perspective on the sextic potential $gx^6+bx^4+mx^2+\beta/x^2$. *J. Phys. A Math. Theor.* **2014**, *47*, 295203, doi:10.1088/1751-8113/47/29/295203.
37. Bender, C.; Dunne, G.V. Quasi-exactly solvable systems and orthogonal polynomials. *J. Math. Phys.* **1996**, *37*, 6–11.
38. Mhaskar, H.N. *Introduction to the Theory of Weighted Polynomial Approximation*; World Scientific Pub. Co. Inc.: Singapore, Singapore, 1996.
39. Handy, C.R. Application of the eigenvalue moment method to the quartic anharmonic double-well oscillator. *Phys. Rev. A* **1992**, *46*, 1663–1666.
40. Grossmann, A.; Morlet, J. Decomposition of Hardy functions into square integrable wavelets of constant shape. *SIAM J. Math. Anal.* **1984**, *15*, 723–736.
41. Chu, C.K. *An Introduction to Wavelets*; Academic: New York, NY, USA, 1992.
42. Handy, C.R.; Murenzi, R. Moment-wavelet quantization: A first principles analysis of quantum mechanics through continuous wavelet transform theory. *Phys. Lett. A* **1998**, *248*, 7–15.
43. Handy, C.R.; Murenzi, R. On the equivalence of moment quantization and continuous wavelet transform analysis. *J. Phys. A Math. Gen.* **1998**, *31*, 9897–10004.