A Nonperturbative Perspective on Inner Product Quantization: Highly Accurate
Solutions to the Schrödinger Equation

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(Received October 7, 2018)

We devise a new and highly accurate quantization procedure for the inner product representation, both in configuration and momentum space. Utilizing the representation $\Psi(\xi) = \sum_i a_i[E]\xi^i R_\beta(\xi)$, for an appropriate reference function, $R_\beta(\xi)$, we demonstrate that the (convergent) zeroes of the coefficient functions, $a_i[E] = 0$, approximate the exact bound/resonance state energies with increasing accuracy as $i \to \infty$. The validity of the approach is shown to be based on an extension of the Hill determinant quantization procedure. Our method has been applied, with remarkable success, to various quantum mechanical problems.

PACS numbers: 02.30.Hq, 03.65.-w, 03.65.Ge

The development of numerically efficient algorithms for quantum mechanical problems continues to be a challenging issue. Within this context, variational approaches based on optimal selection of basis sets remain one of the more successful approaches. Nevertheless, it appears that little attention has been paid to further enhancing such techniques by utilizing basis functions with an inherently analytical (i.e., power series) significance. In this Letter we show that such considerations can greatly reduce the computational effort of variational procedures involving large variational matrices, reduce to solving for the roots of an algebraically generated function. Our approach is based on a relatively simple extension of the Hill determinant quantization procedure.

One of the basic procedures for solving quantum systems is the Hill determinant approach [1]. It involves approximating the bound state wave function in terms of a suitable truncated basis, $\Psi(x) = \sum_{l=0}^{I} v_l B_l(x)$, and solving the finite dimensional problem

$$\sum_{j=0}^{I} M_{ij}x^j v_j = 0,$$

through the Hill determinant equation

$$\text{Det}\left(M(x)^{\text{I}}[x]\right) = 0,$$

for an appropriate reference function $R_\beta(x)$. The function coefficients, $a_i[E]$, depend on the energy variable, $E$, and are readily generated through the standard methods for differential equations. For simplicity, the above expansion assumes that $x = 0$ is a regular point. If the functions $x^j R_\beta(x)$ define a complete basis (not necessarily orthonormal), one can also pursue a Hill determinant analysis for the corresponding representation

$$\Psi(x) = \sum_{l=0}^{I} v_l x^l R_\beta(x).$$

In some cases, the recursive structure of the Hill determinant for increasing values of $I$ can be computed [3]. This allows one to analyze the asymptotic behavior with respect to $I$, for the roots of the Hill-determinant equation. In general, this analysis can be difficult and computationally demanding. It is in this context that we have discovered a remarkable relation whose simplicity has apparently gone unrecognized until now, despite the suggestive, but specialized, nature of the work by Bender and Dunne [4,5]. Specifically, we demonstrate that the convergent zeroes of the coefficient functions:

$$a_{i+1}[E_l^{(i)}] = 0,$$

(where $l$ labels the roots) converge to the exact discrete state energies, $E_l^{(\text{exact})}$, as the expansion order, $i$, increases:

$$\lim_{i \to \infty} E_l^{(i)} = E_l^{(\text{exact})}.$$

The theoretical justification for this proceeds as follows. Assume that $B_l(x) = x^l R_\beta(x)$ and that the corresponding Hill determinant method yields convergent results to the physical energies and wave functions. Let $E$ assume any value, $E = E_c$, for which the infinite matrix $M_{ij}[E_c]$, has no minor sub-matrix with zero determinant. One can recursively generate [6], through an effective LU decomposition method, an infinite set of vectors $\{V^{(i)}[0 \leq I < \infty]\}$ satisfying,
\[
\sum_{j=0}^{I} \mathcal{M}_{l,j}[E_c] V_j^{(l)} = 0,
\]  
(7)

for \(0 \leq i \leq I - 1\), and

\[
\sum_{j=0}^{I} \mathcal{M}_{I,j}[E_c] V_j^{(I)} = \mathcal{D}_I[E_c],
\]  
(8)

where \(V_I^{(l)} = 1\), and \(V_j^{(l)} = 0\), for \(j \geq I + 1\). One also has

\[
\text{Det} \left( \mathcal{M}^{(l)}[E_c] \right) = \prod_{i=0}^{I} \mathcal{D}_i[E_c].
\]

The relation in Eq. (7) involves \(I\) constraints for \(I\) unknowns (recall \(V_I^{(l)} = 1\), thus Eq. (7) is actually an inhomogeneous relation). The second relation, Eq. (8), serves to define \(\mathcal{D}_I[E_c]\).

For a given order \(I\), the roots of Eq. (2) corresponds to the roots of Eq. (8), \(E = E_I^{(l)}\), defined by

\[
\text{Det} \left( \mathcal{M}^{(l)}[E_I^{(l)}] \right) = 0
\]

and \(\text{Det} \left( \mathcal{M}^{(l)}[E^{(l)}] \right) = \mathcal{D}_I[E_I^{(l)}] = 0\). We denote the corresponding vectors by \(V^{(l)}[E_I^{(l)}]\).

From the recursion formula for the \(V\)'s [6], we have:

\[
V_I^{(l+1)}[E_I^{(l)}] = -\sum_{i=0}^{I} \frac{V_i^{(l+1)}[E_I^{(l)}] \mathcal{M}_{l+1,i}[E_I^{(l)}]}{\mathcal{D}_I[E_I^{(l)}]}.
\]  
(9)

Thus, in the \(E \rightarrow E_I^{(l)}\) limit, for a given \(l\), one obtains

\[
V_I^{(l+1)}[E_I^{(l)}] = \pm \infty.
\]  
(10)

By the very nature of the Hill determinant approach, for a sufficiently large order, \(I + 1\), one expects the partial sums

\[
\Psi_I(x) \approx \sum_{i=0}^{I+1} V_i^{(l+1)}[E_I^{(l+1)}] x^i R_\beta(x),
\]

(11)

define good, approximate, solutions to the physical wave functions. The same should hold for the corresponding, renormalized, truncated power series expansion

\[
\Psi_I(x) \approx \sum_{i=0}^{I+1} \frac{a_i[E_I^{(l+1)}]}{a_{l+1}[E_I^{(l+1)}]} x^i R_\beta(x).
\]  
(12)

Note that each of the expansions is normalized by setting the highest degree coefficient to unity.

For fixed, and sufficiently large, values of \(I + 1\), the preceding partial sums are expected to agree, term by term, for each of the roots \(E_I^{(l+1)}\). In particular, based on this concurrence, one expects

\[
\frac{a_I[E_I^{(l)}]}{a_{l+1}[E_I^{(l)}]} \approx V_I^{(l+1)}[E_I^{(l)}],
\]

which upon comparing with Eq.(10) leads to the desired conclusion:

\[
\frac{a_I[E_I^{(l)}]}{a_{l+1}[E_I^{(l)}]} \approx V_I^{(l+1)}[E_I^{(l)}] = \infty,
\]  
(13)

or

\[
a_{l+1}[E_I^{(l)}] = 0,
\]  
(14)

and \(\Psi_I(x) \approx N \sum_{i=0}^{I} a_i[E_I^{(l)}] x^i R_\beta(x)\).

We now demonstrate the capabilities of the preceding method. For the case of exactly solvable models, e.g., \(V(x) = x^2\) or \(V(x) = x^2 + g/x^2\), our approach readily yields the exact solutions, once the proper reference functions are selected: \(R_\beta = \exp(-x^2/2)\), and \(R_\beta = x^\alpha \exp(-x^2/2) (\alpha = (1+\sqrt{1+4g})/2)\), respectively.

Let us now consider the quartic anharmonic oscillator, \(V(x) = x^2 + gx^4\). Using \(R_\beta = \exp(-\beta x^2)\) one obtains the recursion relation:

\[
a_n(E) = \frac{\Omega_n a_{n-2}(E) + (1 - 4\beta^2) a_{n-4}(E) + ga_{n-6}(E)}{n(n-1)},
\]  
(15)

where \(\Omega_n = 4\beta n - 6\beta - E\) and \(a_n = 0\) for \(n < 0\). Table I shows the calculated energies of the ground and first excited states. Our method shows systematic convergence for increasing \(I\), exceeding some of the high accuracy solutions published [6 - 8]. Figure 1 shows the dependence of the ground state energy on the parameter \(g\). Figure 2 shows the corresponding wave functions.

An important version of the quartic anharmonic oscillator potential is the double well problem \(V(x) = -Z^2 x^2 + x^4\). It is well-known that in the deep well limit \((Z^2 \rightarrow \infty)\), the two lowest states are almost degenerate. Application of our method (refer to Table II) readily confirms this, and by its high accuracy significant, disagrees with the predictions of de Saavedra and Buen- dia (SB) [9]. In particular, for \(Z^2 = 25\), we observe that the quasi-degenerate nature of the ground and first excited state energies becomes apparent only after 26 significant digits, not the 16 predicted by SB.

Similar calculations have been carried out for higher degree potentials such as the sextic, octic, and dctic anharmonic potentials. The results are given in Table III.

The generality of our method permits the study of large classes of problems. In particular, transcendental potentials can be analyzed, provided the potential function, \(V(x)\), admits a power series expansion which is monotonically convergent (non-alternating). For instance, in the case of \(V(x) = \exp(x^2) - 1\), we can readily obtain the first three energy levels: \(E_0 = 1.356371240\), \(E_1 = 4.633078503\), and \(E_2 = 8.9706782\). \((R_\beta(x) = e^{-x^2}\), and \(a_n\) generated up to \(n \leq 80\).

Another type of potential which can be investigated is \(V(x) = V_0(x_0 + x)^\alpha\), where \(\alpha > -2\). For the two cases \(-2 < \alpha < 0\) and \(0 < \alpha < \infty\) the asymptotic forms for the wave function can be studied via \(\Psi(x) = \phi_-(x) e^{-\sqrt{-E}x}\) and \(\Psi(x) = \phi_+(x) e^{-\beta x^2}\), respectively. Upon making the transformation \(y = \sqrt{\log(1 + x/x_0)}\), one can readily obtain the corresponding differential equations for \(\phi_\pm(y)\),

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and proceed to generate the necessary power series expansion, \( \phi_{\pm}(y) = \sum a_n^{\pm} y^n \). In Figure 3 we plot \( E[\alpha] \) vs. \( \alpha \) for the cases of \( \{x_0 = 1, V_0 = -2; -2 < \alpha < 0 \} \) and \( \{x_0 = 1, V_0 = 1; 0 < \alpha < 4 \} \).

The selection of the reference function is clearly important. In the case of the sextic anharmonic oscillator \( (V(x) = x^2 + gx^6) \), our method works for the reference functions \( e^{-\beta x^2} \), \( \sigma = 2 \), and 3. For the case \( \sigma = 4 \) (and \( \beta = \frac{\sqrt{x}}{4} \)), which corresponds to the asymptotic form of the wave function, no convergent roots were observed upon solving Eq. (14).

Quantization is a global problem, not a local one. Configuration space analysis, by its manifestly local nature, may not always be a suitable representation in which to quantize. However, a momentum space representation is more appropriate. Specifically, the power series expansion for the Fourier transform of the wave function, \( \tilde{\Psi}(k) = \int dk \ e^{-ikx} \Psi(x) = \sum_{\rho=0}^{\infty} \frac{(-k)^\rho}{\rho!} \mu(\rho) \), involves global quantities, the (Hamburger) power moments, \( \mu(\rho) = \int dx \ x^\rho \Psi(x) \). As such, one would expect that our method would be more effective in momentum space. These observations are at the heart of various moment based quantization approaches [2], particularly the Eigenvalue Moment Method (EMM) [10].

Extending our method into momentum space presents additional features not encountered in configuration space. The most important of these is that new variables (the missing moments within the EMM approach) are encountered, regardless of the spatial dimension, \( D \), of the problem. Solving spatial problems of dimension \( D = 1 \) presents similar theoretical/algorithmic challenges to those in higher dimensions. We outline the essentials.

Limiting ourselves to symmetric \( \Psi(x) \) configurations, for simplicity, the coefficients of the power series expansion for the momentum space wave function, \( \tilde{\Psi}(k) = \int dk \ e^{-ikx} \Psi(x) = \sum_{\rho=0}^{\infty} \frac{(-k)^\rho}{\rho!} \mu(\rho) \) satisfy a linear, moment recursion equation, resulting in the linear relations \( u(\rho) = \sum_{\ell=0}^{m_s} M_{E}(\rho, \ell) u(\ell) \), \( 0 \leq \rho < \infty \); the \( M_{E}(\rho, \ell) \)'s are known, and the missing moment order, \( m_s \), is problem dependent [10].

Implementing our quantization procedure on the representation \( \tilde{\Psi}(k) = \sum_{n=0}^{m_s} a_{2n} k^{2n} e^{-\beta k^2} \), we obtain

\[
 a_{2n}[E, u(0), \ldots, u(m_s)] = \sum_{\ell=0}^{m_s} D_{n,\ell}[E] u(\ell),
\]

where

\[
 D_{n,\ell}[E] = \sum_{\rho_1 + \rho_2 = n} \frac{(-k)^{\rho_1} M_{E}(\rho_1, \ell) \beta^{\rho_2}}{(2\rho_1)! \rho_2!}.
\]

In principle, there will be a sequence of energy and missing moment values satisfying \( a_{2n}[E^{(\infty)}, \{u^{(\infty)}(\ell)\}] = 0 \) converging to the respective physical state values as \( n \to \infty \). Since the \( D_{n,\ell}[E] \)'s are not expected to define a degenerate matrix for all \( E \)'s, as \( n \to \infty \), we can approximate the converging sequence by considering the \([m_s + 1] \times [m_s + 1]\) matrix equation

\[
 \sum_{\ell_2=0}^{m_s} D_{n+\ell_1,\ell_2}[E] u(\ell_2) = 0,
\]

and the ensuing determinant equation,

\[
 Det\left(D^{(n)}[E]\right) = 0.
\]

Implementation of this for the quartic \((m_s = 1)\) and sextic \((m_s = 2)\) anharmonic oscillators yielded results consistent with those cited in Tables I and III.

Some problems can involve no missing moments. One of these is the aforementioned sextic anharmonic oscillator \((m_s = 0)\) formulation, provided one implements the above formalism with respect to the configuration space expression \( \tilde{\Psi}(x) = \Psi(x) e^{-\frac{1}{2}x^2} \).

The same holds for the problem \( V(x) = x^2 + \frac{gx^2}{1 + \lambda x^2} \), provided \( \tilde{\Psi}(x) = \frac{\tilde{\Psi}(x)}{\sqrt{1 + \lambda x^2}} e^{-\frac{1}{2}x^2} \) [11]. Table IV summarizes our results for this case, which surpass the accuracy calculated through an analytic continuation quantization procedure [12].

In summary, we have developed a nonperturbative approach for the inner product quantization procedure which allows one to calculate the energies and wave functions of the Schrödinger equation. We have demonstrated that our method yields excellent numerical results for various quantum mechanical problems. A full account of the approach, including the application to higher dimensional models and resonant states, will be published elsewhere.

This work was supported in part by the National Science Foundation under Grant No. HRD9450386, Air Force Office of Scientific Research under Grant No. F49620-96-1-0211, and Army Research Office under Grant No. DAAH04-95-1-0651.

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TABLE I. The calculated ground and first excited state energies for the quartic anharmonic oscillator with $g = 1$.

| $l$ | $\beta$ | $n$ | $E_n$ |
|-----|---------|-----|-------|
| 10  | 1/2     | 0   | 1.41  |
|     |         | 1   | 4.9   |
|     |         | 0   | 1.392 |
|     |         | 1   | 4.65  |
| 40  | 1/2     | 0   | 1.392 349 |
|     |         | 1   | 4.648 84 |
|     |         | 0   | 1.392 351 641 4 |
|     |         | 1   | 4.648 812 70 |
| 160 | 1/2     | 0   | 1.392 351 641 530 291 |
|     |         | 1   | 4.648 812 704 212 |
|     |         | 0   | 1.392 351 641 530 291 855 657 507 876 |
|     |         | 1   | 4.648 812 704 212 077 536 377 032 91 |

Refs. [4-6] $E_0 = 1.392$ 351 641 351 641 351 641 351 641 351 641 351 641 351 641 351 641 $E_1 = 4.648$ 812 704

TABLE II. The calculated ground and first excited state energies for the potential $V(x) = -Z^2x^2 + x^4$.

| $Z^2$ | Parity | $E_\pm$ |
|-------|--------|---------|
| 0     | +      | 1.060 362 090 484 182 899 647 046 016 |
|       | -      | 3.799 673 029 801 094 278 383 094 188 |
| 1     | +      | 0.657 653 005 180 715 123 059 021 723 |
|       | -      | 2.834 536 202 119 304 214 654 676 208 |
| 5     | +      | -3.410 142 761 239 829 475 297 709 653 |
|       | -      | -3.250 675 362 289 235 980 228 513 775 |
| 10    | +      | -20.633 576 702 947 799 149 958 554 634 |
|       | -      | -20.633 546 884 404 911 079 343 874 899 |
| 15    | +      | -50.841 387 284 381 954 366 250 996 515 |
|       | -      | -50.841 387 284 187 005 154 710 149 735 |
| 25    | +      | -149.219 456 142 190 888 029 163 966 538 |
|       | -      | -149.219 456 142 190 888 029 163 958 974 |

TABLE III. The calculated ground state energies of the sextic, octet and dectic anharmonic potentials for $g = 1$.

| $V(x)$ | $E_0$ (Ref. [4]) | $E_0$ |
|--------|------------------|-------|
| $x^2 + x^8$ | 1.435 624 619 1435 624 619 000 392 231 569 |
| $x^2 + x^8$ | 1.491 019 895 1491 019 895 662 |
| $x^2 + x^{10}$ | 1.546 263 512 6 |

TABLE IV. The first four symmetric state energies for the rational fraction potential $V(x) = x^2 + \frac{x^2}{1+\lambda x}$ for $\lambda = g = 0.1$. 

FIG 1. The calculated ground state energy for the quartic anharmonic oscillator.

FIG 2. The calculated ground and first excited state wave functions for the quartic anharmonic oscillator.

FIG 3. The calculated ground and first excited state energies for the potential $V(x) = V_0(x + x_0)^\alpha$ for $-2 < \alpha < 2$. 

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Figure 1, Submitted to Phys. Rev. Lett.
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Figure 2, Submitted to Phys. Rev. Lett.
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Figure 3, Submitted to Phys. Rev. Lett.
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