PHYSICAL REVIEW
LETTERS

VOLUME 80 | 27 APRIL 1998 | NUMBER 17

New Perspective on Inner Product Quantization

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(Received 27 June 1997)

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) zeros of the coefficient functions, $a_i[E] = 0$, approximate the exact bound state energies with increasing accuracy as $i \to \infty$. The validity of the approach is shown to be based on an approximation to the Hill determinant quantization procedure. Our method has been applied, with remarkable success, to various quantum mechanical problems in one and two space dimensions. [S0031-9007(98)05988-2]

PACS numbers: 03.65.Ge, 02.30.Hq

One of the most 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, $\Psi(x) = \sum_{i=0}^{I} v_i \mathcal{B}_i(x)$, and solving the finite dimensional problem $\sum_{j=0}^{I} \mathcal{M}_{i,j}[E_l^{(I)}]v_j = 0$, through the Hill determinant equation

$$\mathrm{Det}(\mathcal{M}^{(I)}[E_l^{(I)}]) = 0\,, \tag{1}$$

$\mathcal{M}_{ij}^{(I)} = \mathcal{M}_{ij}$, for $0 \le i,\ j \le I$, and $\mathcal{M}_{ij}[E] = \langle \mathcal{B}_i|H|\mathcal{B}_j\rangle - E\langle \mathcal{B}_i \,|\, \mathcal{B}_j\rangle$. For a suitable basis, as $I \to \infty$, the roots of the Hill determinant converge to the true eigenvalues of the Hamiltonian (l indexes the roots):

$$\lim_{I\to\infty} E_l^{(I)} = E_l^{(\mathrm{exact})}. \tag{2}$$

Another basic analytical tool is the power series expansion method [2]:

$$\Psi(x) = \left(\sum_i a_i[E]x^i\right)R_\beta(x)\,, \tag{3}$$

where $R_\beta(x)$ is an appropriate reference function. The coefficient functions, $a_i[E]$, are generated through the standard power series expansion method for differential equations. For simplicity, the above expansion assumes that $x = 0$ is a regular point. If the functions $x^i R_\beta(x)$ define a complete basis (not necessarily orthonormal), one can also pursue a Hill determinant analysis for the corresponding representation,

$$\Psi(x) = \sum_i^I v_i x^i R_\beta(x)\,. \tag{4}$$

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, Dunne, and Moshe [4]. Specifically, we demonstrate that the convergent zeros of the coefficient functions

$$a_i[E_l^{(i-1)}] = 0 \tag{5}$$

converge to the exact discrete state energies, $E_l^{(\mathrm{exact})}$, as i increases. The simplicity of this approach, implemented either in configuration or momentum space, belies its highly efficient and effective computational power, particularly in generating high accuracy eigenenergies and configurations (not discussed here). Other groups have also examined the configuration space coefficients, $a_i[E]$, with respect to their energy dependence. Of particular importance are the works of Rosenthal, Wilson, and Alexander [5]. However, their complicated *algebraic shooting*

method solely concentrates on generating eigenenergy bounds and explicitly overlooks the advantages of Eq. (5).

A heuristic justification of our method proceeds as follows. Let $\mathcal{B}_i(x) = x^i R_\beta(x)$ and assume that the corresponding Hill determinant method yields convergent results for the physical energies and corresponding wave functions. Denote the eigenvector solution to the Hill determinant matrix by $\vec{v} \to \vec{V}^{(I)}[E_l^{(I)}]$:

$$\sum_{j=0}^{I} \mathcal{M}_{i,j}[E_l^{(I)}] V_j^{(I)}[E_l^{(I)}] = 0 \tag{6}$$

for $0 \le i \le I$, where we normalize $V_I^{(I)} = 1$. It follows that as $I \to \infty$, $V_j^{(I)}[E_l^{(I)}] \to \frac{a_j[E_l^{(I)}]}{a_I[E_l^{(I)}]}$, for $0 \le j \le I$, since each sequence of coefficients generates the same wave function:

$$\sum_{j=0}^{I} V_j^{(I)}[E_l^{(I)}] x^j R_\beta(x) \to \sum_{j=0}^{I} \frac{a_j[E_l^{(I)}]}{a_I[E_l^{(I)}]} x^j R_\beta(x) \to \Psi_l(x)\,. \tag{7}$$

In this context we equate the coefficients ($a_I[E_l^{(I)}] \neq 0$):

$$V_j^{(I)}[E_l^{(I)}] = \frac{a_j[E_l^{(I)}]}{a_I[E_l^{(I)}]}, \qquad 0 \le j \le I\,. \tag{8}$$

Case (1): $a_j[E]$ a rational fraction.—This corresponds to most one dimensional configuration space problems and some special momentum space problems. The expression $\mathcal{P}_i[E] \equiv \sum_{j=0}^{I} \mathcal{M}_{i,j}[E] a_j[E]$ will also be a rational fraction in E and continuous at $E = E_l^{(I)}$. From Eqs. (8) and (6), we have $\mathcal{P}_i[E_l^{(I)}] = 0$, so long as $i \le I$. We are interested in evaluating $\mathcal{P}_{i \le I-1}[E]$ at $E = E_l^{(I-1)}$. In this regard, the partial sum $\sum_{j=0}^{I-1} \mathcal{M}_{i,j}[E_l^{(I-1)}] a_j[E_l^{(I-1)}] = a_{I-1}[E_l^{(I-1)}] \sum_{j=0}^{I-1} \mathcal{M}_{i,j}[E_l^{(I-1)}] V_j^{(I-1)}[E_l^{(I-1)}]$ is zero since the latter summation corresponds to Eq. (6) for $I \to I - 1$. Accordingly,

$$\mathcal{M}_{i,I}[E_l^{(I-1)}] a_I[E_l^{(I-1)}] = \mathcal{P}_i[E_l^{(I-1)}] \tag{9}$$

for $0 \le i \le I - 1$. Since $\lim_{I\to\infty}(E_l^{(I-1)} - E_l^{(I)}) \to 0$, and $\mathcal{P}_i[E_l^{(I)}] = 0$, we then have (if $\mathcal{M}_{i \le I-1,I}[E_l^{(I-1)}] \neq 0$

$$\lim_{I\to\infty} a_I[E_l^{(I-1)}] = 0\,. \tag{10}$$

Therefore, the zeros of $a_I[E]$ should converge to the physical energies.

Case (2).—The more general case corresponds to $a_j[E, \vec{\chi}] = \sum_{\ell=0}^{m_s} D_{j,\ell}[E] \chi_\ell$, where the $D_{j,\ell}[E]$'s are rational fractions in E. The preceding "proof" applies provided one works with the continuous function $\mathcal{P}_i[E, \vec{\chi}]$ satisfying $\mathcal{P}_i[E_l^{(I)}, \vec{\chi}_l^{(I)}] = 0$, from Eq. (8).

We now demonstrate the capabilities of the preceding method. It is important to mention that in cases of exactly solvable models, where the wave function can be expressed as a finite polynominal multiplied by an appropriate reference function (usually, the asymptotic form), our method reproduces the exact solutions.

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

I	β	n	E_n
10	1/2	0	1.41
		1	4.9
	1	0	1.392
		1	4.65
40	1/2	0	1.392 349
		1	4.648 84
	1	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
	1	0	1.392 351 641 530 291 855 657 507 876
		1	4.648 812 704 212 077 536 377 032 91
Refs. [6,7]		E_0	1.392 351 641 530 291 85
		E_1	4.648 812 704

Consider a nonexactly solvable problem, such as the quartic anharmonic oscillator, $V(x) = x^2 + gx^4$. Using $R_\beta = \exp(-\beta x^2)$ obtains the recursion relation

$$a_n(E) = \frac{\Omega_n a_{n-2}(E) + (1 - 4\beta^2) a_{n-4}(E) + g a_{n-6}(E)}{n(n-1)}, \tag{11}$$

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 coupling parameter g for $g \le 10$.

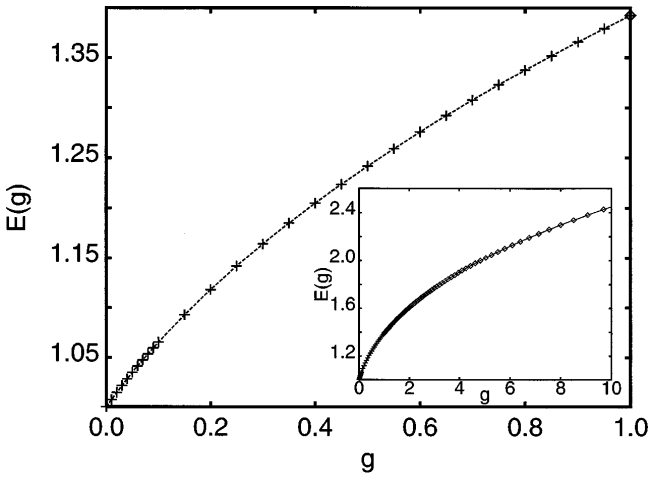

FIG. 1. The ground state energy for the quartic anharmonic oscillator for $0 \le g \le 1$ (inset: $0 \le g \le 10$).

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
	−	3.799 673 029 801 394 168 783 094 188
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

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

The results for higher degree potentials, such as the sextic, octic, and dectic anharmonic potentials, 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 (nonalternating). For instance, in the case of $V(x) = \exp(x^2) - 1$, we can readily obtain the first three energy levels: $E_0 = 1.356\,371\,240$, $E_1 = 4.633\,078\,503$, and $E_2 = 8.970\,678\,2$. [$R_\beta(x) = e^{-x^2}$, 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. In Fig. 2 we plot $E[\alpha]$ vs α for the cases of $\{x_0 = 1, V_0 = -2; -2 < \alpha < 0\}$ and $\{x_0 = 1, V_0 = 1; 0 < \alpha < 4\}$.

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

$V(x)$	E_0 (Ref. [3])	E_0
$x^2 + x^6$	1.435 624 619 0	1.435 624 619 003 392 231 569
$x^2 + x^8$	1.491 019 895	1.491 019 895 662
$x^2 + x^{10}$		1.546 263 512 6

We can readily extend the method to parity nonconserving potentials. In this case, the a_n's are linearly dependent on $\Psi(0)$ and $\Psi'(0)$: $a_n[E, \Psi, \Psi'] = \sum_{l=0,1} M_E(n = N + \delta_n, l)\Psi^{(l)}$, $\delta_n = 0, 1$. Since the $M_E(n, l)$ are expected to be independent for any two successive "n" values, we can solve for the energies by taking $\mathrm{Det}(M_E^{(N)}) = 0$ as $N \to \infty$. For example, for $V(x) = x + x^4$, using $R_\beta = e^{-4x^2}$ we obtain $E_0 = 0.930\,546\,034\,189\,9$, $E_1 = 3.781\,896\,248\,503\,0$, and $E_2 = 7.435\,067\,263\,287$, utilizing $N = 100$.

The selection of the reference function is important. For the potential $V(x) = x^2 + gx^6$, our method works if $R_\beta(x) = e^{-\beta x^\sigma}$, $\sigma = 2$, and 3. For $\sigma = 4$, corresponding to the asymptotic form of the wave function, no convergent roots were observed. We have also checked this for the higher order potentials and have found this property to be true. In general, $R_\beta(x)$ should fall off slower than the asymptotic form of the wave function (except for the special cases of exactly solvable problems).

Our method applied in momentum space presents additional features not encountered in most configuration space problems. The most important of these is that more variables [the *missing moments* within the eigenvalue moment method (EMM) [10] approach] are encountered, regardless of the spatial dimension, $\mathcal{D}$, of the problem. In particular, problems corresponding to $\mathcal{D} \geq 2$ will involve an infinite hierarchy of missing moment variables. Nevertheless, within our formalism, solving $\mathcal{D} = 1$ problems presents similar challenges to those in higher dimensions. We outline the essentials for both ($\mathcal{D} = 1$ and 2).

For simplicity, consider $\Psi(x)$ to be symmetric. The coefficients of the power series expansion for the momentum space wave function, $\hat{\Psi}(k) = \int dk\, e^{-ikx}\Psi(x) = \sum_{\rho=0} \frac{(-k^2)^\rho}{(2\rho)!} u(\rho)$, satisfy a linear moment recursion equation $u(\rho) = \sum_{\ell=0}^{m_s} M_E(\rho, \ell)u(\ell)$, $0 \leq \rho < \infty$; where

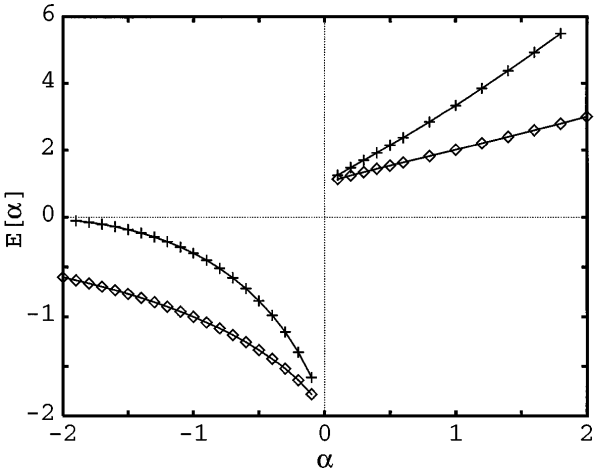

FIG. 2. The calculated ground and first excited state energies for the potential $V(x) = V_0|x_0 + x|^\alpha$ for $-2 < \alpha < 2$.

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 $\hat{\Psi}(k) = (\sum_{n=0} a_n k^{2n}) e^{-\beta k^2}$, we obtain

$$a_n[E, u(0), \ldots, u(m_s)] = \sum_{\ell=0}^{m_s} D_{n,\ell}[E] u(\ell), \qquad (12)$$

where

$$D_{n,\ell}[E] = \sum_{\rho_1+\rho_2=n} \frac{(-1)^{\rho_1} M_E(\rho_1,\ell)\beta^{\rho_2}}{(2\rho_1)!\,\rho_2!}. \qquad (13)$$

In accordance with Eq. (10), there will be a sequence of energy and missing moment values satisfying $a_n[E^{(n)}, \{u^{(n)}(\ell)\}] = 0$ converging to the physical 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

$$\sum_{\ell_2=0}^{m_s} D_{n+\ell_1,\ell_2}[E] u(\ell_2) = 0, \qquad (14)$$

and the ensuing determinant equation,

$$\mathrm{Det}(D^{(n)}[E]) = 0. \qquad (15)$$

Performing this for the quartic ($m_s = 1$) and sextic ($m_s = 2$) anharmonic oscillators yields results consistent with those cited in Tables I and III.

Some problems can involve no missing moments ($m_s = 0$). One of these is the aforementioned sextic anharmonic oscillator, provided one implements the above formalism with respect to the configuration space expression $\tilde{\Psi}(x) = \Psi(x) e^{-\frac{\sqrt{g}}{4}x^4}$. The ensuing calculation yields excellent results. The same holds for the problem $V(x) = x^2 + \frac{gx^2}{1+\lambda x^2}$, provided $\tilde{\Psi}(x) = \frac{\Psi(x)}{1+gx^2} e^{-\frac{1}{2}x^2}$ [11]. Table IV summarizes our results for the case, which surpass the accuracy calculated through an analytic continuation quantization procedure [12].

For problems on the half real axis, $r \geq 0$, despite the Stieltjes nature of the moments $u(\rho) = \int_0^\infty dr\, r^\rho \Psi(r)$, the asymptotic form of the wave function $\Psi(r) \to e^{-\sqrt{|E|}r}$ does not lead to a bounded and analytic Fourier transform. In order to achieve this, one must map the problem onto the real axis: $z^2 = r$, and $\tilde{\Psi}(z) \equiv |z|\Psi(z^2)$, for $-\infty < z < \infty$. Since $\tilde{\Psi}(z) \to e^{-\sqrt{|E|}z^2}$, the corresponding Fourier transform should be better behaved. The even (nonzero) Hamburger moments $\mu(2\rho) = \int_{-\infty}^{\infty} dz\, z^{2\rho} \tilde{\Psi}(z) = u(\rho)$ permit the analysis represented by Eqs. (12)–(15). Application to the Coulomb potential yielded rapidly converging estimates to the exact energies. A similar analysis with respect to $H = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{1}{2}\frac{l(l+1)}{r^2} - \frac{1}{r+b}$ (utilizing the $m_s = 2$ missing moment equations in Ref. [13]) converges to the correct ground state energy $E = -0.082\,862\,42$ ($l = 1$, $b = 1$, $R_\beta(k) = e^{-k^2}$ and $N = 100$). The same applies for the potential $V(x) = \frac{-f}{1+\sigma x^2}$ [i.e., for symmetric states, $u(p) = \int_0^\infty dx\, x^p \Psi(x)$ depend linearly on $\Psi(0)$, $u(0)$, and $u(1)$]. For $f = 1$ and $\sigma = 10^{-3}$ the first three (even parity) energy levels are $-0.969\,109\,93$, $-0.851\,372\,5$, and $-0.744\,905\,9$ ($\beta = 1$, and $N = 44$).

In the case of multidimensional problems, $\mathcal{D} \geq 2$, the momentum space expansion coefficients will assume the form $a_{n,m}[E, u(0,0), \ldots, u(p_{\ell \leq N_{n,m}}, q_{\ell \leq N_{n,m}})]$, involving a linear dependence on the first $1 + N_{n,m}$ missing moments, $\{u(p_\ell, q_\ell) \,|\, 0 \leq \ell < \infty\}$. One must then properly select the finite subset of $\{a_{n,m}\}$ coefficients to be zero, leading in turn to a relation equivalent to Eq. (15). For the $L_z = 0$ angular momentum states of the quadratic Zeeman problem, $H_{QZ} = -\frac{1}{2}\nabla^2 - \frac{1}{r} + \frac{1}{8}B^2(x^2 + y^2)$, in parabolic coordinates ($\xi = r - z > 0$, and $\eta = r + z > 0$) [10b], excellent results are obtained provided we work with $\{a_{n,m} \,|\, n + m = 2L + 1, m \leq L\}$, which depend on the missing moments $\{u(i,i) \,|\, 0 \leq i \leq L\}$. One then implements exactly the same computation as described for the one dimensional case. The first two binding energy levels are given in Table V ($\beta = 1, L = 25$). They are consistent with those of Rosner *et al.* [14].

For the Hamiltonian $H_{xy} = -(\partial_x^2 + \partial_y^2) + x^2 + y^2 + (xy)^2$, the previous formalism was applied to $\{a_{n,m} \,|\, n = L, 0 \leq m \leq L\}$, which depend on the missing moments $\{u(i,0) \,|\, 0 \leq i \leq L\}$. The calculated ground state energy (Table V) agrees with that of Vrscay and Handy ($\beta = 0.5, L = 20$) [15].

In summary, we have developed a highly accurate inner product quantization procedure involving the zeros of the underlying energy dependent coefficient functions. We have applied this method to several representative one dimensional problems in configurations space. We then extend our method into momentum space enabling the study of multidimensional problems.

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.

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

n	E_n
0	1.043 173 713 044 445 233 778 700 870 546 094
2	5.181 094 785 884 700 927 110 409 072 888 3
4	9.272 816 970 035 252 254 582 438 478 9
6	13.339 390 726 973 551 232 933 170 5

TABLE V. First two symmetric energy levels for H_{QZ} ($B = 2$) and H_{xy}.

H	E_{ground}	$E_{\text{first excited}}$
H_{QZ}	1 − 1.02 221 40	1 − 0.173 939 7
H_{xy}	2.195 918 086	7.031 272 466

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