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Application of the eigenvalue moment method to the quartic anharmonic double-well oscillator

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The eigenvalue moment method (EMM) is a precise technique for generating converging lower and upper bounds to the low-lying eigenenergies of singular quantum Hamiltonians. We apply it to the quartic anharmonic double-well oscillator problem, $P^2-Z^2x^2+x^4$, recently studied by Saavedra and Buendia [Phys. Rev. A **42**, 5073 (1990)]. In addition, we introduce important algorithmic modifications to the conventional EMM formulation, leading to more efficient applications.

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Over the past few years the eigenvalue moment method (EMM) has been developed into an effective and simple technique for generating converging lower and upper bounds to the low-lying eigenenergies of multidimensional quantum Hamiltonians [1–4]. Although EMM may not necessarily be the preferred technique for determining all eigenenergies for different Hamiltonian parameter values, it does allow one to test the reliability of other faster, but potentially less precise, methods. A case in point is the recent study by de Saavedra and Buendia [5] on the eigenenergies of the double-well quartic anharmonic oscillator,

$$H=-\partial_x^2-Z^2x^2+x^4 . \tag{1}$$

For the ground-state energy E_g case corresponding to $Z^2=5$, the EMM bounds are $-3.410\,142\,761\,239\,829\,50 < E_g < -3.410\,142\,761\,239\,829\,35$. The calculation by de Saavedra and Buendia predicts $-3.410\,142\,761\,239\,826$. We compare the numerical predictions of both methods in Table I.

In this work we will only focus on the ground-state eigenvalues for the system represented by Eq. (1). The EMM analysis can be readily implemented for the excited states [6]. Our objective is only to emphasize the relevance of an EMM analysis. In addition, we discuss other algorithmic improvements to the original EMM analysis presented in Refs. [2] and [3]. These are discussed in the Appendixes.

Consider the ground-state eigenvalues of the double-well quartic anharmonic oscillator problem

$$[-\partial_x^2-Z^2x^2+x^4]\Psi(x)=E_g\Psi(x) . \tag{2}$$

We will transform the configuration-space problem into a moment problem [7]. The parity-symmetric structure of the ground-state wave function permits the use of Stieltjes moments $u(p)=\int_0^\infty dy\, y^p\Psi(\sqrt{y})/\sqrt{y}$. The corresponding Stieltjes moment equation is then

$$u(p+2)=Eu(p)+Z^2u(p+1)+2p(2p-1)u(p-1) \quad \text{for } p\geq 0 . \tag{3}$$

The energy E appears as a parameter. Once the moments $u(0)$ and $u(1)$ are specified, all the other moments can be generated. The linear dependence on these initialization variables or *missing moments* [1] is made manifest through the relation

$$u(p)=\sum_{j=0}^{l} M_E(p,j)u(j) , \tag{4a}$$

where, also,

$$M_E(i,j)=\delta_{i,j} \quad \text{for } 0\leq i,j\leq 1 . \tag{4b}$$

The (energy-dependent) $M_E(p,j)$ coefficients satisfy the same moment recursion relation as the moments, with respect to the p argument. They can be generated numerically.

Clearly, the homogeneous nature of Eq. (3) motivates the specification of an appropriate normalization. One convenient choice is

$$u(0)+u(1)=1 . \tag{5}$$

Solving for $u(0)$ and performing the appropriate substitution in Eq. (4a) yields the relation

$$u(p)=\hat{M}_E(p,0)+\hat{M}_E(p,1)u(1) , \tag{6}$$

where

$$\hat{M}_E(p,j)=\begin{cases} M_E(p,0) & \text{for } j=0 \\ M_E(p,j)-M_E(p,0) & \text{for } j=1 . \end{cases} \tag{7}$$

It is a well-known theorem that the bosonic ground-state wave function must be of uniform signature [8], which can be taken to be positive. Quantization through the EMM theory takes place by imposing the necessary and sufficient conditions for the moments $\{u(p)\}$ to be the moments of a positive distribution [7]. These take on the form [2,3]

$$\sum_{i,j=0}^{N} C_i u(m+i+j) C_j > 0 , \tag{8}$$

for all Cs, $m=0,1$, and $0 \le i,j \le N$ where $0 \le N < \infty$.

Inserting Eq. (6) into Eq. (8) results in an infinite number of linear constraints on the missing moment $u(1)$. For a given N, one must determine the energy parameter values admitting a $u(1)$ solution set to Eq. (8). This can be done effectively through implementation of a linear programming based *cutting method* applied on Eq. (8) [2,3]. The reader can consult the appropriate references for a detailed description of its implementation. An important part of this procedure is the determination of cutting vectors C which have nonpositive expectation value

TABLE I. Bounds for the ground-state eigenvalue of the double-well quartic anharmonic oscillator. The maximum number of moments used is denoted by P. All computations were done in double precision on the Cray supercomputer.

Z^2	P	Lower bound	Upper bound
1	8	0.63	0.67
	12	0.657 1	0.658 5
	16	0.657 633 75	0.657 660 75
	20	0.657 652 875	0.657 653 375
	24	0.657 652 999 5	0.657 653 007 0
	28	0.657 653 005 16	0.657 653 005 26
	32	0.657 653 005 179 6	0.657 653 005 181 2
	36	0.657 653 005 180 710	0.657 653 005 180 728
	40	0.657 653 005 180 714 95	0.657 653 005 180 715 20
	44	0.657 653 005 180 715 121 75	0.657 653 005 180 715 124 75
	48	0.657 653 005 180 715 123 04	0.657 653 005 180 715 123 07
		(Value given in Ref. [5]: 0.657 653 005 180 715)	
5	8	−3.6	−2.5
	12	−3.46	−3.40
	16	−3.410 5	−3.408 6
	20	−3.410 18	−3.410 13
	24	−3.410 144	−3.410 141
	28	−3.410 142 79	−3.410 142 74
	32	−3.410 142 761 37	−3.410 142 760 59
	36	−3.410 142 761 254 95	−3.410 142 761 237 4
	40	−3.410 142 761 239 974	−3.410 142 761 239 506
	44	−3.410 142 761 239 836	−3.410 142 761 239 828 0
	48	−3.410 142 761 239 829 50	−3.410 142 761 239 829 35
		(Value given in Ref. [5]: −3.410 142 761 239 826)	
15	8	−52.5	−46.5
	12	−50.970	−50.445
	16	−50.875	−50.815
	20	−50.845	−50.840
	24	−50.841 5	−50.841 1
	28	−50.841 395	−50.841 377
	32	−50.841 387 95	−50.841 386 75
	36	−50.841 387 302	−50.841 387 248
	40	−50.841 387 286 25	−50.841 387 283 78
	44	−50.841 387 284 402 1875	−50.841 387 284 311 0625
	48	−50.841 387 284 383 9625	−50.841 387 284 380 9250
	50	−50.841 387 284 382 1625	−50.841 387 284 381 3625
		(Value given in Ref. [5]: −50.841 387 284 381 90)	
25	8	−152	−143
	12	−149.6	−148.5
	16	−149.26	−149.12
	20	−149.227	−149.213
	24	−149.221	−149.219
	28	−149.219 6	−149.219 3
	32	−149.219 46	−149.219 44
	36	−149.219 456 5	−149.219 455 8
	40	−149.219 456 171	−149.219 456 115
	44	−149.219 456 142 89	−149.219 456 139 63
		(Value given in Ref. [5]: −149.219 456 142 1913)	

$\langle C|\mathcal{M}|C\rangle \leq 0$, relative to some appropriate Hankel moment matrix $\mathcal{M}_{i,j}=u(m+i+j)$. In Refs. [2] and [3] such cutting vectors were obtained by determining the negative eigenvectors of the associated Hankel matrix. This procedure is costly; however, a more effective approach is via either an $\mathcal{LU}$ matrix decomposition or through the generation of $\mathcal{M}$-orthogonal vectors $[\langle \mathbf{V}^{(k)}|\mathcal{M}|\mathbf{V}^{(l)}\rangle = N(k)\delta_{k,l}]$. These are discussed in Appendixes A and B, respectively.

The numerical results of the preceding analysis are given in Table I. In order to avoid too large numbers, we rescaled the Stieltjes moments according to $u_\Lambda(p)=u(p)/\Lambda^p$. The corresponding rescaled moment equation is

$$u_\Lambda(p+2)=E\Lambda^{-2}u_\Lambda(p)+Z^2\Lambda^{-1}u_\Lambda(p+1) +2p(2p-1)\Lambda^{-3}u_\Lambda(p-1)\ , \tag{9}$$

where we choose $\Lambda=Z^2$.

Although no numerical error analysis of the basic EMM theory is available, we have always used the following empirical rule for determining the reliability of the generated eigenenergy bounds: so long as there is only one energy interval of allowed (feasible) energy values, the generated bounds are acceptable. That is, if at any order of the calculation we observe intermittent feasible energy intervals (separated by energy intervals which are not allowed or infeasible), then the numerical reliability of the results are suspect.

There are now good theoretical arguments to support this rule. In a recent communication by Ashbaugh and Sundberg [9], they have rigorously argued (from a mathematical perspective) that for most potentials, there can be no segmentation of the feasible energy set (it must be a continuous interval). This is also supported by a different theoretical analysis by Handy and Ndow [10] corresponding to a Euclidean time formulation of the basic EMM analysis. The latter yields automatic bounds on the ground-state energy without having to partition an arbitrary energy interval.

Two additional comments are in order. First, in the original linear programming analysis of the sextic anharmonic oscillator [2], feasible energy interval segmentation was observed. In that work we used both an inefficient linear programming moment theory and algorithm. A reinvestigation of the sextic problem with a more efficient code (corresponding to that employed in Ref. [3]) showed no feasible energy segmentation, in keeping with the previously cited works. Second, in the course of investigating an earlier work by Bessis, Vrscay, and Handy [11], the use of the Jacobi method to recursively generate the Hankel-Hadamard (HH) determinants (an important theoretical component of the EMM theory) gave erroneous bounds, for certain parameter values of the potential function. Such behavior was anticipated because of the presence of small denominators and the consequential propagation of errors. In such cases, a direct calculation of the HH determinants always led to the correct energy bounds, regardless of the parameter values. The numerical structure of the EMM theory is in keeping with the latter.

On the basis of the preceding discussion, we are confident of the results quoted in Table I. Also note that computer time (and not any evidence of numerical instability) limited the extent to which we could generate higher-order bounds.

We have established the relevance of an EMM analysis for calculating precise ground-state energy bounds for the quartic anharmonic double-well oscillator. Also, we have improved the algorithmic efficiency of the conventional EMM analysis through the $\mathcal{LU}$ generation of cutting vectors.

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APPENDIX A: $\mathcal{LU}$-CUTTING PROCEDURE

As indicated previously, an important part of the linear programming based cutting procedure [2,3] involves the determination of vectors with nonpositive expectation values (when they exist) relative to a given symmetric (Hankel) matrix $\langle C|\mathcal{M}|C\rangle \leq 0$. For simplicity, we will assume that the matrix indices are equal to or greater than unity ($\mathcal{M}_{i,j}$ and $i,j \geq 1$). In earlier references [2,3], such cutting vectors were found by determining the appropriate nonpositive eigenvectors of the associated symmetric matrix $\mathcal{M}$. This can be computationally expensive. Alternatively, one may use the more economical $\mathcal{LU}$ decomposition to realize the representation $\mathcal{M}=\mathcal{L}\mathcal{D}\mathcal{L}^t$, where $\mathcal{L}$ is a lower triangular matrix (the t denotes the transpose) with all diagonal entries equal to unity and $\mathcal{D}$ is a purely diagonal matrix [12]. Any diagonal entry that is nonpositive, $\mathcal{D}_i \leq 0$, generates a cutting vector through the relation (i is kept fixed) $\sum_k \mathcal{L}_{kj}C_k=\delta_{ji}$.

The only drawback in using $\mathcal{LU}$-cutting vectors, as opposed to identifying nonpositive eigenvectors, is that more of the former type of cutting vectors may be required in order to "cut" a given "polytope" within the *cutting method* formalism [2,3]. For completeness, we outline the $\mathcal{LU}$-decomposition process for generating a cutting vector. This will also enable the reader to better appreciate an alternate formulation given in Appendix B.

We adopt an inductive strategy. Let $\mathcal{M}$ be a symmetric matrix. Assume that the submatrix formed from the first d rows and columns, $\mathcal{M}_d$, has an $\mathcal{LU}$ representation $\mathcal{M}_d=\mathcal{L}\mathcal{U}$, where $\mathcal{L}$ is a lower triangular matrix whose diagonal entries are all unity, whereas $\mathcal{U}$ is an upper triangular matrix. One can readily argue that $\mathcal{U}=\mathcal{D}\mathcal{L}^t$, where $\mathcal{D}$ is purely diagonal. We will assume that the dth diagonal entry of $\mathcal{M}_d$ is nonzero, $\mathcal{M}_{d,d}\neq 0$; otherwise, one could take $C_i=\delta_{i,d}$ to be a cutting vector. The $d+1$ submatrix can be represented as

$$\mathcal{M}_{d+1}=\begin{bmatrix}\mathcal{L} & \mathbf{0}\\ \mathbf{R} & 1\end{bmatrix}\begin{bmatrix}\mathcal{U} & \mathbf{V}\\ \mathbf{0} & u\end{bmatrix}\ , \tag{A1}$$

where the boldface quantities are either row or column vectors of dimension d. The above representation exists because one can solve for $\mathbf{V}$, $\mathbf{R}$, and u,

$$\sum_{j=1}^{d} (\mathcal{L})_{ij} V_j = \mathcal{M}_{i,d+1} \quad \text{for } 1 \le i \le d \ ,$$
$$\sum_{j=1}^{d} (\mathcal{U})_{ji} R_j = \mathcal{M}_{d+1,i} \quad \text{for } 1 \le i \le d \ , \tag{A2}$$

and

$$\langle \mathbf{R}|\mathbf{V}\rangle + u = \mathcal{M}_{d+1,d+1} \ .$$

The second relation may be rewritten as $\sum_{j=1}^{d} (\mathcal{D}\mathcal{L}^t)_{ji} R_j = \mathcal{M}_{i,d+1}$, or $R_j = V_j \mathcal{D}_j^{-1}$, for each j. Clearly, the latter assumes that none of the diagonal entries is zero. The matrix representation in Eq. (A1) becomes the updated $(d+1)$-dimensional $\mathcal{L}\mathcal{U}$ decomposition with $(\mathcal{U})_{d+1,d+1} = u = \mathcal{D}_{d+1}$.

As noted, the above procedure continues until either the original matrix is completely resolved into $\mathcal{L}\mathcal{U}$ form, or one of the diagonal entries becomes nonpositive, $\mathcal{D}_d \le 0$ (actually, as long as $\mathcal{D}_d < 0$ one can completely decompose $\mathcal{M}$). If the latter occurs, then one can stop and solve for the cutting vector, satisfying

$$\sum_{j=1}^{d} \mathcal{L}_{ji} C_j = \delta_{i,d} \quad \text{for } 1 \le i \le d$$
$$\text{where } C_d = 1, C_j = 0 \text{ for } j > d \ . \tag{A3}$$

Such a $\mathbf{C}^{(d)}$ vector will yield a nonpositive expectation value with respect to the full $\mathcal{M}$ matrix. A simple renormalization will yield a normalized vector, $\mathbf{C}^{(d)}/(\langle \mathbf{C}^{(d)}|\mathbf{C}^{(d)}\rangle)^{1/2}$.

Having obtained a normalized ($\langle \mathbf{C}|\mathbf{C}\rangle = 1$) cutting vector, one may produce another one with smaller $\mathcal{M}$-expectation value by repeating the above with respects to the properly modified matrix $\mathcal{M} - \langle \mathbf{C}|\mathcal{M}|\mathbf{C}\rangle 1$. If this matrix has a (normalized) cutting vector $\mathbf{C}'$ then $\langle \mathbf{C}'|\mathcal{M}|\mathbf{C}'\rangle \le \langle \mathbf{C}|\mathcal{M}|\mathbf{C}\rangle \le 0$. From the cutting method perspective, such iterations can produce "deeper" cutting vectors.

APPENDIX B: GENERALIZED ORTHOGONAL VECTORS

Given a symmetric matrix $\mathcal{M}$, we want to determine the family of orthogonal vectors relative to $\mathcal{M}$, satisfying

$$\langle \mathbf{V}^{(k)}|\mathcal{M}|\mathbf{V}^{(l)}\rangle = N(k)\delta_{k,l} \ , \tag{B1}$$

where $V_k^{(k)} = 1$, and $V_j^{(k)} = 0$ if $j > k$. Assume that such a set of $\mathcal{M}$-orthogonal vectors $O_d \equiv \{\mathbf{V}^{(l)} | 1 \le l \le d\}$ exists, for some d (not necessarily the full dimension). If the submatrix $\mathcal{M}_d$ (as defined in Appendix A) is not positive definite (that is, there exists a cutting vector $\langle C|\mathcal{M}_d|C\rangle \le 0$), then one of the $N(k)$ must be nonpositive. The proof is immediate. Clearly, any d-dimensional vector can be spanned by the orthogonal set O_d: $\sum_{i=1}^{d} c_i \mathbf{V}^{(i)}$. The corresponding expectation value is $\sum_{i=1}^{d} c_i^2 N(i)$. Unless one of the N is nonpositive, the submatrix will be positive definite, a contradiction. Thus the realization of an $\mathcal{M}$-orthogonal set of vectors is intimately connected with the generation of cutting vectors.

We can generate O_d inductively. Assume that such a set exists. Any basis vector $\mathbf{e}^i$ (with components $e_j^i = \delta_{i,j}$ for $1 \le i,j \le d$) can be expressed as a superposition of the form $\mathbf{e}^k = \sum_{j=1}^{k} c_j \mathbf{V}^{(j)}$, with $c_k = 1$. It then follows that the relation in (B1) is equivalent to

$$\langle \mathbf{e}^k|\mathcal{M}|\mathbf{V}^{(l)}\rangle = N(l)\delta_{k,l} \quad \text{if } k \le l \text{ only!} \ . \tag{B2}$$

Alternatively, $\sum_{j=1}^{l} \mathcal{M}_{kj} V_j^{(l)} = 0$ or $N(l)$, depending on whether $k \le l-1$ or $k = l$, respectively. One may use these relations to directly invert and solve for $\{V_j^{(l)}\}$: $\sum_{j=1}^{l-1} \mathcal{M}_{kj} V_j^{(l)} = -\mathcal{M}_{kl}$. However, we can recursively generate the $V_i^{(l)}$ component in terms of the higher-order components $\{V_j^{(l)} | j \ge i+1\}$ and the vectors $\{\mathbf{V}^{(k)} | k < l\}$. Specifically, expanding (B1) and making use of (B2) yields (recall that in general $V_l^{(l)} = 1$ and $V_{j>l}^{(l)} = 0$)

$$\sum_{i,j} V_i^{(k)} \mathcal{M}_{ij} V_j^{(l)} = \sum_{j=1}^{l} \left[\sum_{i=1}^{k} V_i^{(k)} \mathcal{M}_{ij} \right] V_j^{(l)} = 0$$
$$\text{if } k < l \tag{B3}$$

or

$$\sum_{j=k}^{l} \left[\sum_{i=1}^{k} V_i^{(k)} \mathcal{M}_{ij} \right] V_j^{(l)} = 0 \quad \text{if } k < l \ .$$

The last relation follows from $\sum_{i=1}^{k} V_i^{(k)} \mathcal{M}_{ij} = \sum_{i=1}^{k} \mathcal{M}_{ji} V_i^{(k)} = 0$ if $j < k$! Upon solving for $V_k^{(l)}$ (recall that $V_l^{(l)} = 1$), we get

$$V_k^{(l)} = -\left\{ \sum_{j=k+1}^{l} \left[\sum_{i=1}^{k} V_i^{(k)} \mathcal{M}_{ij} \right] V_j^{(l)} \right\} \Big/ \left[\sum_{i=1}^{K} V_i^{(k)} \mathcal{M}_{ik} \right]$$
$$\text{for } k = l-1, l-2, \ldots, 1 \tag{B4}$$

or

$$V_k^{(l)} = -\left\{ \sum_{j=k+1}^{l} \left[\sum_{i=1}^{k} V_i^{(k)} \mathcal{M}_{ij} \right] V_j^{(l)} \right\} \Big/ N(k)$$
$$\text{for } k = l-1, l-2, \ldots, 1 \ . \tag{B5}$$

Equation (B5) may be used to generate all the orthogonal vectors or until, for some l, one generates $N(l) = 0$. As indicated, if any $N(k)$ is nonpositive, its corresponding orthogonal vector is a cutting vector.

Both formalisms in Appendixes A and B are equivalent. The simplest way to see this is to note that the $C^{(d)}$ vectors in (A3) satisfy $\langle C^{(k)}|\mathcal{M}|C^{(l)}\rangle = \mathcal{D}_k \delta_{k,l}$.

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