Moment-method analysis of the ground state of discretized bosonic systems

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The eigenvalue moment method for bosonic systems, recently developed by C. R. Handy and D. Bessis [Phys. Rev. Lett **55**, 931 (1985)], is extended to discrete quantum mechanics. The relevant formalism is described and applied in the context of the discretized harmonic and sextic anharmonic potentials. Rapidly converging bounds to the associated ground-state energies are obtained for fixed lattice spacing a satisfying $a < O(1)$.

INTRODUCTION

The formulation of lattice models for quantum mechanics and field theory has been an ongoing concern for some time, particularly in regards to understanding strong-coupling physics.[1] One particular approach inaugurated by Bender and *et al.*[2] focused on the singular-perturbation aspects of a lattice-regulated strong-coupling field theory. The issues addressed by them motivated a similar analysis of quantum mechanics, and in particular, on the relevance of a moments formulation for a lattice-regulated quantum mechanics.[3] In this regard, it has been established for continuum multidimensional bosonic systems[4–7] that a moments' perspective can achieve important results in the strong-coupling–singular-perturbation regime. In particular, rapidly converging bounds to ground-state energies are attainable. The objective of this paper is to demonstrate that the same holds for discretized quantum mechanics, although we shall limit this presentation to two one-dimensional problems.

Besides the physical motivation for understanding discretized quantum systems, there are also practical considerations. Firstly, from a numerical standpoint lattice approximations usually allow one to practically address continuum systems through a computer.[8] Secondly, lattice models may allow for a better understanding of continuum systems, as was the case when Case and Kac developed their discrete analysis for the inverse scattering problem.[9] The same will hold here. Indeed, an important theorem on the non-negativity of the bosonic ground-state wave function can be readily appreciated within the lattice context; whereas in the continuum, the analogous theorem is not so obvious.[10] This will be one of the first issues to be discussed. Afterwards, we discuss the application of the eigenvalue moment method to two one-dimensional polynomial potential problems: the harmonic and the sextic anharmonic oscillator. The multidimensional generalization of our results follows in a manner similar to that for one-dimensional systems. Much of the necessary formalism has already been explained elsewhere.[4–7] Accordingly, some of the subsequent discussion will be brief.

I. GENERAL PRINCIPLES

The continuum eigenvalue moment method utilizes the exponential falloff and non-negative property of the bosonic ground-state wave function in order to define a moments problem. These issues are also relevant to the discrete formulation. We outline the important features of one-dimensional lattice Hamiltonians that allow for the application of the moment method.

Consider the discretized one-dimensional Schrödinger equation ($\varepsilon^2=\hbar^2/2m$)

$$-(\varepsilon/a)^2\Delta^2\Psi(L)+V(aL)\Psi(L)=E\Psi(L)\ , \tag{1.1}$$

where a is the lattice spacing, $V(aL)$ is the continuum potential function evaluated at the site $x=aL$, L is an arbitrary integer, E is the energy, and the finite-difference second-order operator is taken to be

$$\Delta^2\Psi(L)=\Psi(L+1)+\Psi(L-1)-2\Psi(L)\ . \tag{1.2}$$

The lattice Hamburger moments are

$$\tilde{u}(p)=a\sum_{L=-\infty}^{+\infty}(aL)^p\Psi(L)\ . \tag{1.3}$$

As for the continuum case, the finiteness of the lattice moments is insured by the exponential falloff of the physical discrete wave-function solution to Eq. (1.1). An excellent discussion of this may be found in the text by Bender and Orzag.[11] They argue that the asymptotics of solutions to Eq. (1.2) is determined by the asymptotics of the corresponding continuum solution. For completeness, we include a somewhat different analysis pertaining to polynominal potentials. In the subsequent presentation, we restrict our remarks to the positive limit $L\rightarrow+\infty$, for brevity. The extension to the negative direction follows similarly, and is implicitly assumed.

Let $R_L=\Psi(L+1)/\Psi(L)$. We are primarily interested in "bounded" lattice solutions for which $\lim_{L\rightarrow\infty}R_L\equiv R_\infty$ exists and $|R_\infty|<1$. If the latter holds and $R_\infty\neq0$, then the lattice configuration has an exponential behavior

$$|\Psi(L)|\simeq\exp(-L\,|\ln|R_\infty||\,|)\ .$$

If $R_\infty = 0$, then the falloff of $\Psi(L)$ as $L \to \infty$ is even more rapid than this and in either event, all moments of Ψ are finite. Lattice quantization corresponds to determining the E values for which such bounded solutions exist.

The existence of bound-state solutions for well-behaved potentials can be established by analyzing the nonlinear recursion relation satisfied by R_L,

$$-(\varepsilon/a)^2[R_L+(R_{L-1})^{-1}-2]+V(aL)=E \ . \tag{1.4}$$

Assuming that in the asymptotic limit $L \to \infty$ we may replace R_{L-1} by R_L, it then follows that R_L takes on the functional dependence

$$R_\pm(z)=1+[z \pm z(1+4\lambda/z)^{1/2}]/(2\lambda) \ , \tag{1.5}$$

where $\lambda=(\varepsilon/a)^2$ and $z=V(aL)-E$. The nature of Eq. (1.5) is consistent with the assumption $\lim_{L\to\infty}(R_L/R_{L+1})=1$ if

$$\lim_{L\to\infty}[R_\pm(V_L-E)/R_\pm(V_{L+1}-E)]=1 \ ,$$

where $V_L=V(aL)$. For asymptotically finite and positive potentials the latter is always true because

$$\lim_{L\to\infty}[V(aL)/V(aL+a)]=1 \ .$$

For asymptotically infinite and positive potentials the dominant term in Eq. (1.5) (i.e., $R_- \simeq \lambda/z$) yields the limit behavior

$$\frac{R_-(V_L)}{R_-(V_{L+1})} \to \frac{V_{L+1}}{V_L} \tag{1.6}$$

for bound-state lattice solutions. If the right-hand side approaches unity, then the assumptions leading to Eq. (1.5) are valid. For polynomial potentials, such is the case. These are the kinds of potentials considered in this work.

We now focus on establishing the non-negativity of the discrete bosonic ground-state lattice solution. We will be working within the space of normalized lattice configurations, $\langle \Psi \mid \Psi \rangle = 1$. The self-adjoint lattice Hamiltonian operator will be denoted as $H=-(\varepsilon/a)^2\Delta^2+V(aL)$. For potentials having a lower bound $V(aL) \geq V_{\min}$, the Hamiltonian is bounded from below,

$$V_{\min} < \langle \Psi \mid H \mid \Psi \rangle \ . \tag{1.7}$$

This follows from the simple relation for the kinetic energy

$$(-)\sum_{L=-\infty}^{\infty}\Psi^*(L)\Delta^2\Psi(L)=\sum_{L=-\infty}^{\infty}|\Psi(L+1)-\Psi(L)|^2 \ , \tag{1.8}$$

from which ensues

$$\langle \Psi \mid H \mid \Psi \rangle > \sum_{L=-\infty}^{\infty}[V(aL)-V_{\min}]\,|\Psi(L)|^2+V_{\min} > V_{\min}$$

Realizing that the normalized Ψ's which extremize $\langle \Psi \mid H \mid \Psi \rangle$ are eigenstates of H and conversely, it follows that the ground-state energy must satisfy

$$E_{\rm gr} \leq \langle \Psi \mid H \mid \Psi \rangle \ . \tag{1.9}$$

We will prove that the ground state has a uniform signature and can be taken to be non-negative. This rests upon showing that given any normalized configuration Ψ, the expectation value $\langle \Psi \mid H \mid \Psi \rangle$ is decreased by using a suitably defined non-negative configuration. It can be readily argued that the ground state can be taken to be a real configuration; accordingly, we will restrict our analysis to real configurations only.

The proof of uniform signature and non-negativity proceeds as follows. Let $\Psi(L)$ be of nonuniform signature and nonpositive on the integer set

$$S=\{L \mid I \leq L \leq J\} \ , \tag{1.10}$$

where I and J are integers or $\pm\infty$, $-\infty \leq I \leq J \leq \infty$, with the additional requirements that $\Psi(L)<0$ for some $L \in S$ and $\Psi(I-1)>0$ (absent if $I=-\infty$) and $\Psi(L+1)>0$ (absent if $J=\infty$). Note that since Ψ has nonuniform signature $I=-\infty$ and $J=\infty$ is not a possibility and thus one or the other of these latter two conditions is always present.

Let $\Phi(L)$ correspond to $\Psi(L)$ for $L \notin S$ and $\Phi(L) = -\Psi(L) \geq 0$ for $L \in S$. We want to show that

$$\langle \Phi \mid H \mid \Phi \rangle \leq \langle \Psi \mid H \mid \Psi \rangle \ . \tag{1.11}$$

If L_1 and L_2 simultaneously lie in S or in the complement of S, C_S, we have the product equality $\Phi(L_1)\Phi(L_2)=\Psi(L_1)\Psi(L_2)$. Thus the only terms responsible for Eq. (1.11) come from the kinetic energy, $\Psi(L)\Delta^2\Psi$, at $L=I-1$, I, J, and $J+1$. The relevant contribution to Eq. (1.11) is the relation

$$-2(\varepsilon/a)^2[\Phi(I-1)\Phi(I)+\Phi(J+1)\Phi(J)] \leq -2(\varepsilon/a)^2[\Psi(I-1)\Psi(I)+\Psi(J+1)\Psi(J)] \ , \tag{1.12}$$

which follows from $\Phi(I-1)=\Psi(I-1)>0$, $\Phi(J+1)=\Psi(J+1)>0$, $\Phi(I)=-\Psi(I)\geq 0$, and $\Phi(J)=-\Psi(J)\geq 0$.

As long as either of $\Phi(I)$ and $\Phi(J)$ is not equal to zero, Eq. (1.11) is a strict inequality; otherwise, the energy is not decreased. Thus, assuming that Ψ is a ground-state wave function, the argument above shows that $\Phi(I)=-\Psi(I)$ and $\Phi(J)=-\Psi(J)$ must both be 0 (for otherwise Φ would yield a lower total energy, a contradiction). In this case Ψ and Φ must both be ground-state wave functions. This follows from the variational characterization of minimizers of the Rayleigh quotient $\langle \Psi \mid H \mid \Psi \rangle / \langle \Psi \mid \Psi \rangle$: a minimizer must be a solution to the discretized Schrödinger equation with $E=E_{\rm gr}$. But if Ψ and Φ are ground-state wave functions then so is $\frac{1}{2}(\Phi-\Psi)$. Now this is a function which coincides with Φ on S and is therefore nontrivial [recall that there exists an L in S such that $\Psi(L)<0$]. On the other hand, this function is zero on C_S which extends infinitely to one or both of $\pm\infty$. Since $\frac{1}{2}(\Phi-\Psi)$ must also satisfy the discretized Schrödinger equation and since any solution to this which vanishes at two consecutive lattice sites must be identically zero (observe that we are dealing with a second-order linear recursion relation) we have reached a contradiction. This shows that the ground-state wave function has uniform signature.

In fact, the argument above really shows that the ground-state wave function can never vanish, for if it did we could construct a wave function of nonuniform signature which still minimizes the Rayleigh quotient by appropriate reversals of sign in the given wave function as done above (actually, by more or less reversing the process applied above). Since, by the variational characterization, this new wave function would also be a ground-state wave function (i.e., satisfy the discretized Schrödinger equation for $E=E_{\rm gr}$), we could then arrive at a contradiction as above. Thus we may assume that Ψ, the ground-state wave function, is always positive. From this, in addition, it follows that Ψ is nondegenerate (i.e., by orthogonality the "other" ground state would not be of uniform signature).

II. HARMONIC OSCILLATOR

Let us consider the lattice counterpart to the usual continuum harmonic-oscillator problem

$$-\varepsilon^2\Psi''+x^2\Psi=E\Psi\ , \tag{2.1}$$

$$-(\varepsilon/a)^2\Delta^2\Psi(L)+(aL)^2\Psi(L)=E\Psi(L)\ . \tag{2.2}$$

Applying the moment operator $\sum_{L=-\infty}^{+\infty}a(aL)^p$ to both sides of Eq. (2.2), and defining $\tilde{u}(p)\equiv\sum_L a(aL)^p\Psi(L)$, give

$$-(\varepsilon/a)^2a\sum_{L=-\infty}^{\infty}(aL)^p[\Psi(L+1)+\Psi(L-1)-2\Psi(L)]+\tilde{u}(p+2)=E\tilde{u}(p)\ , \tag{2.3}$$

$$-(\varepsilon/a)^2a\sum_{L=-\infty}^{\infty}a^p[(L-1)^p+(L+1)^p-2L^p]\Psi(L)+\tilde{u}(p+2)=E\tilde{u}(p)\ , \tag{2.4}$$

$$-(\varepsilon/a)^2a\sum_{L=-\infty}^{\infty}a^p\left[2\sum_{\substack{i=2,\\ \text{and even}}}^{p}B(p,i)L^{p-i}\right]\Psi(L)+\tilde{u}(p+2)=E\tilde{u}(p)\ . \tag{2.5}$$

The $B(p,i)$ correspond to the binomial coefficients. Interchanging the two summations in Eq. (2.5) yields the moment equation

$$\tilde{u}(p+2)=E\tilde{u}(p)+2(\varepsilon/a)^2\sum_{\substack{i=2,\\ \text{and even}}}^{p}a^iB(p,i)\tilde{u}(p-i)\ . \tag{2.6}$$

The ground state must be symmetric, hence $\tilde{u}(p=\text{odd})=0$. In the continuum theory[4–7] the even order Hamburger moments correspond to Stieltjes moments. The same is true for the lattice theory, although in a more subtle manner. The even order Hamburger moments are equivalent to the Stieltjes moments of a discrete distribution,

$$\tilde{u}(2p)=u(p)=\int_0^\infty dy\,y^p\left[A_0\delta(y)+\sum_{i=1}^{\infty}A_i\delta(y-y_i)\right]\ , \tag{2.7}$$

$$=\frac{A_0}{2}\delta_{0,p}+\sum_{i=1}^{\infty}A_iy_i^p\ . \tag{2.8}$$

In order to define the y_i's and A_i's, we must transform the Hamburger moments of the symmetric configuration, $\Psi(-L)=\Psi(L)$, according to

$$\tilde{u}(2p)=a\sum_{L=-\infty}^{+\infty}(aL)^{2p}\Psi(L)\ , \tag{2.9}$$

$$=2a\frac{(a\ 0)^{2p}}{2}\Psi(0)+2a\sum_{L=1}^{\infty}[(aL)^2]^p\Psi(L)\ . \tag{2.10}$$

Note that $(a\ 0)^{2p}=\delta_{0,p}$. Comparing Eqs. (2.10) and (2.8) it follows that $y_i=(ai)^2$, and $A_i=2a\Psi(i)$.

The importance of Eq. (2.7) is that for symmetric configurations it simplifies the application of the relevant theorems arising from the "moments problem."[12] For the discrete Stieltjes case, the necessary and sufficient conditions for

$$\{u(p)\,|\,p=0,1,\dots\}$$

to correspond to a non-negative discrete distribution are that the following Hankel-Hadamard determinant inequality constraints be satisfied:[12,13]

$$\Delta_{m,n}[u]=\text{Det}\begin{vmatrix}u(m),u(m+1),\dots,u(m+n)\\ u(m+1),u(m+2),\dots,u(m+n+1)\\ \vdots\\ u(m+n),u(m+n+1),\dots,u(m+2n)\end{vmatrix}>0\quad\text{for } m=0,1 \text{ and } n\geq 0\ . \tag{2.11}$$

The Stieltjes moments are generated through the recursive relation

$$u(p+1)=Eu(p)+2(\varepsilon/a)^2\sum_{i=1}^{p}a^{2i}B(2p,2i)u(p-i)\ . \tag{2.12}$$

We may take $u(0)=1$.

The first nontrivial Hankel-Hadamard determinants are

$$\Delta_{1,0}=E/\varepsilon>0\ , \tag{2.13a}$$

$$\Delta_{1,1}=10(E/\varepsilon)^2+2a^2(E/\varepsilon)-4>0\ , \tag{2.13b}$$

$$\Delta_{0,2}=4[-16(E/\varepsilon)^2+4a^2(E/\varepsilon)+28]>0\ . \tag{2.13c}$$

Combining these inequalities gives us the lowest-order

ground-state energy bounds

$$\frac{-a^2+(a^4+40\varepsilon^2)^{1/2}}{10} \leq E \leq \frac{a^2+(a^4+112\varepsilon^2)^{1/2}}{8} . \tag{2.14}$$

The numerical results for various values of the lattice spacing are quoted in Tables I–V. The basic programming logic is as follows. We partition a given energy interval $[E_{\min},E_{\max}]$ and specify some maximum moment order $p_{\max}$. At each point in the partitioned energy interval, all the Stieltjes moments of order $p \leq p_{\max}$ are calculated. All the corresponding Hankel-Hadamard determinants are evaluated. Only those energy points satisfying Eq. (2.11) are allowed. Through them one can define an updated energy interval $[E'_{\min},E'_{\max}]$. The maximum moment order parameter is increased by 1, $p_{\max} \rightarrow p_{\max}+1$, and the entire procedure is repeated. Rapidly converging lower and upper bounds to the ground-state energy are obtained for $a < 0(1)$.

The results for the continuum case, $a=0$ (in Table I), are consistent with the order-of-magnitude estimates in Ref. 4 (Table I). However, the bounds cited in Ref. 4, at best, are not as accurately determined as those given here; and at worst, seem to be systematically off, in order-of-magnitude estimate, by a factor of 5.

III. DISCUSSION OF NUMERICAL RESULTS FOR THE HARMONIC OSCILLATOR

The results cited in Tables I–V show that the moment approach yields rapidly converging bounds for relatively small values of the lattice spacing a. For $a=5$, no tight bounds are possible. Already for $a=1$ there is a clear reduction in the rate that the bounds converge on the physical value, in comparison to the cited results for $a=0$, 0.01, and 0.1. For the large lattice spacing limit $a \rightarrow \infty$, an alternate formulation in terms of the "trigonometric moment problem" works very well. This is discussed in a sequel by Handy, Mantica, and Gibbons.[14] For completeness, we make note of some simple bounds attainable for a rescaled theory.

The rescaled lattice Stieltjes moments, $\hat{u}(p)=u(p)/a^{2p}$, satisfy the recursion relation

$$\hat{u}(p+1)=(E/a^2)\hat{u}(p) + 2(\varepsilon/a^2)^2 \sum_{i=1}^{p} B(2p,2i)\hat{u}(p-i) . \tag{3.1}$$

If we relabel $E/a^2=e$, then the rescaled moments are explicitly dependent on e and $(\varepsilon/a^2)^2$. In the limit $a \rightarrow \infty$, the moments are given by $\hat{u}_{\infty}(p)=e^p$. This asymptotic moment solution can be shown (i.e., Carleman's condition[12,13]) to uniquely correspond to a discrete *continuum* Dirac distribution

$$\hat{\Psi}=[\delta(x-e^{1/2})+\delta(x+e^{1/2})]/2 . \tag{3.2}$$

Note that there is *no unique non-negative* solution with respect to the "energy" variable e. However, if we also impose the Hankel-Hadamard inequalities prior to taking

TABLE I. Eigenvalue bounds for the lattice harmonic oscillator ($a=0$, $\varepsilon=1$).

$p_{\max}$	Lower bound	Upper bound
6	0.912	1.045 12
7	0.983 884 8	1.042 457 6
8	0.984 470 528 0	1.006 142 464
9	0.997 690 409 0	1.005 925 745
10	0.997 772 762 3	1.000 819 837
11	0.999 692 419 1	1.000 819 837
12	0.999 703 693 2	1.000 109 564
13	0.999 959 391 5	1.000 109 564
14	0.999 960 893 2	1.000 014 955
15	0.999 994 952 2	1.000 014 415
16	0.999 994 952 2	1.000 001 959
17	0.999 999 366 3	1.000 001 819
18	0.999 999 366 3	1.000 000 225
19	0.999 999 915 6	1.000 000 225
20	0.999 999 921 8	1.000 000 030

TABLE II. Eigenvalue bounds for the lattice harmonic oscillator ($a=0.01$, $\varepsilon=1$).

$p_{\max}$	Lower bound	Upper bound
6	0.912	1.045 12
7	0.983 884 80	1.042 457 6
8	0.984 470 528	1.006 142 464 0
9	0.997 690 409 0	1.005 925 745 0
10	0.997 772 762 3	1.000 819 837 0
11	0.999 692 419 1	1.000 819 837 0
12	0.999 692 419 1	1.000 109 564 0
13	0.999 951 048 6	1.000 105 392 0
14	0.999 954 135 5	1.000 008 156 0
15	0.999 988 708 4	1.000 008 156 0
16	0.999 988 708 4	0.999 995 709 4
17	0.999 993 119 1	0.999 995 569 4
18	0.999 993 119 1	0.999 993 976 7
19	0.999 993 666 8	0.999 993 976 7
20	0.999 993 671 0	0.999 993 779 1

TABLE III. Eigenvalue bounds for the lattice harmonic oscillator ($a=0.1$, $\varepsilon=1$).

$p_{\max}$	Lower bound	Upper bound
6	0.908 24	1.043 92
7	0.982 864	1.042 563 2
8	0.984 057 984	1.005 549 696 0
9	0.996 953 011 2	1.005 549 696 0
10	0.997 038 978 0	1.000 305 718 0
11	0.999 031 689 6	1.000 240 383 0
12	0.999 055 863 5	0.999 490 993 3
13	0.999 329 995 2	0.999 490 993 3
14	0.999 331 605 2	0.999 391 174 5
15	0.999 368 538 2	0.999 389 983 1
16	0.999 368 967 1	0.999 376 687 2
17	0.999 373 830 8	0.999 376 687 2
18	0.999 373 859 3	0.999 374 887 7
19	0.999 374 507 2	0.999 374 877 4
20	0.999 374 514 6	0.999 374 644 2

TABLE IV. Eigenvalue bounds for the lattice harmonic oscillator ($a=1$, $\varepsilon=1$).

$p_{\max}$	lower bound	upper bound
6	0.78	1.052
7	0.8752	1.052
8	0.8752	0.972 44
9	0.909 234	0.972 44
10	0.909 866 06	0.949 053 78
11	0.921 622 376	0.948 661 902 8
12	0.921 892 771 3	0.940 550 044 8
13	0.926 557 089 6	0.940 550 044 8
14	0.926 557 089 6	0.937 331 665 1
15	0.928 604 259 0	0.937 331 665 1
16	0.928 604 259 0	0.936 022 554 2
17	0.929 420 271 4	0.936 022 554 2
18	0.929 420 271 4	0.935 428 348 7
19	0.929 720 675 3	0.935 428 348 7
20	0.929 720 675 3	0.935 257 118 5

the $a\to\infty$ limit, then from Eq. (2.14) a simple relation follows for $e=E/a^2$,

$$\frac{-1+(1+40\varepsilon^2/a^4)^{1/2}}{10}\le e\le\frac{1+(1+112\varepsilon^2/a^4)^{1/2}}{8}\ . \tag{3.3}$$

The *asymptotic bounds* for e are $0\le e\le\frac{1}{4}$. Thus, contrary to the discussion pertaining to the asymptotic theory defined by Eq. (3.2), e is not unboundedly arbitrary, as suggested by Eq. (3.3). Thus we interpret this as an indication that the limit $a\to\infty$ is *not* inaccessible because of a breakdown in the ground state's uniqueness of positivity, as is confirmed by Ref. 14.

IV. DISCRETIZED SEXTIC ANHARMONIC OSCILLATOR

We now consider a more difficult problem, that of the discretized sextic anharmonic oscillator. The corresponding lattice equation is

$$-(\varepsilon/a)^2\Delta^2\Psi+[(aL)^2+(aL)^6]\Psi=E\Psi\ . \tag{4.1}$$

Repeating the technical procedures used in deriving Eq. (2.6) for the lattice Hamburger moments, one obtains the sextic moment's equation,

$$\bar{u}(p+6)=E\bar{u}(p)-\bar{u}(p+2)+2(\varepsilon/a)^2\sum_{\substack{i=2,\\ \text{and even}}}^{p}a^iB(p,i)\bar{u}(p-i)\ . \tag{4.2}$$

TABLE V. Eigenvalue bounds for the lattice harmonic oscillator ($a=5$, $\varepsilon=1$). These results were obtained by rescaling the Stieltjes moments according to $u(p)/a^{2p}$, thus avoiding large numbers. The Hankel-Hadamard relations are unchanged. Refer to Eq. (3.1).

$p_{\max}$	Lower bound	Upper bound
6	0.066	6.339 96
⋮	unchanged	unchanged
20	0.066	6.339 96

For the symmetric ground state, we may work with the Stieltjes moments corresponding to $u(p)\equiv\bar{u}(2p)$, for $p\ge0$. The moment equation for $u(p)$ is given by

$$u(p+3)=Eu(p)-u(p+1)+2(\varepsilon/a)^2\sum_{i=1}^{p}B(2p,2i)a^{2i}u(p-i)\ . \tag{4.3}$$

The above moment equation corresponds to a third-order finite-difference equation. The three initial values $u(0-2)$, the "missing moments," must be specified before all the remaining moments can be generated. The energy E appears as a parameter in the difference equation. Because of the homogeneous nature of Eq. (4.3), we are free to choose any normalization, so long as it is consistent with the underlying non-negativity of the physical solution. Contrary to the simple choice $u(0)=1$ adopted for the harmonic oscillator, it will be necessary to choose

$$\sum_{p=0}^{2}u(p)=1\ . \tag{4.4}$$

Note that the missing moments are automatically bounded, $0<u(0-2)<1$.

In principle, we could use the Hankel-Hadamard determinant inequalities to constrain and determine the physical values for the energy and the missing moments. Practically, this would involve a three-parameter search (E, and two independent missing moments) in order to determine where the *nonlinear* Hankel-Hadamard inequalities are satisfied. This is very inefficient. Problems involving three or more independent missing moments become impossible. Indeed, all multidimensional problems involve an infinite hierarchy of missing moments.[5–7] Because of this, in Refs. 6 and 7 we reformulated the nonlinear Hankel-Hadamard moment method in terms of an *equivalent* linear theory in the missing moments.

Two important theoretical and practical factors enable us to develop an equivalent linear formulation of the nonlinear Hankel-Hadamard moment method. The first of these is outlined in the context of Eqs. (4.7) and (4.8). It makes use of well-known linear inequality relations traditionally used in deriving the nonlinear Hankel-Hadamard inequalities.[12,13]

The second important factor is the use of the powerful theory of linear programming[15] to determine if for a given energy value there cannot exist (infeasibility) a solution to the aforementioned set of linear inequalities. We outline below the basic structure of the linearized moment method.

The missing moments will become the "independent variables" in our linear formalism. These variables must be bounded in order to be able to use linear programming methods; thus the reason for choosing Eq. (4.4).

The dependence of the $u(p)$'s on the missing moments may be represented by

$$u(p)=\sum_{q=0}^{2}M(E;p,q)u(q)\ , \tag{4.5a}$$

where

$$M(E;p,q)=\delta_{p,q}\quad\text{for } 0\le p,q\le2\ . \tag{4.5b}$$

The M matrices are only dependent upon the energy, and can be generated through the moment equation (4.3) upon making use of the initialization conditions in Eq. (4.5b). The constraint relation in Eq. (4.4) allows us to solve for $u(0)$ in terms of the other missing moments. We can incorporate this into Eq. (4.5a), obtaining

$$u(p)=\sum_{q=0}^{2}\hat{M}(E;p,q)\hat{u}(q)\ , \tag{4.6a}$$

where

$$\hat{u}(q)=\begin{cases}1 & \text{if } q=0\\ u(q) & \text{if } q=1,2\end{cases} \tag{4.6b}$$

and

$$\hat{M}(E;p,q)=\begin{cases}M(E;p,0) & \text{if } q=0\\ M(E;p,q)-M(E;p,0) & \text{if } q=1,2\ .\end{cases} \tag{4.6c}$$

Let $N(L)$ denote a non-negative lattice function. We can define an associated discrete distribution by

$$D(y)=\sum_{L=-\infty}^{+\infty}aN(L)\delta(y-aL)\ .$$

The Hankel-Hadamard determinant inequalities [refer to Eq. (2.11)] express the necessary and sufficient conditions in order for $D(y)$ [or equivalently, $N(L)$] to be non-negative. These inequalities are traditionally derived from the following equivalent relations:[12,13]

$$\int_{-\infty}^{\infty}dy\left[\sum_{i=0}^{I}C_i y^i\right]^2 D(y)\geq 0 \quad \text{for all } C\text{'s and } I\geq 0\ , \tag{4.7a}$$

or alternatively, using $u(p)=\int_{-\infty}^{\infty}dy\,y^p D(y)$,

$$\sum_{i=0}^{I}\sum_{j=0}^{I}C_i u(i+j)C_j\geq 0 \quad \text{for all } C\text{'s and } I\geq 0\ . \tag{4.7b}$$

The imposition of Eq. (4.7b) on $D(y)$ and $yD(y)$ would guarantee that $D(y)=0$, for $y<0$, and $D(y)\geq 0$, for $y=0$. Thus, for a Stieltjes distribution, the following quadratic form constraints insure non-negativity on the non-negative lattice axis:

$$\sum_{i=0}^{I}\sum_{j=0}^{I}C_i' u(i+j)C_j'\geq 0 \tag{4.8a}$$

and

$$\sum_{i=0}^{I}\sum_{j=0}^{I}C_i'' u(1+i+j)C_j''\geq 0$$

$$\text{for all } C''\text{s, } C'''\text{s, and } I\ . \tag{4.8b}$$

Inserting Eq. (4.6a) into Eqs. (4.8) yields the following infinite number of linear inequality constraints for the missing moments, at any arbitrary E value:

$$\sum_{q=1}^{2}-u(q)\sum_{i=0}^{I}\sum_{j=0}^{I}C_i'\hat{M}(E;i+j,q)C_j'$$

$$\leq\sum_{i=0}^{I}\sum_{j=0}^{I}C_i'\hat{M}(E;i+j,0)C_j'\ , \tag{4.9a}$$

$$\sum_{q=1}^{2}-u(q)\sum_{i}^{I}\sum_{j=0}^{I}C_i''\hat{M}(E;1+i+j,q)C_j''$$

$$\leq\sum_{i=0}^{I}\sum_{j=0}^{I}C_i''\hat{M}(E;1+i+j,0)C_j''\ . \tag{4.9b}$$

For future reference, we also include the bounds $u(0-2)<1$, or

$$\sum_{q=1}^{2}\hat{M}(E;p,q)u(q)<1-\hat{M}(E;p,0)\quad \text{for } p=0,1,2\ . \tag{4.9c}$$

The above infinite set of linear inequalities [with respect to the independent variables $u(1)$ and $u(2)$] will only have a solution for the exact physical energy value.[4] A rigorous proof of this, with respect to the equivalent Hankel-Hadamard formulation, has been established by Ashbaugh and Sundberg.[16] Clearly, in order to determine if a given energy value is unphysical, it is not necessary to solve the uncountably infinite number of inequalities. If one can determine a finite subset of C' and C'' vectors (each of finite dimension) for which the associated inequality relations are invalid, then one can say that the given energy value is unphysical. In Refs. 6 and 7, Handy and co-workers describe a "cutting" procedure for quickly determining such optimal finite subsets of C vectors. As indicated earlier, it is at this stage that the methods of linear programming are used.

Linear programming is concerned with the following two issues.

(1) Determining the existence (feasibility) or nonexistence (infeasibility) of a solution set to the generic linear inequality problem

$$A\mathbf{X}\leq\mathbf{B}\ ,$$

where A and $\mathbf{B}$ are a given matrix and vector, respectively (the solution set is a convex "polytope" bounded by intersecting hyperplanes).

TABLE VI. Ground state for discretized sextic oscillator.

Lattice spacing a	Feasible energy interval	$p_{\max}$	n_{dx}
0	(1.41,1.47)	8	12
	(1.423,1.438)	10	20
	(1.4352,1.4364)	12	34
	(1.4355,1.4357)	14	39
0.01	(1.41,1.47)	8	20
	(1.423,1.438)	10	22
	(1.4352,1.4364)	12	33
	(1.4355,1.4357)	14	40
0.1	(1.40,1.46)	8	21
	(1.421,1.436)	10	23
	(1.4331,1.4344)	12	30
	(1.4334,1.4337)	14	42
1	(1.17,1.30)	8	18
	(1.19,1.27)	20	42

(2) Optimizing some given linear "objective" function within the solution set.

In most texts, it is the optimization aspect which receives the greatest attention. An objective function is not explicitly ingrained in the equations corresponding to Eq. (4.9). It is clear that these relations are concerned with feasibility [existence of a $u(1),u(2)$ convex subdomain]. Despite this, the specification of certain appropriate objective functions is crucial in the deployment of the cutting methods in Refs. 6 and 7. A central aspect of such cutting techniques is locating a "deep" interior point for a given polytope. In Ref. 6, the deep interior point is taken to be the average over all "extremal vertices." In Ref. 7, the deep interior point is defined by the center of the largest sphere that can be inscribed within the given polytope. The latter is a faster procedure (by at least a factor of two times the number of missing moments). It is the one adopted in this work.

The numerical results for the discretized sextic anharmonic oscillator are cited in Table VI. Note that the parameter $p_{\max}$ corresponds to the maximum moment order generated $[M(E;p,q)$ for $p \leq p_{\max}]$, while, n_{dx} is the approximate number of C' and C'' vectors required to determine infeasibility. For the continuum case, $a=0$, the cited ground-state energy agrees with those of Hioe *et al.*[17]

CONCLUSION

We have extended the moment method for generating rapidly converging eigenvalue bounds to the discretized Schrödinger equation. Essential to this program is the development of a linear programming reformulation of the original Hankel-Hadamard formalism. This enables us to solve any multidimensional, linear quantum system, regardless of the number of missing moments.

In addition to the above theoretical interests, the present lattice formulation encourages us to solve *nonlinear* problems by combining the moment methods of the present work with the lattice high-temperature expansion techniques of Bender *et al.*[2] The moments of certain nonlinear problems can be generated through such methods.[3]

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[1]M. Creutz, Phys. Rev. Lett. **45**, 313 (1980).
[2]C. M. Bender, F. Cooper, G. S. Guralnik, and D. H. Sharp, Phys. Rev. D **19**, 1865 (1979).
[3]C. R. Handy, Phys. Rev. D **24**, 378 (1981).
[4]C. R. Handy and D. Bessis, Phys. Rev. Lett. **55**, 931 (1985).
[5]D. Bessis and C. R. Handy, Int. J. Quantum Chem. Symp. **20**, 21 (1986).
[6]C. R. Handy, D. Bessis, and T. D. Morley, Phys. Rev. A **37**, 4557 (1988).
[7]C. R. Handy, D. Bessis, G. Sigismondi, and T. D. Morley, Phys. Rev. Lett. **60**, 253 (1988).
[8]W. F. Ames, *Numerial Methods for Partial Differential Equations* (Academic, New York, 1977).
[9]K. M. Case and M. Kac, J. Math. Phys. **14**, 594 (1973).
[10]M. Reed and B. Simon, *Methods of Modern Mathematical Physics* (Academic, New York, 1978).
[11]C. M. Bender and S. A. Orzag, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978).
[12]J. A. Shohat and J. D. Tamarkin, *The Problem of Moments* (American Mathematical Society, Providence, RI, 1963).
[13]G. A. Baker, Jr., *Essentials of Padé Approximants* (Academic, New York, 1975).
[14]C. R. Handy, G. Mantica, and J. B. Gibbons, Phys. Rev. A (to be published).
[15]V. Chvatal, *Linear Programming* (Freeman, New York, 1983).
[16]M. Ashbaugh and C. Sundberg (private communication of a joint collaboration between the Departments of Mathematics of the University of Missouri and the University of Tennessee, respectively).
[17]F. T. Hioe, D. MacMillen, and E. W. Montroll, J. Math. Phys. **17**, 1320 (1976).