Rapidly Convergent Lower Bounds for the Schrödinger-Equation Ground-State Energy

Carlos R. Handy
Department of Physics, Atlanta University, Atlanta, Georgia 30314

and

Daniel Bessis[(a)]
School of Mathematics, Georgia Institute of Technology, Atlanta, Georgia 30332
(Received 18 March 1985)

We present a new and fundamental approach for generating rapidly convergent lower and upper bounds to the ground-state energy of a bosonic system, E_g. The bosonic ground-state wave function defines a moments problem because it both is nonnegative and exhibits rapid asymptotic decrease. Through the use of the Hankel-Hadamard determinant inequalities associated with this moments problem one can constrain E_g through exponentially convergent bounds. Extensions to excited bosonic states and fermionic systems are briefly outlined.

PACS numbers: 31.15.+q, 02.30.+g, 03.65.Ge

The development of effective methods for generating rapidly convergent *lower* and upper bounds to the quantum ground-state energy, E_g, has been an important problem for many decades.[1] Until now, this problem had remained unsolved. Although there are many other techniques for calculating eigenvalues, none of these can give systematically convergent bounds; therefore, most eigenvalue estimates are inaccurate. This is an important concern for the two-dimensional *Zeeman* problem with superstrong magnetic fields.[2,3] The multidimensional generalization of our approach will be applied to this important problem in future works. Nonetheless, the superstrong-magnetic-field case for the *spherically symmetric Zeeman* problem is readily solved here. The *laser physics* problem of Lai and Lin[4] affords an example of the shortcomings of some eigenvalue calculation schemes. Their combined Padé, Hellman-Feynman hypervirial analysis leads to $E_g = 1.017\,281\,60$ ($\lambda = 0.1$, $g = 2$); however, a more accurate answer is provided by our method,[5] $1.017\,176 < E_g < 1.017\,185$.

We present our approach in the context of one-dimensional quantum systems with rational-fraction potential functions. Many important problems in *charmonium physics* and *atomic physics* are of this type, including the spherically symmetric Zeeman problem.[6] In addition, many polynomial-potential problems, such as the quartic[7] and sextic[3] potentials, have played a fundamental theoretical role in our understanding of strongly coupled quantum systems. These two cases are solved here through our approach. As has been argued by Handy,[8,9] moments are relevant to *strong-coupling physics.* As such, because the *moments problem*[10–12] plays a key role in our method, it is not too surprising that our technique is so effective for many strong-coupling quantum problems.

We will focus on bosonic ground states because the associated wave function is nonnegative[13] in a coordinate-basis representation. However, our method is extendable to any system (i.e., excited bosonic states, fermionic states) once the signature properties of the associated wave function are known. For example, because the nth excited bosonic state must have n nodes,[14] we may represent it in the form $\Psi_n = P_n(x) \times F(x)$, where $F(x)$ is nonnegative, and P_n is an n-degree polynomial. The coefficients of P_n and E_n, the eigenvalue, can then be determined through our method. Some examples of this are given in a related work by Handy and Msezane.[15]

Consider a d-dimensional bosonic quantum system with wave function $\Psi(\mathbf{x})$. The Hamburger moments are defined as

$$\mu(n_1, \ldots, n_d) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \prod_{i=1}^{d} x_i^{n_i} \Psi(\mathbf{x})\, dx_1 \cdots dx_d. \tag{1}$$

The asymptotic properties of the ground-state bosonic wave function, Ψ_g, insure that the corresponding Hamburger moments exist.[16,17] In addition, the nonnegativeness[13] of Ψ_g permits us to normalize things according to $\mu(\mathbf{0}) = 1$. The combination of these two facts (existence of moments, nonegativity of Ψ_g) define a moments problem through which eigenvalue quantization, through convergent bounds, is possible. We demonstrate this through the class of one-dimensional rational-fraction–potential problems.

We denote by $V(x) = N(x)/D(x)$ the rational-fraction potential function involving $N(x) = \sum_{k=0}^{p} n_k \times x^k$ and $D(x) = \sum_{k=0}^{q} d_k x^k$. The associated normalized Schrödinger equation is $-D(x)\Psi'' + [N(x) - E_g D(x)]\Psi = 0$. Through the necessary "integration by parts" analysis, a recursive relation for the Hamburger moments follows:

$$-\left[\sum_{k=0}^{q} d_k (m+k)(m+k-1)\mu_{m+k-2}\right] + \sum_{k=0}^{p} n_k \mu_{m+k} - E_g \left(\sum_{k=0}^{q} d_k \mu_{m+k}\right) = 0. \tag{2}$$

The Schrödinger equation admits physical and unphysical (unbounded) solutions. Only the former are implicitly assumed in Eq. (2); otherwise infinite asymptotic "boundary" terms would be present. If we set $m=0$ in Eq. (2), the highest-order moment μ_t, $t=\max\{p,q\}$, is seen to depend on all the lower-order moments $\mu_{t-1},\ldots,\mu_1$ and on E_g. Once these are specified, all the higher-order moments are determined. We call this the "missing moment problem."

For parity-invariant systems $\Psi(x)$ is symmetric; thus, only even-order Hamburger moments are nonzero. These are equivalent to the Stieltjes moments of a different function measure. Specifically, through a simple change of variables one has $\hat{\mu}_p=\mu_{2p}$, where $\hat{\mu}_p=\int_0^\infty y^p[\Psi(\sqrt{y})/\sqrt{y}]dy$. The Stieltjes moment problem tells us[10-12] that the Hankel-Hadamard determinant inequalities express the necessary and sufficient conditions for a sequence of numbers to be the moments of a nonnegative function. The Hankel-Hadamard determinants are defined as follows:

$$\Delta(m,n)=\det\begin{vmatrix}\hat{\mu}_m & \hat{\mu}_{m+1} & \cdots & \hat{\mu}_{m+n}\\ \vdots & & & \vdots\\ \hat{\mu}_{m+n} & \hat{\mu}_{m+n+1} & \cdots & \hat{\mu}_{m+2n}\end{vmatrix}. \tag{3}$$

The specific inequalities of concern to us are $\Delta(0,n)>0$ and $\Delta(1,n)>0$, for $n\geqslant 0$. Given the first $M+1$ $\hat{\mu}$ moments, it is apparent from Eq. (3) that all of the determinants $\Delta(0,n)$, for $0\leqslant 2n\leqslant M$, and $\Delta(1,n)$, for $0\leqslant 2n\leqslant M-1$, are calculable. We shall study how successive increases in M lead to improved bounds for the true ground-state energy and any missing moments. An examination of the data shows that as more and more determinant inequalities are used, stronger constraints, more restrictions, are being imposed on E_g, etc. These constraints come from the requirement that all of the relevant determinant inequalities be satisfied *simultaneously*.

For the harmonic-oscillator problem, $-\Psi''+\frac{1}{4}x^2\Psi=E_g\Psi$, the Stieltjes moment recursion relation is $\hat{\mu}_{p+1}=4[E_g\hat{\mu}_p+2p(2p-1)\hat{\mu}_{p-1}]$. It follows that $\hat{\mu}_1=4E_g$, $\hat{\mu}_2=(4E_g)^2+8$, $\hat{\mu}_3=(4E_g)^3+56(4E_g)$, and $\hat{\mu}_4=(4E_g)^4+176(4E_g)^2+960$. The first nontrivial Hankel-Hadamard determinant inequality is $\Delta(1,0)>0$, or $E_g>0$. It also follows that $\Delta(1,1)=40\times(4E_g)^2-64$ and $\Delta(0,2)=-1024[(4E_g)^2-7]$. The $\Delta(1,1)>0$ and $\Delta(0,2)>0$ inequalities yield the bounds $0.3162<E_g<0.6615$ for the ground state. The higher-order determinants are polynomials in E_g and can be numerically determined. All higher-order determinant numerical analysis can be restricted to the above interval for E_g.

Given the first $m+1$ moments $\hat{\mu}_0,\ldots,\hat{\mu}_m$ we let $E_m^{(\pm)}$ denote the upper and lower bounds on the true ground-state energy E_g^*. For the harmonic-oscillator case, Table I contains the positive deviations $\delta_m^{(\pm)}$ relative to $E_g^*=\frac{1}{2}$. It will be noted that as the number of moments is increased by one, only one of the bounds is improved; furthermore, this pattern alternates between the lower and upper bounds. Because of this, it is convenient to define the "deviation parameters" in accordance with

TABLE I. Deviations from exact ground-state energy $E_g^*=\frac{1}{2}$ for $V(x)=\frac{1}{4}x^2$. m is the maximum order of moments used.

m	$\delta_m^{(-)}=E_g^*-E_m^{(-)}$	$\delta_m^{(+)}=E_m^{(+)}-E_g^*$
10	5×10^{-3}	1×10^{-3}
11	1×10^{-3}	1×10^{-3}
12	1×10^{-3}	1×10^{-4}
13	1×10^{-4}	1×10^{-4}
14	1×10^{-4}	1×10^{-5}

$$\delta_m^{(\pm)}=c_\pm 10^{-\alpha_\pm m},\quad m=\text{even}. \tag{4}$$

The data in Table I correspond to $c_\pm\simeq 1$ and $\alpha_\pm\simeq 0.3$, thereby manifesting an exponential convergence.

The sextic-potential problem $V=mx^2+gx^6$ $(g>0)$ has a symmetric ground state. A Stieltjes formulation follows, resulting in the recursive moment relation

$$\hat{\mu}_{p+3}=g^{-1}[E_g\hat{\mu}_p-m\hat{\mu}_{p+1}+2p(2p-1)\hat{\mu}_{p-1}],$$

where E_g, $\hat{\mu}_1$, and $\hat{\mu}_2$ are undetermined. This two-missing-moment problem can be reduced to a zero-missing-moment problem through the transformation $e^S\Psi=\Phi$, where $S=-\frac{1}{4}g^{1/2}x^4$.

A simple analysis of the sextic problem gives us the asymptotic form of the general solution, $\Psi(x)\simeq\exp(\pm\frac{1}{4}g^{1/2}x^4)$. Unphysical solutions correspond to $+\frac{1}{4}$. If a Hankel-Hadamard approach is to yield useful lower energy bounds then the transformation $\Psi\rightarrow\Phi$ must insure that the Φ-space recursive moment equations do not admit unphysical solutions. This means that $\Psi_{\text{unphysical}}$ must have *infinite* Φ moments, $\mu_p=\int x^p\Phi\,dx$. Also note that the uniqueness of the nonnegativity of the ground state is preserved under $\Psi\rightarrow\Phi$.

The ensuing Stieltjes moments for Φ satisfy $\hat{\mu}_{p+1}=U(p)/\Omega(p)$, where $\Omega(p)=g^{1/2}(4p+3)+m$, $U(p)=E_g\hat{\mu}_p+2p(2p-1)\hat{\mu}_{p-1}$. As long as $g>0$ a ground state must exist, and its moments must be finite and nonzero. The $\Omega(i)$ denominator can vanish if $m=-g^{1/2}(4i+3)$, for integer i. It must then follow that $U(i)=0$. For $i=0,1$ this type of analysis leads to $E_g=0$ and $E_g=-2\sqrt{2}g^{1/4}$, respectively.

The lower-order determinants yield the bounds

TABLE II. Deviations from exact ground-state energy $E_g^* = 1.435\,6247$ for $V(x) = x^2 + x^6$.

m	$\delta_m^{(-)} = E_g^* - E_m^{(-)}$	$\delta_m^{(+)} = E_m^{(+)} - E_g^*$
10	0.62×10^{-3}	0.18×10^{-3}
11	0.12×10^{-3}	0.18×10^{-3}
12	0.12×10^{-3}	0.15×10^{-4}
13	0.47×10^{-5}	0.15×10^{-4}
14	0.47×10^{-5}	0.13×10^{-5}

$[\Gamma = (3g^{1/2} + m)2^{-1/2}g^{-1/4}]$

$$0 < E_g < \Gamma, \quad \text{for } m > -3g^{1/2}, \tag{5}$$

$$\Gamma < E_g < 0, \quad \text{for } -7g^{1/2} < m < -3g^{1/2}, \tag{6}$$

$$E_g < \Gamma, \quad \text{for } m < -7g^{1/2}. \tag{7}$$

Equation (5) follows from $\Delta(0,1) > 0$ and $\hat{\mu}_1 > 0$. Examination of $\Delta(1,1) > 0$ leads to $-2g^{1/2}E_g^4 + \beta E_g^2 - 2D_1^2 D_3 > 0$, where $\beta = D_1 D_2 + 6D_2^2 - 2D_1 D_3$ and $D_i = g^{1/2}(4i-1) + m$. For the case $m = g = 1$ one obtains thereby the bounds $1.0997 < E_g < 2.8285$. All higher-order determinant numerical analysis can be restricted to this interval. The data in Table II confirm an exponential rate of convergence to the value $E_g^* = 1.435\,6247$ of Hioe, MacMillen, and Montroll,[18] where $c_\pm \simeq 1$ and $\alpha_\pm \simeq 0.4$.

The Bohr atom, $r\Phi'' + (\gamma - \frac{1}{4}r)\Phi = 0$ $[\Phi(0) = 0]$,[19] corresponds to a rational-fraction potential problem which is purely Stieltjes, whose moments satisfy $\mu_{m+1} = 4[\gamma\mu_m + m(m+1)\mu_{m-1}]$. The lower-order determinant inequalities yield the bounds $0.50 < \gamma < 1.59$. The true value is $\gamma = 1$. Table III supports an exponential rate of convergence; $c_- \simeq 3$, $c_+ \simeq 6$, and $\alpha_\pm \simeq 0.3$.

The spherically symmetric Zeeman problem,[6] $-\frac{1}{2}\nabla^2\Psi - (Z/r)\Psi + \lambda r^2\Psi = E\Psi$, becomes a zero-missing-moment problem upon working with the moments of $F(r) = re^{-\alpha r^2}\Psi$, where $\alpha = (\lambda/2)^{1/2}$. The associated recursion relation is

$$\mu_{m+1} = [Z\mu_m + \tfrac{1}{2}m(m+1)\mu_{m-1}]/D_m,$$

$$D_m = \alpha(2m+3) - E.$$

From the requirement that the moments be positive, it follows that $E_g < 3\alpha$. The lower-order determinant inequalities bound E_g to $\tilde{E} < E_g < 3\alpha - Z(2\alpha)^{1/2}$, where $\tilde{E}$ corresponds to the most-positive-root solution of the cubic polynomial $(x = 3\alpha - \tilde{E})$

$$-x^3 + (2Z^2 - 4\alpha)x^2 + 6\alpha Z^2 x + [12(\alpha Z)^2 - 2\alpha Z^4] > 0.$$

For the superstrong-magnetic-field case, $\lambda = 1$ and $Z = 1$, we get $0.593\,7711 < E_g < 0.593\,7717$ on the basis of using the first fifteen moments. For $\lambda = 1$, $Z = 3$, $-4.197\,8716 < E_g < -4.197\,8712$, with use of nineteen moments. For $\lambda = 0.1$, $Z = 1$, $-0.296\,0880 < E_g < -0.296\,0870$, with use of fifteen moments. In all cases there was monotonic convergence. Table III has the pertinent data for the superstrong-field case; $c_+ \simeq 6$, $c_- \simeq 1$, $\alpha_+ \simeq 0.5$, $\alpha_- \simeq 0.4$.

TABLE III. Deviations from the ground-state energy $\gamma^* = 1$, $E^* = 0.593\,77$, for the Bohr and Zeeman atomic potentials, respectively ($Z = 1$, $\lambda = 1$).

m	$\delta_m^{(-)} = \gamma^* - \gamma_m^{(-)}$	$\delta_m^{(+)} = \gamma_m^{(+)} - \gamma^*$	$(\delta_E^{(-)})_m$	$(\delta_E^{(+)})_m$
10	2×10^{-2}	4×10^{-3}	4×10^{-4}	6×10^{-5}
11	3×10^{-3}	4×10^{-3}	2×10^{-5}	6×10^{-5}
12	3×10^{-3}	6.4×10^{-4}	2×10^{-5}	6×10^{-6}
13	3.3×10^{-4}	6.4×10^{-4}	1×10^{-6}	6×10^{-6}

The quartic anharmonic oscillator, $-\Psi'' + (mx^2 + x^4)\Psi = E_g\Psi$, leads to a one-missing-moment problem for its Stieltjes moments,

$$\hat{\mu}_{p+2} = [E_g\hat{\mu}_p - m\hat{\mu}_{p+1} + 2p(2p-1)\hat{\mu}_{p-1}].$$

The determinant inequalities simultaneously constrain E_g and $\hat{\mu}_1$. In particular, $\Delta(0,1) > 0$ yields the bound $E_g > \hat{\mu}_1(m + \hat{\mu}_1)$; thereby duplicating the well-known theorem $E_g > \text{Infinum}\{V\}$. The inequality $\Delta(1,1) > 0$ leads to $E_g^2 - E_g\hat{\mu}_1(m + \hat{\mu}_1) - 2\hat{\mu}_1 < 0$. Combining these two Δ inequalities results in $e_1 < E_g < \frac{1}{2}[e_1 + (e_1^2 + 8\hat{\mu}_1)^{1/2}]$, where $e_1 = \hat{\mu}_1(m + \hat{\mu}_1)$. The numerical behavior of the higher-order determinant inequalities further constrains E_g to a value consistent with that quoted in Ref. 3, $E_g^* = 1.060\,3621$. The data in Table IV show the exponential convergence resulting from the use of the first fifteen moments: $c_\pm^{(E,\mu)} \simeq 1$, $\alpha_\pm^{(E,\mu)} \simeq 0.3$. The superscripts refer to the energy and moment entries. Our actual numerical analysis involved the first 22 moments, leading to continued exponential convergence to the values $1.060\,362\,05 < E_g < 1.060\,362\,10$ and $0.635\,924\,42$

TABLE IV. Deviations for E_g and $\hat{\mu}_1$ from the ground-state values $E_g^* = 1.060\,362\,09$ and $\hat{\mu}_1^* = 0.635\,924\,43$ for $V(x) = x^4$.

m	$(\delta_E^{(-)})_m$	$(\delta_E^{(+)})_m$	$(\delta_\mu^{(-)})_m$	$(\delta_\mu^{(+)})_m$
10	0.14×10^{-2}	0.16×10^{-2}	0.19×10^{-2}	0.11×10^{-2}
11	0.14×10^{-2}	0.54×10^{-3}	0.22×10^{-3}	0.28×10^{-3}
12	0.14×10^{-3}	0.52×10^{-3}	0.12×10^{-3}	0.24×10^{-3}
13	0.14×10^{-3}	0.18×10^{-4}	0.12×10^{-3}	0.36×10^{-4}
14	0.22×10^{-4}	0.18×10^{-4}	0.14×10^{-5}	0.30×10^{-4}

$< \hat{\mu}_1 < 0.635\,924\,44$.

Clearly, the scope of our approach is quite extensive. Its extension to the multidimensional realm will be the subject of future works.

We express our appreciation to Professor W. Ames, Professor M. Barnsley, Professor J. Geronimo, Professor E. Harrell, Professor A. Msezane, and Professor E. R. Vrscay for fruitful discussions. The work of one of us (C.R.H.) was supported in part by a National Science Foundation Grant RII-8312.

[(a)]On leave from Centre d'Etudes Nucléaires de Saclay, Saclay, France.

[1]M. F. Barnsley, J. Phys. A **11**, 55–68 (1978); L. Nitti, M. Pellicoro, and M. Villani, J. Math. Phys. **21**, 834 (1980); M. Barnsley and G. Turchetti, Comput. Phys. Commun. **22**, 325 (1981); A. Weinstein, Mem. Sci. Math. No. 88 (1937); P. O. Löwdin, Phys. Rev. **139**, A357 (1965); F. Ortolani and G. Turchetti, J. Phys. B **11**, L207 (1978); G. Turchetti, F. Ortolani, and C. Sagretti, Nuovo Cimento **44A**, 211 (1978).

[3]J. Cizek and E. R. Vrscay, Int. J. Quant. Chem. **21**, 27 (1982).

[4]C. S. Lai and H. E. Lin, J. Phys. A **15**, 1495 (1982).

[5]C. R. Handy, to be published.

[6]E. R. Vrscay, Phys. Rev. Lett. **53**, 2521–2524 (1984).

[7]C. M. Bender and T. T. Wu, Phys. Rev. **184**, 1231 (1969).

[8]C. R. Handy, Phys. Rev. D **24**, 378 (1981).

[9]C. R. Handy, Phys. Rev. D **31**, 3168 (1985).

[10]N. I. Akhiezer, *The Classical Moment Problem and Some Related Questions in Analysis* (Oliver and Boyd, Edinburgh, 1965).

[11]G. A. Baker, Jr., *Essentials of Padé Approximants* (Academic, New York, 1975).

[12]J. A. Shohat and J. D. Tamarkin, *The Problem of Moments* (American Mathematical Society, Providence, R.I., 1963).

[13]M. Reed and B. Simon, *Methods of Modern Mathematical Physics,* (Academic, New York, 1978), p. 206, Theorem XIII-46.

[14]A. Messiah, *Quantum Mechanics,* translated by G. M. Temmer (Wiley-Interscience, New York, 1961), Vol. 1, Chap. 3, Sect. 12.

[15]C. R. Handy and A. Msezane, to be published.

[16]Shmuel Agmon, *Lectures on the Exponential Decay of Solutions of Second Order Elliptic Equations,* Mathematical Notes Series No. 29 (Princeton Univ. Press, Princeton, N.J., 1983).

[17]I. M. Glazman, *Direct Methods of Qualitative Spectral Analysis of Singular Differential Operators* (Israel Program for Scientific Translation, Jerusalem, 1969), p. 179, Theorem 1.

[18]F. T. Hioe, D. MacMillen, and E. W. Montroll, J. Math. Phys. **17**, 1320 (1976).

[19]R. M. Eisberg, *Fundamentals of Modern Physics* (Wiley, New York, 1967).