PHYSICAL REVIEW A

GENERAL PHYSICS

THIRD SERIES, VOLUME 37, NUMBER 12 JUNE 15, 1988

Generating quantum energy bounds by the moment method: A linear-programming approach

C. R. Handy and D. Bessis*
Department of Physics, Atlanta University, Atlanta, Georgia 30314-4391

T. D. Morley
School of Mathematics, Georgia Institute of Technology, Atlanta, Georgia 30332
(Received 24 March 1987)

Recently, Handy and Bessis derived, for singular multidimensional Schrödinger equations, infinite sets of hierarchical inequalities fulfilled by the moments of the ground-state wave function. These inequalities, when increasing in number, provide tighter lower and upper bounds to the ground-state energy. This analysis makes use of nonlinear multivariate determinant functionals (Hankel-Hadamard determinants) which define complicated convex sets in the space of the "missing moments." It is possible to reformulate all the above in terms of *linear programming*. The previous sets are now replaced by new sets defined by *linear inequalities*. This new formulation makes the general moment approach highly practical. We describe the general formalism and give a simple one-dimensional example to illustrate it. The three-dimensional quadratic Zeeman problem, in the transition region, is analyzed by this method. Preliminary results for values of the magnetic field $B=0.2$, 2, and 20 (in atomic units) are given.

I. INTRODUCTION

In an earlier work Handy and Bessis[1] showed how a moment analysis for bosonic systems led to the generation of rapidly convergent *lower and upper bounds* to quantum eigenvalues. This approach is particularly effective for strongly coupled systems requiring some type of singular perturbation analysis.[2]

The need for such methods as the above is self-evident, for without bounds no absolute statements of accuracy can be made. Also, the results of our method when applied to many strong coupling problems[3-6] greatly complement conventional perturbation-theory techniques. In addition to these, the moment approach enjoys several other important properties.

(i) The moment method is readily applicable to unbounded, or otherwise singular, potentials, as demonstrated in Sec. IV.

(ii) The presence of a continuum spectrum (scattering states) in the Hamiltonian does not affect the moment formulation. Those scattering states are projected out in an *exact* manner. This property is an important one. Some methods are affected by the existence of a continuous part to the spectrum of the Hamiltonian operator. This is discussed in a recent work by Cizek and Vrscay.[7]

(iii) The moment method applies to excited states, provided the nodal zones are known. For instance, in some three-dimensional problems considerations of parity will determine the nodal zone of the first excited state. For one-dimensional problems, one takes as unknown the nodes of the excited state; the method then provides bounds to the location of the nodes and to the energy of the excited state.

The original moment formulation[1] made use of nonlinear moment inequality constraints involving Hankel-Hadamard determinants,

$$\Delta_{m,n}\{u\}>0\ , \tag{1.1}$$

dependent upon the moments $\{u\}$ of the ground-state wave function for the system in question. Refer to the Appendix for a discussion of the "moment problem"[8] and the definition and properties of the Hankel-Hadamard (HH) determinants. The HH determinants, symbolized by Eq. (1.1), correspond to *nonlinear* multivariate functionals of the moments.

For many finite-dimensional quantum systems, the moments will satisfy a recursive homogeneous linear difference equation in which the energy appears as a parameter. The order and dimensionality of this linear difference equation will determine the number of initial moments that must be specified before all other moments can be determined. We designate the former as *missing moments*. Clearly, all remaining moments will be linearly

dependent upon the missing moments.

It follows from the discussion above that the HH determinants will become nonlinear multivariate functionals of the missing moments and energy. It has been argued in Ref. 1 that the only solution to the HH inequalities corresponds to the physical ground-state energy and missing-moment values. At the practical level, for a given finite set of HH inequalities and arbitrary energy value one must determine if there *exists* or *not* a missing moment subset that can satisfy all the HH inequalities. If such a subset exists, then the associated energy value is a possible physical value. If no subset exists, then the associated energy value is physically impossible. In the case of singular strong coupling quantum systems, it has been our experience that relatively few HH inequalities need to be considered in order to determine an accurate answer for the physical ground-state energy. Furthermore, the accuracy obtainable is dramatic because it comes by way of *rapidly converging lower and upper bounds.*

Given an arbitrary energy value, the determination of the feasibility (existence) or infeasibility (nonexistence) of a missing moment subset, consistent with the HH inequalities, is generally difficult through a direct analysis of the nonlinear multivariate Hankel-Hadamard determinant functionals. For quantum systems with at most three missing moments one can do this. Some theoretically important problems fall in this category.[3-6] Unfortunately, for many one-dimensional problems, and for all multidimensional systems, this is not the case. Indeed, the latter will always involve an infinite number of missing moments.

The principal objective of this work is to develop an equivalent *linear formulation* to the HH moment method for calculating rapidly converging lower and upper bounds to the bosonic ground-state eigenvalue.[1] As will be shown in the following sections, such a linear reformulation is possible through the theory of *linear programming.*[9] The development and use of linear programming techniques has been very prominent in mathematics, economics, and operations research.

The impact of the linearization program to the general moment method is important. It allows for far-reaching practical applications to multidimensional quantum systems. In this paper we shall concentrate on one of these, the quadratic Zeeman effect for strong magnetic fields.[7,10] This problem has been the focus of much theoretical research for the past 25 years, as documented in the comprehensive work by Le Guillou and Zinn-Justin.[10]

In Sec. II we give a comprehensive overview of the essential logical structure of the linear-programming reformulation. An explicit one-dimensional example is considered in Sec. III, that of the sextic potential. Finally, in Sec. IV we extend the method to the three-dimensional quadratic Zeeman problem. For this problem we can obtain unprecedented energy bounds for magnetic field strengths B in the "transition regime" ($B \geq 1$, measured in atomic units). More efficient codes are presently being developed that will allow us to extend these results to the hyperstrong regime ($B < 2 \times 10^4$) (refer to Sec. V). Despite this, the energy-bound results quoted in this paper for the transition regime surpass available bound results, as developed in the excellent work of Cizek and Vrscay.[7]

II. BRIEF OVERVIEW

In the following sections and the Appendix we present a detailed discussion of the linearized moment method for generating convergent bounds to bosonic ground-state eigenvalues. As indicated in the Introduction, the method can also be applied to excited states once their non-negative structure is understood. In this section we outline the basic logic, as applied to the ground state, so as to facilitate the discussion given in the remaining sections.

The first important issue is the fact that for any multidimensional nondegenerate (finite degree of freedom) bosonic system, the ground state must be *non-negative*[11] and have finite power moments, as summarized by Eqs. (2.1) and (2.2). In this work, "non-negative" is used in the conventional sense and in addition denotes a function which is positive on a support of nonzero measure. Accordingly, for the ground state we have

$$\Psi_{\text{ground}}(x) \geq 0 , \tag{2.1}$$

$$m(p) \equiv \int \mathbf{x}^{\mathbf{p}} \Psi_{\text{ground}}(\mathbf{x}) D\mathbf{x} < \infty , \tag{2.2}$$

where $\mathbf{x}^{\mathbf{p}} = \prod_i x_i^{p_i}$.

The relations above are *necessary* and *sufficient.* That is, the only solution of the Schrödinger equation satisfying Eqs. (2.1) and (2.2) is the ground state.[1]

The second phase of the general moment method requires obtaining a moment equation for the particular Schrödinger equation being considered. This is usually straightforward.

(i) When the potential is a rational fraction in the components of $\mathbf{x}$, the Schrödinger equation can be written as

$$L\Psi = 0 , \tag{2.3}$$

where L is a second-order linear (partial) differential operator with polynomial coefficients. By multiplying (2.3) by $\mathbf{x}^{\mathbf{p}}$ and integrating by parts, one gets a linear recursion relation for the physical moments. Implicit in the integration by parts is the fact that physically bounded solutions exhibit fast asymptotic decrease to zero. Accordingly, there are no end-point contributions.

(ii) For the quadratic Zeeman problem to be considered, the potential is not a rational fraction in $\mathbf{x}^{\mathbf{p}}$; it involves square roots. By transforming to parabolic coordinates one can recast the problem into a form consistent with (2.3). It is often possible to transform a given system into one consistent with (2.3).

(iii) The focus on rational fraction potentials is mandated if one wants to work with ordinary power moments. Alternatively, one can work with generalized moments. As an example, certain magnetohydrodynamic tokamak stability models[12] work with effective potentials of the form

$$V(x)=P(x,\sin(x),\cos(x)) , \tag{2.4}$$

where P is a polynomial. The generalized moments are

$$\mu_{m,n}=\int_{-\infty}^{\infty} x^m \exp(inx)\Psi_{\text{ground}}(x)dx . \tag{2.5}$$

It is easy to derive a linear recursion relation for these moments. It is also straightforward to obtain the necessary and sufficient conditions for the generalized moments in (2.5) to correspond to a non-negative function measure.

We do not intend to overwhelm the reader with all possible cases that can be analyzed in terms of the moment method. However, it should be clear that a very large class of problems can be addressed.

As alluded to in the Introduction, the moment equation referred to above will serve to distinguish two sets of moments. One of these will be the "missing moments." Only by specifying these can the remaining moments be determined. The latter define the second set of moments and are linearly dependent upon the former.

The aforementioned moments equation combined with the non-negativity property of the ground-state wave function define a "moments problem."[1,8] The traditional moments problem concerns itself with the specification of the necessary and sufficient constraints that a set of moments must satisfy in order that they correspond to a non-negative function measure. These take on the form of the Hankel-Hadamard determinant inequalities referred to in the Introduction, and are discussed in greater detail in the Appendix.

The energy E appears as a parameter in the moment equation. Accordingly, the moments will be dependent on the missing moments as well as on the energy. Through the infinite hierarchy of HH moment inequality constraints, both the missing moments and energy will be constrained to a progressively decreasing, physically allowed, subdomain. Thus, not only can lower and upper bounds be established for the physical energy, but also the same can be realized for the missing moments.

Of additional practical significance is the fact that for singular strongly coupled systems the size of the missing moment and energy domain decreases very rapidly as more moments are considered. This is demonstrated in all of the cited works (for two-missing-moment problems), and will also be shown here to apply to the infinite-missing-moment case as well.

As indicated in the Introduction, the nonlinear nature of the original Hankel-Hadamard moment formulation[1] is impractical for systems with more than three missing moments. Firstly, because of the homogeneous nature of Schrödinger's equation, the associated moment equation will also be homogeneous. Consequently, through any appropriate choice of normalization, one can always reduce the number of missing moments by 1. For a three-missing-moment problem, the imposition of an appropriate normalization prescription will yield two independent missing moments. Thus for such problems, the determination of the energy-missing-moment subset consistent with the HH inequalities will require a three-dimensional numerical search. Clearly, for problems with many missing moments, such numerical searches are impossible. To remedy this difficulty, we were motivated to reformulate the nonlinear moment method (HH inequality constraints) in terms of a linear theory. In this we have been successful. That is, we shall establish the existence of an equivalent linear formulation of the nonlinear Hankel-Hadamard moment approach.

As referred to in the Introduction, given a finite number of HH determinants (corresponding to a matrix dimensionality less than or equal to some given maximum dimensionality), if for some energy value there exists a missing-moment subset consistent with the HH inequalities, that missing moment subset must be convex. This will be proven in the subsequent discussion. The boundary of this missing-moment subset will correspond to intersecting nonlinear hypersurfaces. It will be shown that this subset can be considered as the envelope of an uncountably infinite number of intersecting hyperplanes. All of this will comprise the first phase of our linearization program.

The second phase of the linearization program will be to determine which of the infinitely many hyperplanes are more important in adequately enveloping the nonlinear missing-moment bounded convex subset. The identification of these "optimal" hyperplanes will make our program more efficient. In particular, they will enable us to quickly determine if for some arbitrary energy value there does not exist a missing-moment subset, thereby allowing us to conclude that that energy value is physically impossible.

In order to make the previous discussion more specific we consider the general one-dimensional problem. The Hamburger moments of a non-negative function $\Psi(x)$, when they exist, are defined by

$$m(p)=\int_{-\infty}^{\infty} x^p \Psi(x)dx . \tag{2.6}$$

For the first $2I+1$ moments $\{m(p), 0\le p\le 2I\}$, a finite number of nonlinear (in the moments, and therefore in the missing moments as well) determinant inequality constraints [see Eq. (2.9)] are derivable from the expressions[8]

$$\int_{-\infty}^{\infty}\left[\sum_{i=0}^{I} C_i x^i\right]^2 \Psi(x)dx>0$$

$$\text{for all real } C_i \text{ (not all 0)} \tag{2.7}$$

or

$$\sum_{i,j=0}^{I} C_i m(i+j) C_j>0$$

$$\text{for all real } C_i \text{ (not all 0) .} \tag{2.8}$$

The quadratic form relation in (2.8) expresses that the m matrix has only positive eigenvalues or, equivalently, that the Hankel-Hadamard determinants must be positive:[8]

$$\Delta_{0,k}=\det\begin{vmatrix} m(0) & m(1) & m(2) & \cdots & m(k) \\ m(1) & m(2) & m(3) & \cdots & m(k+1) \\ \vdots & & & & \vdots \\ m(k) & m(k+1) & m(k+2) & \cdots & m(2k) \end{vmatrix} > 0 , \tag{2.9}$$

for $k=0,1,\ldots,I$.

Both Eqs. (2.9) and (2.8) are equivalent. It is important to note that they clearly show that a *finite* number of nonlinear (in the moments) HH inequalities are equivalent to an *infinite* number of linear (in the moments) inequalities (because the C's can take on any value).

Let us *symbolize* the linear-moment–missing-moment dependence by $m(p)=\sum_{l=0}^{L}\hat{M}(p;l;E)u_l$, where u_l are the L missing moments ($u_0=1$) and $\hat{M}(p;l;E)$ is an energy (E) -dependent coefficient recursively obtainable from the moment equation. Inserting this relation into (2.8) and interchanging the summations yields

$$\sum_{l=1}^{L} A_l[E;C]u_l < B[E;C] \quad \text{for all } C_i , \tag{2.10}$$

where

$$A_l[E;C]=\sum_{i,j=0}^{I} -C_i\hat{M}(i+j;l;E)C_j$$

and

$$B[E;C]=-A_0[E;C] .$$

For fixed E and I, (2.10) corresponds to an uncountably infinite set of inequality constraints for the missing moments u_l due to the arbitrariness of the C's. It is clear that these linear inequality constraints define in the missing-moment space the hyperplanes that completely envelope and determine the nonlinear missing-moment subset implicitly defined by (2.9). It is known from linear-programming theory[9] that if there is a solution subset to (2.10) then it must be convex. Thus all of the preceding discussion corresponds to the first phase of our linearization program, as previously described.

One of the major contributions of this work is a prescription for identifying a finite subset of **C** vectors which will quickly tell us if a physical missing-moment convex subdomain exists (for a given E value). Let us assume that such an optimal finite set of vectors is given and see how a linear-programming formulation develops for the missing moments.

For a system with L missing moments let us index the aforementioned optimal set of vectors by $\mathbf{C}(n)$, for $1\le n\le N$ ($N=$"NDX"). We can then generate from (2.10) the corresponding set of linear inequality constraints for the missing moments u_l. This is represented, symbolically, by ($A_{nl}(E)=A_l[E;\mathbf{C}^{(n)}]$)

$$\sum_{l=1}^{L} A_{nl}(E)u_l < B_n(E), \quad 1\le n\le N . \tag{2.11}$$

The determination as to whether or not a u solution exists for (2.11) is addressed through the theory of linear programming.[9] It is important to stress that what is of importance is the issue of existence (feasibility) or nonexistence (infeasibility) of a u_l-solution subset. The usual description of linear-programming theory in most texts is in the context of optimizing some *objective function.* This is not what we are *immediately* interested in. The theory of linear programming is first concerned with feasibility (existence of a solution subset) and second with optimizing some linear objective function within the feasible–convex-solution subset. Indeed, the linear-programming code that we used [International Mathematics and Scientific Library (IMSL) code ZX3LP] defines feasibility as a Phase-1 problem, and optimization of some specified objective function as a Phase-2 problem.

Once a finite set of $\mathbf{C}^{(n)}$ vectors has been defined, one would use the Phase-1 version to determine if a missing-moment subset is feasible or not. If there is no u_l solution (infeasible), then the associated energy value is physically impossible.

The preceding discussion assumed that the $\mathbf{C}^{(n)}$'s had been specified. The actual procedure for generating these vectors is more complicated. Let us adopt an inductive strategy and assume that for some energy value we have a feasible missing-moment subset S_N corresponding to $\mathbf{C}^{(n)}$ for $n\le N$ ["NDX"$=N$ in Eq. (2.11)]. We wish to generate more **C** vectors which will "reduce" S_N into a much smaller convex missing-moment subset or even totally reduce the region into nothing, that is, infeasibility, thereby concluding that the associated energy is unphysical. To achieve this we must find the *extremal vertices* for the *bounded domain* S_N.

For the kth coordinate u_k, the extremal vertices are the two vertex points of S_N for which the u_kth coordinate value is a maximum or minimum. This can be determined by considering (2.11) and the linear objective function $\pm u_k$ (where the choice of sign corresponds to the maximum or minimum extremal kth vertex). This enables us to use the Phase-2 linear-programming code to determine all the extremal vertices.

Because of convexity, the average of all the extremal vertex points of S_N will also be a point within S_N. At this *deep* interior point we can define a matrix (refer to Sec. III) such that its nonpositive eigenvalue eigenvectors correspond to the desired new $\mathbf{C}^{(N+1)},\mathbf{C}^{(N+2)},\ldots,$ vectors that reduce the S_N subset.

By partitioning an arbitrary energy interval in small steps, and implementing the program above at each E point, energy bounds can be obtained. The bounds become narrower as the dimensionality I is increased. The multidimensional extension of the linear-programming formalism above remains exactly the same. This is made clear in Sec. IV and in the Appendix.

III. ONE-DIMENSIONAL EXAMPLE

Consider the sextic potential problem

$$-\Psi''+(\lambda x^2+gx^6)\Psi=E\Psi \ . \tag{3.1}$$

Define the Hamburger moments by

$$m(p)=\int_{-\infty}^{\infty} x^p\Psi(x)dx \ . \tag{3.2}$$

Due to parity invariance, the ground state is a symmetric configuration: the odd-order moments will be zero. Accordingly, through the change of variables $x^2=y$, the even-order Hamburger moments will become the Stieltjes moments of a corresponding function,

$$\begin{aligned} m(2p)&=\int_0^{\infty} y^p[\Psi(\sqrt{y})/\sqrt{y}\,]dy \\ &=u(p) \ . \end{aligned} \tag{3.3}$$

It is known that the bosonic ground-state wave function is non-negative.[11] This, together with the moment recursion relation given in the following [obtained from Eq. (3.1) by multiplying by x^{2p} and integrating from $-\infty$ to $+\infty$], define a moment problem through which the quantization of E, the energy, can be obtained.

From Eq. (3.1) it follows that the Stieltjes moments satisfy

$$\begin{aligned} u(p+3)=&[2p(2p-1)u(p-1)-\lambda u(p+1) \\ &+Eu(p)]/g \ . \end{aligned} \tag{3.4}$$

It will be noted that $u(0)$, $u(1)$, and $u(2)$ must be specified (as well as E) before the remaining moments can be generated. These are denoted as the "missing moments." Of course, the implicit arbitrariness of Ψ's normalization allows us to reduce the number of missing moments by 1. Contrary to the trivial choice $u(0)=1$, used in Ref. 1, it will become necessary to take the more subtle choice

$$u(0)+u(p_{\max})=1 \ . \tag{3.5}$$

The expression $p_{\max}$ ("PMX") corresponds to the *maximum* moment order generated. It will be progressively increased. The reason for the choice (3.5) is that for linear-programming purposes one should work within a bounded region of the missing-moment space. Note that in addition to the necessary physical bound $0<u(p)$ (for all p), Eq. (3.5) leads to other bounds,

$$\begin{aligned} u(p)&=\int_0^{\infty} y^p[\Psi(\sqrt{y})/\sqrt{y}\,]dy \\ &=\int_0^1 y^p[\Psi(\sqrt{y})/\sqrt{y}\,]dy \\ &\quad+\int_1^{\infty} y^p[\Psi(\sqrt{y})/\sqrt{y}\,]dy \ , \end{aligned} \tag{3.6a}$$

$$\begin{aligned} &\le\int_0^1[\Psi(\sqrt{y})/\sqrt{y}\,]dy \\ &\quad+\int_1^{\infty} y^{p_{\max}}[\Psi(\sqrt{y})/\sqrt{y}\,]dy \ , \end{aligned} \tag{3.6b}$$

$$\le u(0)+u(p_{\max})=1 \quad \text{for } p\le p_{\max} \ .$$

Therefore, with the choice of normalization in (3.5), one concludes

$$0<u(p)<1 \quad \text{for } 0\le p\le p_{\max} \ . \tag{3.7}$$

As can be seen, Eq. (3.7) will limit the set of the effective missing moments [$u(1)$ and $u(2)$] to within the unit square.

The choice represented by (3.5) is not unique. For the three-dimensional quadratic Zeeman problem (see Sec. IV) we shall be working with the analogue of $u(0)+u(1)+u(2)=1$. This choice will not limit all the moments to be between 0 and 1; however, for linear-programming purposes, this alternate normalization will also be adequate. It also bounds the missing moments.

From Eq. (3.4) it is clear that the homogeneous linear dependence of all moments on $u(0)$, $u(1)$, and $u(2)$ may be expressed by

$$u(p)=\sum_{q=0}^{2} M(p;q)u(q) \ , \tag{3.8}$$

where

$$M(p;q)=\delta_{p,q} \quad \text{for } 0\le p\le 2 \ . \tag{3.9}$$

Clearly the M-matrix elements satisfy Eq. (3.4) for fixed q, and can be recursively generated through the initialization conditions in (3.9):

$$\begin{aligned} M(p+3;q)=&[2p(2p-1)M(p-1;q)-\lambda M(p+1;q) \\ &+EM(p;q)]/g \ . \end{aligned} \tag{3.10}$$

From (3.5) it follows that

$$u(0)+u(p_{\max})=u(0)+\sum_{q=0}^{2} M(p_{\max};q)u(q)=1 \tag{3.11}$$

or

$$u(0)=\left[1-\sum_{q=1}^{2} M(p_{\max};q)u(q)\right]\Big/[1+M(p_{\max};0)] \ . \tag{3.12}$$

Substituting in Eq. (3.8), one obtains

$$u(p)=\sum_{q=0}^{2} \hat{M}(p;q)\hat{u}(q) \ , \tag{3.13}$$

where

$$\hat{u}(q)=\begin{cases} 1 & \text{if } q=0 \ , \\ u(q) & \text{if } q=1,2 \ , \end{cases} \tag{3.14}$$

and

$$\hat{M}(p;q)=\begin{cases} M(p;0)/[1+M(p_{\max};0)] & \text{if } q=0 \\ M(p;q)-M(p;0)M(p_{\max};q)/[1+M(p_{\max};0)] & \text{if } q=1,2 \ . \end{cases} \tag{3.15}$$

From the Appendix, the necessary and sufficient conditions for the $u(p)$ to be the moments of a non-negative function are

$$\int_0^\infty \left[\sum_{i=0}^{I} v_i y^i\right]^2 [\Psi(\sqrt{y})/\sqrt{y}]dy > 0 \tag{3.16}$$

and

$$\int_0^\infty y\left[\sum_{i=0}^{I} w_i y^i\right]^2 [\Psi(\sqrt{y})/\sqrt{y}]dy > 0 , \tag{3.17}$$

for all possible v_i, w_i, and I.

The integral inequalities above are equivalent to the quadratic form inequalities

$$\sum_{i,j=0}^{I} v_i u(i+j) v_j > 0 \quad \text{for } \mathbf{v} \neq \mathbf{0} \tag{3.18}$$

and

$$\sum_{i,j=0}^{I} w_i u(i+j+1) w_j > 0 \quad \text{for } \mathbf{w} \neq \mathbf{0} . \tag{3.19}$$

In principle, only for the physical energy E_{ph} will the inequalities above, uncountably infinite in number be satisfied.

In the Hankel-Hadamard formulation[1] one replaces the positivity of the quadratic forms (3.18) and (3.19) by the corresponding nonlinear determinant inequalities, given in the following and explained in the Appendix,

$$\Delta_{m,n} > 0 \quad \text{for } 2n+1 \leq p_{\max},\ m = 0,1 . \tag{3.20}$$

One would then have to implement a three-dimensional search in order to determine the corresponding bounded, physically allowed, subdomain for the missing moments [$u(1)$ and $u(2)$] and E.

As indicated in Sec. II we wish to develop an alternate, yet equivalent, linear formulation of (3.20). The inspiration for this is already provided by the equivalence between the finite number of nonlinear inequalities in (3.20) and the infinite number of linear inequalities in (3.18) and (3.19). In addition, it is possible to select from among the uncountably many **v**'s and **w**'s an optimal finite set which will quickly determine if (3.18) and (3.19) have a $u(1)$-$u(2)$ solution set for given E. This will be the focus of the following discussion.

Substituting Eq. (3.13) into (3.18) and (3.19), there follow the relations

$$\sum_{q=0}^{2} \hat{u}(q) \left[\sum_{i,j=0}^{I} v_i \hat{M}(i+j;q) v_j\right] > 0 , \tag{3.21}$$

$$\sum_{q=0}^{2} \hat{u}(q) \left[\sum_{i,j=0}^{I} w_i \hat{M}(i+j+1;q) w_j\right] > 0 , \tag{3.22}$$

for all nonzero **v** and **w**.

Recalling the definition for $\hat{u}(q)$ [refer to Eq. (3.14)], we may rewrite Eqs. (3.21) and (3.22) in a manifestly linear-programming representation (refer to the discussion in Sec. II with regard to the feasibility and optimization aspects of the general linear-programming problem)

$$\sum_{q=1}^{2} -\mathcal{M}^{(0)}_{\mathbf{v},E,I}(q) u(q) < \mathcal{M}^{(0)}_{\mathbf{v},E,I}(0) , \tag{3.23}$$

$$\sum_{q=1}^{2} -\mathcal{M}^{(1)}_{\mathbf{w},E,I}(q) u(q) < \mathcal{M}^{(1)}_{\mathbf{w},E,I}(0) , \tag{3.24}$$

for any choice of nonzero **v**'s and **w**'s. We have made explicit the fact that the coefficients $\mathcal{M}^{(0)}_{\mathbf{v},E,I}(q)$ and $\mathcal{M}^{(1)}_{\mathbf{w},E,I}(q)$ depend upon the **v**-**w** vectors, E and I. The E dependence comes from the implicit energy dependence of the $\hat{M}$ coefficients defined in (3.15), and explicitly referred to in the following relations which define the $\mathcal{M}^{(0,1)}$ coefficients:

$$\mathcal{M}^{(0)}_{\mathbf{v},E,I}(q) = \sum_{i,j=0}^{I} v_i \hat{M}_E(i+j;q) v_j , \tag{3.25}$$

$$\mathcal{M}^{(1)}_{\mathbf{w},E,I}(q) = \sum_{i,j=0}^{I} w_i \hat{M}_E(i+j+1;q) w_j . \tag{3.26}$$

As stated earlier, we cannot solve the infinite number of inequality constraints (3.23) and (3.24) (I fixed, **v** and **w** arbitrary) in order to determine whether or not, for given E, there exists (feasible) or not (infeasible) a $u(1), u(2)$ subdomain satisfying the inequalities. Clearly, in order to determine if the choice for E is unphysical, it is not necessary to solve all of these inequalities. It is sufficient to determine if there exists a finite subset of inequalities (that is, a finite number of **v** and **w** vectors) for which no $u(1), u(2)$ solution is possible. Before describing one algorithm for achieving this, we must clarify the significance of a "convex" set.

The theory of linear programming[9] is built around the concept of convex sets. More specifically, the solution set to an arbitrary linear-programming problem of the generic form (regardless of the objective function)

$$\sum_{l=1}^{L} M_{nl} u_l < B_n , \quad 1 \leq n \leq N \tag{3.27}$$

corresponds to a convex set U_{convex}. A convex set is defined by the property that if two points lie within it, so too must all points along the straight line connecting them. From this it follows that the linear superposition (with positive weights) of any collection of points in U_{convex} must also belong to U_{convex}; in particular, so must their average. We shall make use of this in the algorithm to be described below.

We present a general description of our programming logic. The set of inequalities under consideration is those of Eqs. (3.23) and (3.24), as well as those resulting from $0 < u(p) < 1$ for $0 \leq p \leq p_{\max}$ [refer to Eq. (3.7)]. Thus we have

$$\begin{aligned} &\sum_{q=1}^{2} -\mathcal{M}^{(0)}_{\mathbf{v},E,I}(q) u(q) < \mathcal{M}^{(0)}_{\mathbf{v},E,I}(0) , \\ &\sum_{q=1}^{2} -\mathcal{M}^{(1)}_{\mathbf{w},E,I}(q) u(q) < \mathcal{M}^{(1)}_{\mathbf{w},E,I}(0) , \end{aligned} \tag{3.28}$$

and

$$\sum_{q=1}^{2} \hat{M}(p;q) u(q) < 1 - \hat{M}(p;0) \quad \text{for } p \leq p_{\max} . \tag{3.29}$$

For a given E we first generate the $\hat{M}$ matrices (clearly $1+2I \leq p_{\max}$). We make use of (3.29) [which includes $0<u(1),\ u(2)<1$] to initialize our linear-programming algorithm. That is, the inequalities in (3.29) will immediately limit the possible physical $u(1),u(2)$ values to within the unit square. The corresponding feasible region is necessarily convex. We symbolize it in the illustration in Fig. 1.

Using the standard linear-programming code ZX3LP available through the IMSL computer library, we determine all the vertices of the convex region above corresponding to extremal values for each of the coordinates (refer to the discussion in Sec. II). Referring to the symbolic illustration in Fig. 1, the points P_1 and P_3 correspond to the vertices for which the $u(1)$ coordinate assumes its minimum and maximum values, respectively. The points P_4 and P_2 correspond to the minimum and maximum for the $u(2)$ coordinate. We now take the average of these four points, $\bar{P}_1=(\bar{u}_1,\bar{u}_2)$. It must lie within the convex domain.

At the point $\bar{P}_1$ we determine if there are any nonpositive eigenvalues of the matrices $T^{(\sigma)}$ with components defined by

$$T_{ij}^{(\sigma)}=\sum_{q=0}^{2}\hat{\bar{u}}(q)\hat{M}(\sigma+i+j;q),\quad \sigma=0,1 \tag{3.30}$$

where

$$\hat{\bar{u}}(q)=\begin{cases}1 & \text{if } q=0\ ,\\ \bar{u}_q & \text{if } q=1,2\ .\end{cases} \tag{3.31}$$

Let us assume that $T^{(\sigma)}$ has some *nonpositive* eigenvalues. We may assign the corresponding eigenvector(s) to be the **v** or **w** coefficient vectors in (3.23)–(3.26), depending on σ's value. For each of these nonpositive eigenvalues, the associated **v** or **w** vector will define inequality relations which invalidate the requirements of the moment problem, as defined by Eqs. (3.21) and (3.22). Geometrically, these inequalities correspond to lines which cut the feasible region in Fig. 1 into a much smaller feasible region, as depicted in Fig. 2. For each "cutting" line, $\bar{P}_1$ must lie on the side being cut.

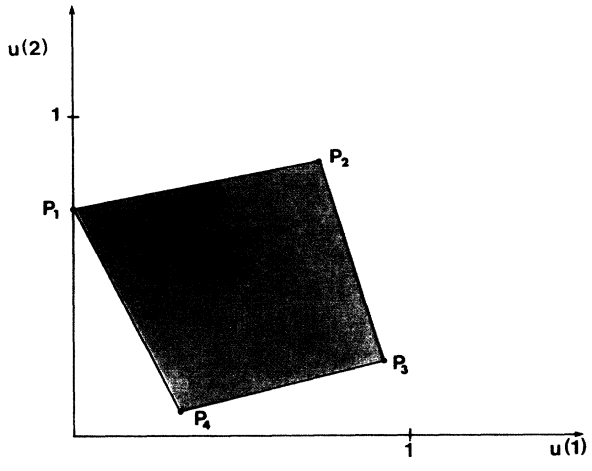

FIG. 1. Symbolic "feasible region" for the sextic potential problem.

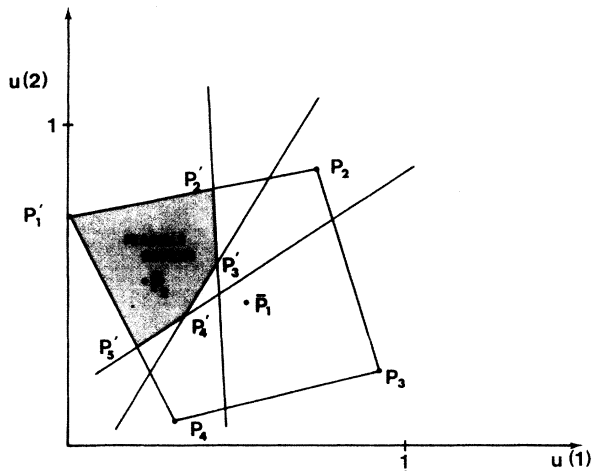

FIG. 2. Symbolic inductive "cutting" procedure obtained through the linear-programming method.

With respect to Fig. 2, the updated convex region is defined by the vertices P_1', P_2', P_3', P_4', and P_5'. We now repeat the application of the linear programming code ZX3LP and determine the new vertices corresponding to extremal values for each of the coordinates. By taking the average of these, a new interior point $\bar{P}_2$ can be defined. At this new point we again determine the inequalities that will reduce the updated feasible region. The preceding inductive process is repeated until one of two things happens (bearing in mind that $p_{\max}$ is fixed at some arbitrary value).

(a) After a finite number of "reductions" no feasible region remains for the chosen E value [no solution exists for Eqs. (3.23)–(3.26)].

(b) After a finite number of reductions, an average point $\bar{P}_k$ is reached for which only positive T eigenvalues exist.

For given E, if case (a) arises, then clearly E is unphysical. If case (b) is manifested, then we say that E is a physically possible value, for the $p_{\max}$ "order" used. For the latter case, progressively increasing $p_{\max}$ will also increase the maximum dimensionality of the underlying **v**-**w** vector space. The inductive application of the *cutting* procedure will quickly result (for some $p_{\max}$ value) in case (a) for a given unphysical E value. In this manner one obtains a fast decreasing energy interval of allowed energy values. The end points of this interval will define the lower and upper bounds to the true physical ground-state energy.

For the case $\lambda=g=1$, the data in Table I give the results obtained for the ground-state energy. For some $p_{\max}$ values, more than one possible energy interval appears. In every case, all but one of these disappeared at the next higher $p_{\max}$ value. We also quote the typical number of inequality relations required for determining the infeasibility (nonexistence) of a $u(1),u(2)$ solution subdomain for given $p_{\max}$. This number is referred to as N [refer to Eq. (2.11)]. This is an important parameter

TABLE I. Linear-programming results for the ground-state energy bounds of $-\Psi''+(x^2+x^6)\Psi=E\Psi$.

$p_{\max}$	Possible energy intervals	N
6	(1.31,1.61), (2.01,3.61), (4.71,5.0)	10
7	(1.38,1,61)	17
8	(1.41,1.48)	20
9	(1.422,1.476)	24
10	(1.422,1.438), (1.438,1.444)	25
11	(1.4345,1.4380)	28
12	(1.4352,1.4366), (1.4366,1.4369)	35
13	(1.4352,1.4357)	37
14	(1.43555,1.43570)	43

because it shows the relatively small number of inequalities necessary in order to obtain good results. Linear-programming codes can handle hundreds of independent variables (i.e., missing moments) and thousands of inequality constraints. Our problems, including the three-dimensional quadratic Zeeman problem (discussed in Sec. IV), fall far short of the typical large-scale linear-programming applications of operations research and economics.

IV. QUADRATIC ZEEMAN PROBLEM

As an example of how to implement the preceding formalism on a multidimensional problem, we consider the important quadratic Zeeman effect for superstrong magnetic fields.[7,13] In atomic units, the Schrödinger equation is

$$\left[-\frac{1}{2}\Delta+\frac{B^2}{8}(r^2-z^2)-Z/r-E\right]\Psi=0 . \tag{4.1}$$

The z axis is taken along the direction of the uniform magnetic field B. The magnetic field is measured in units of 2.35×10^9 G and the length in units of the Bohr radius. The electric charge Z is in proton electric charge units, while for the energy, the rydberg is one-half in these units.

Simple scale invariance shows that

$$E(Z,B)=Z^2E(1,B/Z^2) , \tag{4.2}$$

where $E(Z,B)$ is the ground-state energy. We may therefore take $Z=1$ in our calculations without loss of generality.

One of the main difficulties of the system above, besides the totally unbounded nature of the potential and the presence of a continuum (scattering states), comes from the fact that at large distances ($r\to+\infty$, in the z direction) it is the Coulomb potential Z/r which binds the system. However, this Coulomb potential is of third order with respect to the magnetic potential at large transverse distances. This makes the problem extraordinarily difficult. It is therefore not surprising that the attainment of reliable and precise ground-state energy values has attracted many researchers for the past 25 years.[10]

Upper bounds, using the Rayleigh-Ritz variational principle, with various ansatz, have been obtained by many authors. Lower bounds coming close to the upper bounds are totally absent from the literature for magnetic field strengths in the transition region $B\gtrsim1$. We refer the reader to the work of Cizek and Vrscay.[7]

Many methods have been devised to solve the quadratic Zeeman problem. The nature of these techniques fall into the various categories specified in the following: (i) variational, (ii) adiabatic, (iii) Padé approximation to $(2\varepsilon)^{1/2}$ [refer to Eq. (4.7)], (iv) super adiabatic, and (v) analytic resummation methods. Although some of the results of the calculations using two methods as different as (i) and (v) come very close, the discrepancy in the result increases with B, as quoted in the tables given in the comprehensive work of Le Guillou and Zinn-Justin.[10]

Some authors quote "error" bounds. These are certainly meaningful in the sense that *inside their own approximation scheme* the author can estimate the error. However, to confirm the high quality of some of these calculations, the knowledge of true lower bounds that converge to the Rayleigh-Ritz upper bounds[14] is necessary.

Returning to the moments analysis of (4.1), we transform the system to parabolic coordinates,

$$\xi=r-z>0, \quad \eta=r+z>0 . \tag{4.3}$$

It is also convenient to work within the $\rho(\xi,\eta)$ representation defined by

$$\Psi_{\text{ground}}(\xi,\eta)=\rho(\xi,\eta)\exp(B\xi\eta/4) . \tag{4.4}$$

We now transform (4.1) into

$$\frac{\partial}{\partial\xi}\left[\xi\frac{\partial\rho}{\partial\xi}\right]+\frac{\partial}{\partial\eta}\left[\eta\frac{\partial\rho}{\partial\eta}\right]+\tfrac{1}{2}B\xi\eta\left[\frac{\partial\rho}{\partial\xi}+\frac{\partial\rho}{\partial\eta}\right]+\rho[\tfrac{1}{2}(E+\tfrac{1}{2}B)(\xi+\eta)+Z]=0 . \tag{4.5}$$

It will be noted that the asymptotic behavior of the ground state is

$$\Psi_{\text{ground}}\sim\exp[-B(r^2-z^2)/4-(2\varepsilon)^{1/2}|z|] \quad \text{as } r\to\infty , \tag{4.6}$$

where

$$\varepsilon=B/2-E . \tag{4.7}$$

Because of (4.6) it follows that within the ρ representation no unphysical Ψ solutions (unbounded configurations with infinite moments) will appear. This is so because such configurations would also have infinite moments within the ρ representation. As such, only the physical ground-state solution is the unique solution of the two-dimensional Stieltjes-moment problem formulation given in (4.5).

The two-dimensional Stieltjes moments within the parabolic coordinate representation are defined by

$$u(m,n)=\int_0^\infty d\xi\int_0^\infty d\eta\,\xi^m\eta^n\rho(\xi,\eta) . \tag{4.8}$$

These will satisfy the "star" relation

$$n^2u(n-1,m)+m^2u(n,m-1)-\tfrac{1}{2}(Bn+\varepsilon)u(n,m+1)$$
$$-\tfrac{1}{2}(Bm+\varepsilon)u(n+1,m)+Zu(n,m)=0 . \quad (4.9)$$

Because the ground state is symmetric,

$$\Psi_g(r,z)=\Psi_g(r,-z) , \quad (4.10)$$

it follows that

$$\rho(\xi,\eta)=\rho(\eta,\xi) ; \quad (4.11)$$

accordingly,

$$u(m,n)=u(n,m) . \quad (4.12)$$

It can be immediately seen that the missing moments correspond to the set $\{u(q,q) \mid 0\le q<\infty\}$. In order to see how all the moments can be generated, let us adopt an inductive strategy and assume that all the moments on the first $2k-1$ antidiagonals $\{u(i,j) \mid 0\le i+j\le 2k-1\}$ are given, as well as $u(k,k)$, for some arbitrary "k." One can then generate all the moments along the $2k$ antidiagonal by taking $n=k-i$ and $m=k+i-1$ for $i=1,2,\ldots,k$. That is, solve for $u(n,m+1)$ recursively through (4.9). Taking $m=n=k$, one can then solve for $u(k,k+1)$. Finally, all the moments along the $2k+1$ antidiagonal are generated by taking $n=k-i$ and $m=k+i$, $i=1,2,\ldots,k$. Once the $u(n,m+1)$ moment (for $n\le k$) is determined, $u(m+1,n)$ is also determined through (4.12). By induction, all moments up to the $2(q_{\max})+1$ antidiagonal can be generated, given all the missing moments up to order $u(q_{\max},q_{\max})$ ($q_{\max}$ ="MSN").

It is clear from the preceding that although the full Zeeman problem is an *infinite* missing-moment problem, we can always work with a finite number of missing moments, $1+q_{\max}$ and allow $q_{\max}$ to increase. Consistent with this, the homogeneous and linear dependence of $u(m,n)$ upon the missing moments can be expressed by

$$u(m,n)=\sum_{q=0}^{q_{\max}} M(m,n;q)u(q,q) , \quad (4.13)$$

for $0\le m+n\le 2(q_{\max})+1$.

The $M(m,n;q)$ matrix elements satisfy the same star relation that the moments do, for fixed values of q. The necessary initialization conditions are

$$M(k,k;q)=\delta_{k,q} \quad \text{for } 0\le k,q\le q_{\max} . \quad (4.14)$$

We shall adopt the following normalization condition:

$$\sum_{q=0}^{q_{\max}} u(q,q)=1 . \quad (4.15)$$

We may solve for the zeroth-order moment $[u(0,0)]$ in terms of the other missing moments. Accordingly, one obtains

$$u(m,n)=\sum_{q=0}^{q_{\max}} \hat{M}(m,n;q)\hat{u}_q , \quad (4.16)$$

where

$$\hat{u}_q=\begin{cases}1 & \text{if } q=0 ,\\ u(q,q) & \text{if } q>0 ,\end{cases} \quad (4.17)$$

and

$$\hat{M}(m,n;q)=\begin{cases}M(m,n;0) & \text{if } q=0 ,\\ M(m,n;q)-M(m,n;0) & \text{if } q>0 .\end{cases} \quad (4.18)$$

Note that due to the choice of normalization [Eq. (4.15)] all the missing moments stay within the unit hypercube in the missing-moment space,

$$0<\hat{u}_q<1, \quad 1\le q\le q_{\max} . \quad (4.19)$$

From the discussion in the Appendix, the complete set of necessary and sufficient conditions for the two-dimensional Stieltjes moments to correspond to a nonnegative function measure are

$$\sum_{q=1}^{q_{\max}} -\left[\sum_{k,l=1}^{Dm(\sigma_1,\sigma_2)} \Omega_{i_k,j_k}^{(\sigma_1,\sigma_2)}\hat{M}(\sigma_1+i_k+i_l,\sigma_2+j_k+j_l;q)\Omega_{i_l,j_l}^{(\sigma_1,\sigma_2)}\right]\hat{u}_q$$
$$<\sum_{k,l=1}^{Dm(\sigma_1,\sigma_2)} \Omega_{i_k,j_k}^{(\sigma_1,\sigma_2)}\hat{M}(\sigma_1+i_k+i_l,\sigma_2+j_k+j_l;0)\Omega_{i_l,j_l}^{(\sigma_1,\sigma_2)} , \quad (4.20)$$

where $\sigma_1,\sigma_2=0$ or 1. Some of the expressions appearing in (4.20) are defined below.

For each $\sigma_{1,2}$ value selection, the $\Omega_{i,j}^{(\sigma_1,\sigma_2)}$ correspond to different independent variables. The $(i_k,j_k)=(i,j)_k$ correspond to a particular coordinate pair ordering (not a moment ordering),

$$(0,0)_1,(1,0)_2,(0,1)_3,(2,0)_4,(1,1)_5,(0,2)_6,\ldots,(0,q_{\max}-1)_a,(q_{\max},0)_b,\ldots,(0,q_{\max})_c,\ldots , \quad (4.21)$$

where

$$a=(q_{\max})(q_{\max}+1)/2 ,$$
$$b=a+1 , \quad (4.22)$$
$$c=(q_{\max}+1)(q_{\max}+2)/2 .$$

In Eq. (4.20), $Dm(\sigma_1,\sigma_2)$ is the dimensionality of the appropriate Ω-vector space. Because of the symmetric property given in (4.11) only the cases $(\sigma_1=0,\sigma_2=0)$, $(\sigma_1=1,\sigma_2=0)$, and $(\sigma_1=1,\sigma_2=1)$ need to be considered. Refer to the Appendix for additional clarification. Once $q_{\max}$ and $\sigma_{1,2}$ are specified, the dimen-

TABLE II. Linear-programming results for the quadratic Zeeman problem; $B=0.2$, 2, and 20 a.u. ($Z=1$).

B	$q_{\max}$	Maximum dimension $D_m(1,0)$	Feasible energy Interval (bounds)	N
0.2	3	8	(0.38,0.74)	18
0.2	3	9	(0.52,0.71)	20
0.2	3	10	(0.54,0.62)	25
0.2	4	11	(0.546,0.620)	35
0.2	4	12	(0.548,0.618)	40
0.2	4	13	(0.550,0.610)	42
0.2	4	14	(0.570,0.605)	45
0.2	4	15	(0.582,0.595)	47
0.2	5	20	(0.58870,0.59205)	70
2	3	8	(0.75,1.11)	15
2	3	9	(0.89,1.05)	20
2	3	10	(0.97,1.05)	22
2	4	11	(0.970,1.044)	40
2	4	12	(0.970,1.044)	40
2	4	13	(0.976,1.041)	43
2	4	14	(0.982,1.029)	45
2	4	15	(1.006,1.027)	50
2	5	16	(1.008,1.027)	58
2	5	18	(1.010,1.026)	60
2	5	20	(1.0205,1.0232)	70
2	5	21	(1.0209,1.0224)	80
20	3	8	(1.95,2.40)	30
20	5	17	(2.17,2.25)	40

sionality must be chosen consistent with

$$Dm(\sigma_1,\sigma_2)\leq\begin{cases}(q_{\max}+1)(q_{\max}+2)/2 & \text{if } (\sigma_1,\sigma_2)\neq(1,1)\\ (q_{\max})(q_{\max}+1)/2 & \text{if } \sigma_1=\sigma_2=1\end{cases}. \tag{4.23}$$

The reason for the above is simple. The sequence defined by (4.21) orders the (i,j) in terms of increasing $i+j$. Thus if $(i,j)_{k,l}$ satisfy $1\leq k,l\leq(q_{\max}+1)(q_{\max}+2)/2$, then $i_k+i_l+j_k+j_l\leq 2(q_{\max})$ and $1+i_k+i_l+j_k+j_l\leq 2(q_{\max})+1$. Both of these correspond to moments generated from the $q_{\max}$ missing moments. That is, the sums above identify the antidiagonals of maximum order $2(q_{\max})+1$, which in turn correspond to the moments that can be generated from the first $q_{\max}$ missing moments.

If $1\leq k,l\leq(q_{\max})(q_{\max}+1)/2$, then $2+i_k+i_l+j_k+j_l\leq 2(q_{\max}-1)+2$. This also corresponds to the set of moments which can be generated from the first $q_{\max}$ missing moments.

The programming logic for the system defined by (4.19) and (4.20) is *completely* identical to the one-dimensional system described in the Sec. III. Some results are given in Table II for the magnetic-field-strength values $B=0.2$, 2, and 20 a.u.

V. CONCLUSION

We have developed a linear-programming reformulation of the general moment method for generating lower and upper bounds to energy levels of multidimensional singular Schrödinger equations. We have applied this new method to the three-dimensional quadratic Zeeman effect in the transition region. Our bounds compare well with the most reliable results given in Ref. 10.

The reason why we have not yet provided lower and upper bounds with more significant figures, and for more magnetic field values, is that we are using available linear-programming software not specifically designed for our needs. The type of linear-programming application required by us is not of the standard kind. As such, we need to develop a more suitable code. An example of our needs is the fact that to achieve higher precision in our data, we must work with extremely small convex domains at the threshold of feasibility. We are currently developing such an algorithm,[15] and will communicate a more comprehensive set of results in a future work. In particular, we shall focus on bounds for the second transition region, corresponding to field strengths of 10^8–10^{13} G. Despite the preceding remarks, the results quoted in Table II provide definite and unprecedented information on the ground state of the system.

ACKNOWLEDGMENTS

One of us (C.R.H.) gratefully acknowledges support through National Science Foundation (NSF) Grant No. RII-8312. In addition, we thank Professor J. Cizek and Professor E. Vrscay for useful discussions and their support.

APPENDIX

We give below all of the necessary results of the "problem of moments" relevant to our work. We shall first

consider the one-dimensional problem.[8]

Historically, the Stieltjes-moment problem was first solved in 1895. In 1921, the Hamburger-moment problem was solved. Although the latter includes the former, we shall present these in their proper historical order. As indicated in Sec. II, "non-negative" is used in the conventional sense and also refers to a function which is positive on a support set of nonzero measure.

1. Stieltjes-moment problem

Given a sequence $u(p)$, $p=0,1,2,\ldots$, there exists a non-negative function $f(x)$ defined on $[0,\infty)$ such that $u(p)=\int_0^\infty dx\, x^p f(x)$, if and only if

$$\Delta_{m,n}>0 \quad \text{for } m=0,1, \quad n\geq 0\ , \tag{A1}$$

where

$$\Delta_{m,n}[u]\equiv\det\begin{bmatrix} u(m) & u(m+1) & \cdots & u(m+n) \\ u(m+1) & u(m+2) & \cdots & u(m+n+1) \\ \vdots & \vdots & \vdots & \vdots \\ u(m+n) & u(m+n+1) & \cdots & u(m+2n) \end{bmatrix}\ . \tag{A2}$$

The $\Delta_{m,n}$'s are referred to as Hankel-Hadamard determinants. The Stieltjes theorem by itself is indeterminate. That is, there may be more than one non-negative distribution having the same moments. Additional information, such as the satisfaction of the Carleman conditions,[8] is required before one can conclude that a unique solution exists. The fact that our applied interests involve moment recursion relations associated with determined physical systems should make our entire moment approach completely deterministic with respect to identifying the unique physical solution desired. This is clearly supported by the numerical results cited.

The "necessary" aspect of the Stieltjes-moment theorem follows from the fact that on the half-real axis $[0,\infty)$ any non-negative real polynomial $P(x)\geq 0$ must be of the form $P(x)=x^i(\sum_i C_i x^i)^2$, where $i=0,1$, and the C's are real and arbitrary. The inequalities in (A1) follow from considering the integral relations $\int_0^\infty P(x)f(x)\geq 0$ for all non-negative polynomials on the half-real axis. The "sufficiency" aspect of the Stieltjes theorem (i.e., proving the existence of some non-negative distribution on the half-real axis) is much more difficult. We refer the reader to the relevant references for further details.[8]

2. Hamburger-moment problem

Given a sequence $m(p)$, $p=0,1,2,\ldots$, there exists a non-negative function $g(x)$ defined on $(-\infty,+\infty)$ such that $m(p)=\int_{-\infty}^{\infty} g(x)x^p dx$, $p=0,1,2,\ldots$, if and only if

$$\Delta_{0,n}[m]>0 \quad \text{for all } n\geq 0\ . \tag{A3}$$

As for the Stieltjes case, the "necessary" aspect of the Hamburger-moment theorem follows from the integral inequalities $\int_{-\infty}^{\infty} dx\, P(x)g(x)\geq 0$ for all non-negative polynomials on the entire real axis. Unlike the Stieltjes case, any non-negative polynomial on $(-\infty,+\infty)$ must be of the form $P(x)=(\sum_i C_i x^i)^2$. The converse or "sufficiency" aspect of the Hamburger-moment theorem is involved, and once again the reader is referred to the relevant references.

It is natural to seek at an intuitive level some understanding of how the Stieltjes- and Hamburger-moment theorems are interrelated. Indeed, suppose $f(x)$ is defined on the entire real axis $(-\infty,+\infty)$ and the nature of f's Hamburger moments are such that uniqueness is ensured [i.e., the only distribution on $(-\infty,+\infty)$ having f's moments is f]. We may then ask, what are the necessary and sufficient conditions on f's Hamburger moments in order for $f(x)$ to be zero on the negative axis and non-negative on $[0,+\infty)$? One simple solution would be to impose (A3) on the functions $f(x)$ and $xf(x)$. One would then conclude that $f(x)\geq 0$ and $xf(x)\geq 0$ for all x. The only consistent answer is that $f(x)=0$ for $x<0$ and $f(x)\geq 0$ throughout $[0,\infty)$. Furthermore, the Hamburger moments would effectively become Stieltjes moments. This line of reasoning correctly leads us to the actual Stieltjes-moment relations, as summarized by the inequality relations in (A1).

Intuitive speculations can be paradoxically erroneous. Thus one may ask, suppose $Z(x)$ is zero throughout the negative real axis, could we not then use the Hamburger-moment theorem to specify conditions under which it would be non-negative throughout the non-negative real axis $[0,\infty)$? This would lead to only one set of determinant inequalities $\Delta_{0,n}>0$ for all n. This is clearly wrong from the perspective of the Stieltjes-moment theorem which requires two sets of determinant inequalities. Indeed, because of its indeterminate nature the Hamburger-moment-theorem inequalities could not be used to conclude that the only non-negative distribution on $(-\infty,+\infty)$ having Z's moments is Z. Thus we could not conclude that $Z(x)\geq 0$ for $x\geq 0$. Instead, we can only conclude that there exists some non-negative distribution on $(-\infty,+\infty)$ having Z's moments.

To summarize all of the preceding, the Stieltjes- and Hamburger-moment theorems are indeterminate. The Hamburger problem is potentially more indeterminate than the Stieltjes case. Indeed, as indicated on page X of the comprehensive work by Shohat and Tamarkin,[8] it is possible for a given Hamburger problem to be indeterminate; however, if the Hamburger moments $m(p)$ are taken to be the Stieltjes moments of some distribution on $[0,\infty)$, $m(p)=u(p)$, the Stieltjes problem can be determinate.

As indicated previously, the derivation of the Hamburger Hankel-Hadamard inequalities for a non-negative

function $g(x)$ follows from the following integral inequalities, valid for arbitrary C_i's (not all zero):[8]

$$\int_{-\infty}^{\infty} dx \left[\sum_{i=0}^{I} C_i x^i \right]^2 g(x) > 0, \quad I \geq 0 . \tag{A4}$$

An alternate form for (A4) is the quadratic-form expression

$$\sum_{i,j=0}^{I} C_i m(i+j) C_j > 0 \quad \text{for } C_{0,1,\ldots,I} \text{ not all zero} . \tag{A5}$$

The expression above requires that all the eigenvalues of the symmetric moment matrix be positive. This is equivalent to requiring that the Hankel-Hadamard determinants (A3) be positive.[8] The proof that (A4) or (A5) are sufficient for establishing that $g(x)$ must be non-negative, on the entire real axis, is much harder, and we refer the reader to the relevant references. The importance of the integral formulation in (A4) is that it serves to define a linear formulation of the nonlinear moment inequalities in (A3) and to motivate the multidimensional generalization of the Hankel-Hadamard inequalities.

3. Multidimensional generalizations

We now describe the multidimensional analogue of the preceding formalism. We shall not give the form of the multidimensional Hankel-Hadamard conditions. They can be readily deduced from the linear-quadratic-form relations to be given below.[3,16] Of greater importance to us will be the linear relations that ensue.

Let us define the integral function $I_D(x)$ with respect to some two-dimensional function $h(x,y)$:

$$I_D(x) = \int_{-\infty}^{\infty} dy \left[\sum_{j=0}^{J} D_j y^j \right]^2 h(x,y) , \tag{A6}$$

where the D_j's and J are arbitrary and fixed. If one imposes the conditions (A3) or (A4) on $I_D(x)$ then it follows that $I_D(x) \geq 0$ for all x. If we now vary the D_j's and J, then we can conclude that at each x value, the function $h(x,y)$ must be non-negative for all y. It therefore follows that requiring

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \left[\sum_{i=0}^{I} C_i x^i \right]^2 \left[\sum_{j=0}^{J} D_j y^j \right]^2 h(x,y) > 0 , \tag{A7}$$

for all C_i, D_j (not all C_i's or D_j's equal to 0), $0 \leq i \leq I$, $0 \leq j \leq J$, establishes $h(x,y)$ as non-negative throughout the two-dimensional plane.

Bearing in mind that the set of all two-dimensional polynomials $(\sum_{i,j=0}^{I} \Omega_{ij} x^i y^j)$, for $I \geq 0$, includes the special case $(\sum_i C_i x^i)(\sum_j D_j y^j)$, it follows that an alternate and more effective set of necessary and sufficient conditions for $h(x,y)$ to be non-negative is

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \left[\sum_{i,j=0}^{I} \Omega_{ij} x^i y^j \right]^2 h(x,y) > 0 , \tag{A8}$$

for all possible Ω_{ij} values (not all 0) and I.

The two-dimensional Stieltjes-moment problem would correspond to imposing (A8) on $f(x,y)$, $xf(x,y)$, and $yf(x,y)$. One would conclude that each of these must be non-negative throughout the entire two-dimensional x-y plane. That is, $f(x,y) \geq 0$ for the non-negative quadrant and zero elsewhere. In addition, the Hamburger moments for such an $f(x,y)$ would really be Stieltjes moments.

As for the one-dimensional case, (A8) can be easily converted into a quadratic-form expression involving the moment matrix $m(i_k+i_l, j_k+j_l)$, provided some coordinate pair sequence ordering is adopted [i.e., $(0,0)_1, \ldots, (i,j)_k, \ldots$]. The multidimensional counterpart to the one-dimensional Hankel-Hadamard nonlinear moment inequalities immediately follows.[3,16]

As for the one-dimensional case, the integral representation previously mentioned also serves to define the linear formulation of the multidimensional moment method. Because the quadratic Zeeman problem discussed in Sec. IV is developed in terms of a Stieltjes problem, we focus on such cases in the remainder of this discussion.

The missing-moment structure of the quadratic Zeeman problem (refer to Sec. IV) dictates the appropriate coordinate pair ordering to be

$$(0,0)_1, (1,0)_2, (0,1)_3, (2,0)_4, (1,1)_5, (0,2)_6, (3,0)_7, \ldots . \tag{A9}$$

Thus the $(i,j)_k$th pair occupies the $k = (i+j)(i+j+1)/2 + j + 1$ position. Note that the pairs are grouped in terms of increasing $i+j$. In the following discussion we shall implicitly assume that the coordinate pairs $(i,j)_k = (i_k, j_k)$ are ordered in accordance with the preceding.

As discussed in Sec. IV, upon transforming to parabolic coordinates the symmetric nature of the ground state $[f(x,y) = f(y,x)]$ ensures that the non-negativity conditions for the two-dimensional Stieltjes function $f(x,y)$ (restricted to $x \geq 0$, $y \geq 0$) are completely specified by demanding non-negativity for the Hamburger extensions $h_1(x,y) = f(x,y)$ and $h_2(x,y) = xf(x,y)$ [apply (A8) to $h_{1,2}$]. That is, because of the x-y exchange symmetry no new constraints are to be obtained by looking at $yf(x,y)$. This is a matter of principle. However, since in practice we can only work with a finite number of constraints, it is possible that some numerical enhancement of the tightness of the eigenvalue bounds can be obtained by working with additional types of moment relations. Indeed, such improvement is found by also considering the non-negativity conditions for the Hamburger extension of $h_3(x,y) = xyf(x,y)$. Thus for the quadratic Zeeman problem the necessary and sufficient conditions for non-negativity of $f(x,y)$, on the non-negative quadrant, are to be obtained from applying (A8) to each of the functions $f(x,y)$, $xf(x,y)$, and $xyf(x,y)$.

In keeping with all the specifications in the preceding, the relevant quadratic-form expressions for the two-dimensional Stieltjes-moment problem, as applied to the quadratic Zeeman effect, are $(u(i,j)$

$$= \int_0^\infty dx \int_0^\infty dy\, x^i y^j f(x,y))$$

$$\sum_{k,l=1}^{Dm(\sigma_1,\sigma_2)} \Omega_{i_k j_k}^{(\sigma_1,\sigma_2)} u(\sigma_1+i_k+i_l, \sigma_2+j_k+j_l) \Omega_{i_l j_l}^{(\sigma_1,\sigma_2)} > 0 , \tag{A10}$$

where $(\sigma_1,\sigma_2)=(0,0)$, (1,0), and (1,1). For each of these three cases, the $\Omega_{i_k j_k}^{(\sigma_1,\sigma_2)}$ correspond to different sets of variables. The dimensionality $Dm(\sigma_1,\sigma_2)$ is specified in (4.23).

*On leave from Centre d'Etudes Nucléaires de Saclay, 91191 Gif-sur-Yvette, France.

[1]C. R. Handy and D. Bessis, Phys. Rev. Lett. **55**, 931 (1985).
[2]C. M. Bender and S. A. Orzag, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978).
[3]D. Bessis and C. R. Handy, Int. J. Quantum Chem. Quantum Chem. Symp. **20**, 21 (1986).
[4]C. R. Handy, J. Phys. A **18**, 3593 (1985).
[5]D. Bessis, E. R. Vrscay, and C. R. Handy, J. Phys. A **20**, 419 (1987).
[6]C. R. Handy, D. Bessis, and R. M. Williams, J. Math. Phys. **29**, 717 (1988).
[7]J. Cizek and E. R. Vrscay, Int. J. Quantum Chem. **21**, 27 (1982); **28**, 665 (1985).
[8]J. A. Shohat and J. D. Tamarkin, *The Problem of Moments* (American Mathematical Society, Providence, RI, 1963); G. A. Baker, Jr., *Essentials of Padé Approximants* (Academic, New York, 1975).
[9]V. Chvatal, *Linear Programming* (Freeman, New York, 1983).
[10]J. C. Le Guillou and J. Zinn-Justin, Ann. Phys. (N.Y.) **147**, 57 (1983).
[11]M. Reed and B. Simon, *Methods of Modern Mathematical Physics, Vol. IV, Analysis of Operators* (Academic, New York, 1978).
[12]T. M. Antonsen, Jr., A. Ferreira, and J. J. Ramos, Plasma Phys. **24**, 197 (1982).
[13]J. Avron, I. Herbst, and B. Simon, Phys. Rev. Lett. **62A**, 214 (1977).
[14]P. O. Lowdin, Int. J. Quantum Chem. **21**, 69 (1981).
[15]C. R. Handy, D. Bessis, G. Sigismondi, and T. D. Morley, Phys. Rev. Lett. **60**, 253 (1988).
[16]A. Devinatz, Duke Math. J. **24**, 481 (1957).

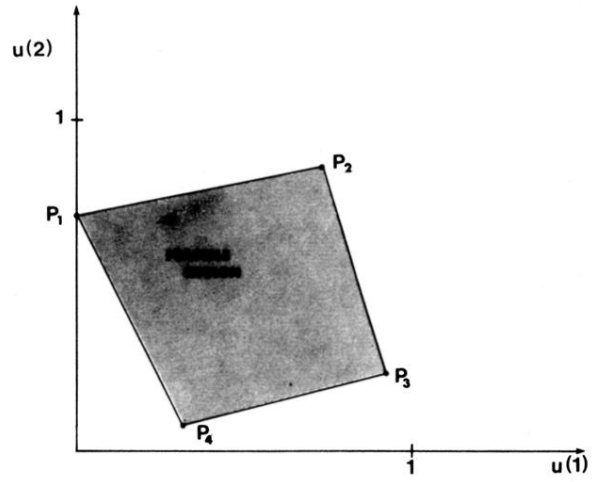

FIG. 1. Symbolic "feasible region" for the sextic potential problem.

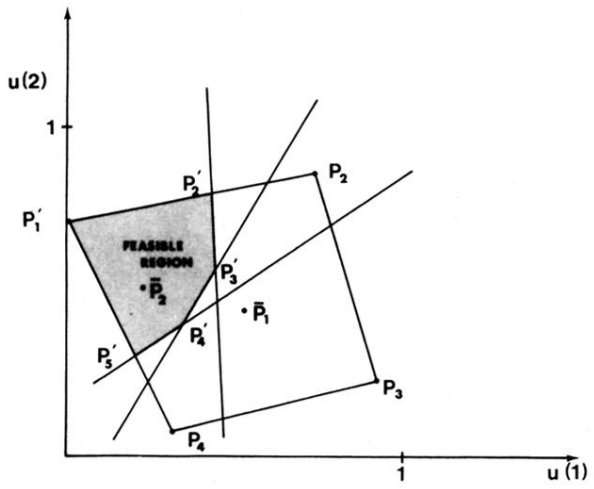

FIG. 2. Symbolic inductive "cutting" procedure obtained through the linear-programming method.