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Euclidean time formulation of the eigenvalue moment method: a moment problem-convexity analysis of Barnsley's theorem

C R Handy and G L Ndow

Department of Physics and Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia 30314, USA

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Abstract. Over the last few years, the eigenvalue moment method (EMM) has been shown to be very effective in generating converging lower and upper bounds to the discrete low-lying spectrum of singular multidimensional Hamiltonians. In this work we adapt the EMM approach to the Euclidean time-dependent Schrödinger equation. The result is a new EMM theory which significantly overlaps with other eigenenergy bounding theories and which leads to a more rigorous algorithmic formulation than previously available.

1. Introduction

The eigenvalue moment method (EMM) is a non-perturbative theory for generating converging lower and upper bounds to the low-lying energy eigenvalues of quantum Hamiltonians. It has been particularly successful in the analysis of singular problems for which standard methods, such as large-order perturbation theory, are ineffective (Handy and Bessis 1985, Handy *et al* 1988a, b).

The conventional EMM theory formulation involves the transformation of the time-independent Schrödinger equation eigenvalue problem, $H\Psi = E\Psi$, into a pure moment problem involving the moments of the wavefunction $\{u(p)\}$. An analysis of the positivity structure of the wavefunction leads to an infinite family of constraints on the energy, E, and the moments as symbolized by (for one-space dimension problems)

$$\Delta_{m,n}\{E; u\} \geqslant 0 \qquad \text{for } m = 0, 1 \text{ and } n \geqslant 0 \tag{1.1}$$

where the constraints correspond to Hankel-Hadamard (HH) determinants.

Given a maximum HH-order, N (i.e. $n \leqslant N$), one must determine all the energy parameter values for which the corresponding finite set of HH constraints admit a moment-solution, $\mathbf{U}_N(E)$. Generally, the admissible set of energy values, $\mathbf{F}_N$, will define an open interval $(E_N^{(-)}, E_N^{(+)})$. As the order N increases, the endpoints define converging lower and upper bounds to the corresponding physical eigenenergy value, E_p.

For an arbitrary energy parameter value, E, the determination of the existence or non-existence of $\mathbf{U}_N(E)$ may be obtained by either directly solving the nonlinear HH constraints or solving an equivalent set of linear moment constraints (made possible by an appropriate linearization of the HH constraints). The latter involves the application of a linear programming (LP) based *cutting method* (Handy *et al* 1988a, b).

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Regardless of which approach is adopted, from a practical perspective, one must always partition an arbitrary energy interval and determine at each partition point whether all the HH inequalities, up to order N, are satisfied. Those partition points admitting moment solutions are then used to approximate the feasible energy interval, $(E_N^{(-)}, E_N^{(+)})$.

Within the conventional multidimensional EMM theoretical formulation, there is no proof available that ensures that the feasible set of energy values (as $N \to \infty$) is indeed an interval; although the EMM theory does guarantee that the infimum and supremum to $\mathbf{F}_N$ define converging lower and upper bounds, respectively, to the true physical eigenenergy value. In principle, there could be several or many feasible energy intervals (to be referred to as *feasible energy interval segmentation*). In practice, this has not been observed (the analysis of the sextic anharmonic oscillator in Handy *et al* (1988a) has programming errors; subsequent investigations showed no feasible energy interval segmentation). Numerically, it appears that at each order of the HH analysis only one continuous feasible energy interval remains. Indeed, for the one-dimensional Schrödinger problem, Ashbaugh and Sundberg (1991) have given a rigorous mathematical proof that no 'feasible energy interval segmentation' can occur for most potentials.

From an algorithmic standpoint, the preceding issues are clearly important (particularly for multidimensional problems) and underscore the necessity for being careful in selecting an adequately small mesh size for the energy space partition; otherwise, it is possible that the existence of several or many feasible energy intervals can go undetected and affect the accuracy of the generated bounds.

In this work we will develop an alternate formulation of the EMM theory which has none of the above theoretical/algorithmic limitations. Specifically, we will study both finite and infinite dimensional (with regards to the number of moment variables) analogues of the generic Euclidean time dependent problem

$$H\Psi(x, t) = \partial_t \Psi(x, t) \tag{1.2}$$

analysed from a *moment problem* (Shohat and Tamarkin 1963) perspective, in order to determine the proper initialization (at '$t = 0$') corresponding to a configuration space solution which evolves for all time as a bounded (finite power moments) and positive function.

The immediate outcomes of the Euclidean-time EMM formulation (ET-EMM) to be presented are:

(1) The ET-EMM approach generates energy bounds automatically.

(2) The ET-EMM generated feasible energy values define an open interval.

(3) The ET-EMM theory will take on a structure (within the moments' representation) analogous to that of Barnsley's theorem (Barnsley 1978) in configuration space (the 'bath-tub' theorem) which states that for a given Schrödinger Hamiltonian, H, and an arbitrary positive wavefunction configuration, $\Phi(x)$, the infimum over x of the ratio $H\Phi(x)/\Phi(x)$ is an immediate lower bound to the ground state energy, E_g:

$$\inf_x \{[H\Phi(x)]/\Phi(x)\} \leqslant E_g. \tag{1.3}$$

It is well known that this theory has two important shortcomings: (i) it can be numerically difficult to locate the infimum; (ii) there is no systematic way of improving the lower bounds; that is, one does not know how to update a given $\Phi(x)$ so as to

yield an improved lower bound. In contrast, ET-EMM offers a better theoretical formulation by which to effectively address these issues.

Despite all the above, the Euclidean time formulation is not as robust as the time independent formulation (EMM). That is, the convergence rates of the eigenenergy bounds cited in the tables are rather slow. The temptation is to say that because one is working with many more variables or *missing moments* (i.e. a much larger dimensioned space) it is reasonable to expect a slower convergence rate. Nevertheless, from a theoretical standpoint ET-EMM has much to offer. In particular, as alluded to before, it suggests that the general (multidimensional) time-independent EMM formulation is more than likely not plagued by feasible energy interval segmentation, as also argued (for the one space dimension case) by Ashbaugh and Sundberg (1991).

Finally, this work is a consequence of applying the basic principles governing the use of the general moment method (Handy and Lee 1991). We do not present an exhaustive study of the numerical nature of the results. Instead, we are more interested in assessing the consistency and consequences of the basic theory itself, as articulated in the subsequent discussion.

2. The Euclidean-time EMM theory

2.1. Finite dimensional systems

Although EMM theory can be (and has been) applied to arbitrary excited states (Handy and Lee 1991), for simplicity we will limit all of the remaining discussion in this paper to the ground state case only.

Consider the following finite dimensional analogue of equation (1.2) (unless otherwise indicated, repeated indices denote implicit summations)

$$[\mathbf{M}_{ij} - \varepsilon\delta_{ij}]v_j(t) = \partial_t v_i(t) \qquad 1 \leqslant i, j \leqslant D \tag{2.1}$$

where D is the dimension. The significance of the ε parameter will be explained shortly. We will assume that the matrix $\mathbf{M}$ is symmetric and of Sturm-Liouville (SL) type. The latter condition requires that the ground state (lowest eigenvalue) eigenvector have all its components non-zero and of uniform signature, which can be taken to be positive. Accordingly, the ground state eigenvector will be referred to as a positive vector. This property is also shared by all bosonic ground state wavefunctions (Handy and Bessis 1985). Returning to (2.1), it follows that each 'excited' eigenvector (including any superposition of degenerate vectors) must have at least one negative component (because of mutual orthogonality with the ground state eigenvector).

From the Rayleigh-Ritz variational theorem, it can be immediately concluded that if a Hermitian matrix has all its off diagonal elements negative (non-zero) then it is of SL type. It is interesting to note that a (symmetric) discretization of the Schrödinger Hamiltonian operator results in an SL matrix.

With respect to (2.1) we now ask:

Is there a unique solution to equation (2.1) which is positive for all time and has finite (Stieltjes) power moments for each compound:

$$0 < w_i(p) \equiv \int_0^\infty \mathrm{d}t\, t^p v_i(t) < \infty?$$

If the answer is yes, then the basic EMM theory guarantees that converging lower and upper bounds to the ground state eigenvalue can be generated (Handy and Lee 1991). This is immediately true if the matrix is of SL type and the ε parameter lies between the ground (λ_1) and first excited (λ_2) state eigenvalues: $\lambda_1 < \varepsilon < \lambda_2$. The proof is easy. First, as implied by the previous notation, let us denote the eigenvectors of $\mathbf{M}$ by ϑ^j, where $j = 1$ corresponds to the ground state. The associated eigenvalues are denoted by λ_j, $\mathbf{M}\vartheta^j = \lambda_j \vartheta^j$.

The general solution to (2.1) satisfies

$$v(t) = \sum_{j=1}^{D} c_j \vartheta^j \exp([\lambda_j - \varepsilon]t). \tag{2.2}$$

As long as $\lambda_1 < \varepsilon \leqslant \lambda_2$, then the only bounded solution with finite $w_i(p)$ power moments is that corresponding to $c_i = 0$, for $i \geqslant 2$. In addition, this solution is positive for all time as long as the trivial factor, c_1, is positive. Thus in this case, application of the EMM philosophy (in a manner to be described below) must result in converging lower and upper bounds to the ground state eigenvalue.

The preceding argument did not require positivity. If we relax the condition $\lambda_1 < \varepsilon < \lambda_2$ and allow

$$\lambda_1 < \lambda_2 < \ldots < \lambda_k < \varepsilon \leqslant \lambda_{k+1} \tag{2.3}$$

for some arbitrary 'k' value, then one can still show that there is a unique solution that is positive and has finite power moments. Consider the sum

$$\sum_{j=1}^{k} c_j \vartheta^j \exp([\lambda_j - \varepsilon]t) \tag{2.4}$$

for arbitrary c_js. This represents the general solution to (2.1) which is asymptotically bounded under condition (2.3), and consequently has finite power moments.

A simple asymptotic analysis shows that at sufficiently large times, only the slowly varying solution corresponding to $j = k$ will dominate; however, unless $k = 1$, the corresponding eigenvector cannot have all its components positive. Accordingly, the ground state vector term in (2.4) generates the only bounded and positive solution for all time. *Thus, as long as ε is an upper bound to the ground state eigenvalue, there is no additional restriction on it.* The same argument should apply to continuous systems.

Proceeding with the necessary ET-EMM analysis, we can transform (2.1) into a multicomponent Stieltjes moment equation upon integrating both sides by $\int_0^\infty \mathrm{d}t\, t^p$:

$$[\mathbf{M}_{ij} - \varepsilon\delta_{ij}]w_j(p) = -\delta_{0,p}v_i - pw_i(p-1). \tag{2.5}$$

The v_i expression denotes the $t = 0$ value of the time dependent 'solution' to (2.1).

From (2.5) one can generate all the w-moments, once the v_i's are specified. Clearly, this dependence is linear. Specifically:

$$[\mathbf{M}_{ij} - \varepsilon\delta_{ij}]w_j(0) = -v_i \tag{2.6}$$

$$[\mathbf{M}_{ij} - \varepsilon\delta_{ij}]w_j(p) = -pw_i(p-1) \qquad \text{for } p \geqslant 1. \tag{2.7}$$

One can express the linear dependence of the ws on the vs through the relation

$$w_i(p) = \sum_{j=1}^{D} M(p; i, j)v_j \tag{2.8}$$

where the $M(p; i, j)$ coefficients satisfy the relation

$$[\mathbf{M}_{ij} - \varepsilon\delta_{ij}]M(p; j, k) = -\delta_{p,0}\delta_{i,k} - pM(p-1; i, k). \tag{2.9}$$

It is readily apparent that the w–v system is homogeneous. We may then impose a convenient normalization:

$$\sum_{i=1}^{D} v_i = 1. \tag{2.10}$$

We will constrain v_1 through the above. Substituting

$$v_1 = 1 - \sum_{i=2}^{D} v_i$$

into (2.8), we obtain

$$w_i(p) = N(p; i, 1) + \sum_{j=2}^{D} N(p; i, j)v_j \tag{2.11}$$

where

$$N(p; i, j) = \begin{cases} M(p; i, 1) & \text{if } j = 1 \\ M(p; i, j) - M(p; i, 1) & \text{if } j \geqslant 2. \end{cases} \tag{2.12}$$

Applying the EMM philosophy, we can 'quantize' or determine the ground state solution by imposing on the w-moments (and thereby on the v-initialization variables) the requirement that they correspond to a positive solution for all time: $v(t) > \mathbf{0}$, for $t \geqslant 0$. Note, the fact that we are implicitly working with finite ws automatically restricts us to the space of bounded time-dependent configurations with finite power moments, as discussed earlier.

Given the representation in (2.11), we proceed to impose the *necessary and sufficient* constraints for the w-moments to correspond to the moments of a positive function. This can be done through the appropriate nonlinear (in the moments) Hankel-Hadamard (HH) inequality constraint relations (Handy and Bessis 1985):

$$\text{Det}\{w_i(m + n_1 + n_2; v)\} > 0 \qquad \text{for } 1 \leqslant i \leqslant D \qquad m = 0, 1 \tag{2.13}$$

and

$$0 \leqslant n_1, n_2 \leqslant N \qquad \text{where } 0 \leqslant N < \infty.$$

For fixed 'i', 'm' and 'N' values, the expression within the brackets corresponds to a Hankel matrix of dimension $N+1$. We have made explicit the w's dependence on the vector v. Thus, one can regard (2.13) as defining constraints within the positive sector of the D-dimensional space $v_1 \otimes v_2 \otimes \ldots \otimes v_D$.

Let us denote by $\mathbf{V}_N$ the solution set to (2.13) up to order N. It can be shown that it must be convex. In the infinite limit $N \to \infty$, $\mathbf{V}_\infty$ must reduce to a D-dimensional point corresponding to the initialization values of the true solution to (2.1), subject to the normalization in (2.10), and denoted by ϑ^1.

2.2. Generating eigenvalue bounds

It is manifestly clear that no explicit reference to an eigenvalue parameter appears within the preceding formalism. How then is one then to generate converging eigenvalue bounds?

The first observation is that the desired v-solution, ϑ^1, must lie in each of the $\mathbf{V}_N$, for arbitrary N. This is because it always satisfies the HH constraints at each order N.

Secondly, if we denote by ϑ_i^1 the ith component of the true solution, then (note: no summation over 'i')

$$[\vartheta_i^1]^{-1}\left[\sum_{j=1}^{D}\mathbf{M}_{ij}\vartheta_j^1\right]\equiv\lambda_1 \qquad \text{for each } i. \tag{2.14}$$

Let us define the ratios:

$$R_i[v]\equiv[v_i]^{-1}\left[\sum_{j=1}^{D}\mathbf{M}_{ij}v_j\right]. \tag{2.15}$$

It must then follow that for each $R_i[v]$, its infimum and supremum values over the set $\mathbf{V}_N$ must define lower and upper bounds, respectively, to the true ground state eigenvalue, λ_1. That is:

$$\inf_{\mathbf{V}_N}\{R_i[v]\}<\lambda_1<\sup_{\mathbf{V}_N}\{R_i[v]\} \tag{2.16}$$

since $R_i[\vartheta^1]=\lambda_1$ and ϑ^1 lies in $\mathbf{V}_N$.

For future reference, we shall denote each of the extremal values by:

$$R_i^-\equiv\inf_{\mathbf{V}_N}\{R_i[v]\} \tag{2.17}$$

$$R_i^+\equiv\sup_{\mathbf{V}_N}\{R_i[v]\}. \tag{2.18}$$

We note several important features of (2.16). First, it (as well as its Schrödinger equation counterpart to be discussed) involves the analogous ratios as those appearing within Barnsley's theory (refer to equation (1.3)). Second, eigenvalue bounds are generated automatically without having to numerically define a partitioning of the λ-space.

At first glance one might expect that the manifest nonlinear v-dependence of the $R_i[v]$ ratios might complicate the determination of the extremal values over the set $\mathbf{V}_N$. Actually, this is not the case. For given 'i' the $R_i[v]$ function is linearly dependent on the variables $1/v_i$ and $\{v_j/v_i|j\neq i\}$.

The set $\mathbf{V}_N^{(-,i)}\equiv\{(v_1/v_i, v_2/v_i, \ldots, v_i^{-1}, v_{i+1}/v_i, \ldots, v_D/v_i)|v\in\mathbf{V}_N\}$ is convex. The most immediate proof follows from the linear programming reformulation of the basic EMM theory (the *cutting method*) which says that $\mathbf{V}_N$ (a bounded set, refer to (2.10)) can be defined by an infinite set of linear inequalities of the form

$$\sum_{j=1}^{D}A_{lj}v_j\leqslant B_l \qquad \text{for } l=1,\ldots,\infty.$$

Since $v_i>0$, upon dividing all the linear inequalities by v_i there follows the infinite *family of linear inequalities:*

$$\sum_{j=1}^{i-1}A_{lj}v_j/v_i-B_l/v_i+\sum_{j=i+1}^{D}A_{lj}v_j/v_i\leqslant -A_{li}.$$

A basic theorem of linear programming theory is that the solution set to any family of linear inequalities must be convex (Chvatal 1983). Thus $\mathbf{V}_N^{(-,i)}$ is convex. The importance of this result is that in principle the determination of the extremal values

in (2.16) is much simpler than that of Barnsley's theorem. The former simply involves the determination of the extremal values of a linear function over a nonlinear convex set. Indeed, the extremal values must lie on the boundary of the set $(\partial \mathbf{V}_N^{(-,i)})$. This corresponds in principle to a readily implementable optimization problem with no multiminima ambiguities. Barnsley's theory can be plagued by multiminima ambiguities depending on the nature of the chosen positive configuration, as discussed in the context of (1.3).

One can proceed to implement the above optimization program provided the boundary set $\partial \mathbf{V}_N^{(-,i)}$ can be readily (numerically) identified. This can be difficult because of the increasing degree of nonlinearity as the Hankel matrix dimension, $N+1$, increases. Nevertheless, one can still implement the above program in the context of a linear programming formulation as presented in the following subsection.

2.3. Linear programming generation of eigenvalue bounds

Instead of finding the extremal values of R_i one can ask if there exists a subset $\mathbf{V}_{N,r}$ of $\mathbf{V}_N$ satisfying the additional constraint $R_i[v]=r_i$, for some arbitrary r_i value. Since $R_i[v]$ is a continuous function, only r_i values lying within the interval $[R_i^-, R_i^+]$ can yield a non-null $\mathbf{V}_{N,r}$; conversely, if r_i lies outside this interval, then $\mathbf{V}_{N,r}=\varnothing$. One can now numerically partition an arbitrary subset of the real line and determine if $\mathbf{V}_{N,r}$ exists or not. Clearly, this process can yield arbitrarily accurate lower and upper bound estimates to the values R_i^- and R_i^+, respectively. Note that although we are again using partitioning, as in the time-independent formulation of the EMM theory, the ET-EMM formulation guarantees that only one continuous feasible r_i interval exists.

One effective method for determining the existence or non-existence of $\mathbf{V}_{N,r}$ is to use the linear programming based *cutting method*. This will also entail using r_i (or equivalently R_i) as a parameter. Proceeding with the latter, we must invert the $R_i - v$ dependence (2.15) and constrain one of the vs. Any of the $R_i[v]$ functions may be considered; however, for the $i=1$ case the fact that v_1 is constrained through (2.10) complicates the ensuing analysis. For this reason, we prefer the restriction: $i>1$.

Combining (2.10) and (2.15) we have

$$R_i = \left[\mathbf{M}_{i1} \left\{ 1 - \sum_{j=2}^{D} v_j \right\} + \sum_{j=2}^{D} \mathbf{M}_{ij} v_j \right] \Big/ v_i \tag{2.19}$$

or

$$v_i R_i = \mathbf{M}_{i1} + \sum_{j=2}^{D} [\mathbf{M}_{ij} - \mathbf{M}_{i1}] v_j \tag{2.20}$$

that is, if we assume that $i \neq D$, then

$$v_i [R_i - \mathbf{M}_{ii} + \mathbf{M}_{i1}] = \mathbf{M}_{i1} + \sum_{j=2 \text{ and } \neq i}^{D} [\mathbf{M}_{ij} - \mathbf{M}_{i1}] v_j. \tag{2.21}$$

It is evident from (2.21) that if one solves for v_i in terms of the other vs and R_i, then there is the potential problem of encountering singularities as R_i is varied. Accordingly, it is preferable to eliminate anyone of the other v_js, since no R_i dependent denominator is encountered. We shall eliminate v_D:

$$[\mathbf{M}_{i1} - \mathbf{M}_{iD}] v_D = \mathbf{M}_{i1} + \sum_{j=2}^{D-1} [\mathbf{M}_{ij} - \mathbf{M}_{i1} - R_i \delta_{ij}] v_j. \tag{2.22}$$

We will regard R_i as a variable parameter and $\{v_2, \ldots, v_{D-1}\}$ as the independent variables (from the *cutting method* perspective). Notice that the preceding analysis has assumed that

$$2 \leqslant i \leqslant D-1. \tag{2.23}$$

The final step is to incorporate (2.22) into (2.11). First define

$$v_D = \Omega_1 + \sum_{j=2}^{D-1} \Omega_j v_j \tag{2.24}$$

where

$$\begin{aligned} \Omega_1 &= \mathbf{M}_{i1}/[\mathbf{M}_{i1} - \mathbf{M}_{iD}] \\ \Omega_j &= [\mathbf{M}_{ij} - \mathbf{M}_{i1} - R_i\delta_{ij}]/[\mathbf{M}_{i1} - \mathbf{M}_{iD}] \qquad 2 \leqslant j \leqslant D-1. \end{aligned} \tag{2.25}$$

Incorporating (2.24) into (2.11) yields

$$w_j(p) = \mathbf{N}_s(p; j, 1) + \sum_{k=2}^{D-1} \mathbf{N}_s(p; j, k) v_k \tag{2.26}$$

where

$$\mathbf{N}_s(p; j, k) = N(p; j, k) + N(p; j, D)\Omega_k. \tag{2.27}$$

Table 1. ET-EMM formulation for the ground-state eigenvalue bounds of a $D=3$ dimensional (symmetric storage mode $\mathbf{M}_{ij}$, $i=1, \ldots, D$ and $j=1, \ldots, i$): 3, −11, 0, −4, −1, 1. Actual eigenvalues: −10.608 858 623 3, 1.527 632 114 23, 13.081 225 919 7. The 'i' refers to the index associated with the chosen $R_i[v]$ function ($2 \leqslant i \leqslant D-1$); while the N refers to the expansion order in (2.28). The ε denotes the chosen eigenvalue shift parameter (equation (2.3)).

i	N	Lower bound	Upper bound
$\varepsilon = -5.0$			
2	3	−16.0	−6.5
2	4	−12.8	−8.8
2	5	−11.5	−9.8
2	6	−10.97	−10.32
2	7	−10.75	−10.49
2	8	−10.67	−10.56
2	9	−10.64	−10.59
2	10	−10.619	−10.601
2	11	−10.613	−10.606
2	12	−10.610 4	−10.607 7
2	13	−10.609 5	−10.608 4
2	14	−10.609 15	−10.608 66
$\varepsilon = -0.1$			
2	3	−10.8	−10.5
2	4	−10.63	−10.58
$\varepsilon = 0.1$			
2	3	−10.80	−10.50
2	4	−10.63	−10.58
2	5	−10.614	−10.602

Table 2. ET-EMM formulation for the ground-state eigenvalue bounds of a $D=4$ dimensional matrix (symmetric storage mode $\mathbf{M}_{ij}$, $i=1,\ldots,D$ and $j=1,\ldots,i$): 3, −11, 2, −4, −1, 1, −2, −3, −6, 2. First three eigenvalues: −11.890 458 099 5, −1.235 757 241 69, 6.962 316 121 33. The 'i' refers to the index associated with the chosen $R_i[v]$ function ($2 \leqslant i \leqslant D-1$); while the N refers to the expansion order in (2.28). The ε denotes the chosen eigenvalue shift parameter (equation (2.3)).

i	N	Lower bound	Upper bound
$\varepsilon=-5.0$			
2	3	−17.1	−8.1
2	4	−13.61	−10.38
2	5	−12.5	−11.32
2	6	−12.107	−11.682
2	7	−11.971	−11.816
2	8	−11.919	−11.864
$\varepsilon=-0.1$			
3	2	−12.0	−11.8
3	3	−12.0	−11.8
3	4	−11.91	−11.87
$\varepsilon=5.0$			
3	2	−11.91	−11.86
3	3	−11.892	−11.889
3	4	−11.890 6	−11.890 3

Utilizing the representation in (2.26) one is ready to use the standard cutting method to obtain bounds for the lowest eigenvalue. Specifically, an equivalent linear formulation of the constraints in (2.13) is provided by the quadratic form-linear (in the moments) inequalities (Handy *et al* 1988a, b):

$$\sum_{n_1 n_2=0}^{N} C_{n_1} w_i(m+n_1+n_2; v) C_{n_2} > 0 \qquad \text{for } m=0, 1;\ N=0, 1, \ldots, \infty \tag{2.28}$$

and arbitrary C_{ni}s. Substituting (2.26) into (2.28) results in the standard linear programming based cutting method utilized in the basic EMM theory. The results of this analysis are summarized in tables 1-3. All the results are consistent with the preceding analysis.

3. ET-EMM analysis for the Schrödinger equation

We now extend the preceding formalism to the continuum case corresponding to the one-dimensional Schrödinger equation. For pedagogic reasons, we limit this discussion to the simple harmonic oscillator case. In general, the ET-EMM formulation requires working with an infinite set of variables (although at any order of the calculation one is working with a finite number of these variables); accordingly, the bounds generated through ET-EMM are slowly convergent. The real contribution of the ET-EMM theory lies in its theoretical structure which is very rich and may suggest more practical reformulations.

Consider the continuum space problem corresponding to the harmonic quantum oscillator (m = mass):

$$-\partial_x^2 \Psi(x, t) + \{mx^2 - \varepsilon\}\Psi(x, t) = \partial_t \Psi(x, t). \tag{3.1}$$

Table 3. ET-EMM formulation for the ground-state eigenvalue bounds of a $D=5$ dimensional matrix (symmetric storage mode $\mathbf{M}_{ij}$, $i=1,\ldots,D$ and $j=1,\ldots,i$): 3, −11, 2, −4, −1, 1, −2, −3, −6, 2, −1, −4, −2, −3, 4. First three eigenvalues: −13.292 380 835 8, −1.305 260 021 42, 4.390 746 126 47. The 'i' refers to the index associated with the chosen $R_i[v]$ function ($2 \leq i \leq D-1$); while the N refers to the expansion order in (2.28). The ε denotes the chosen eigenvalue shift parameter (equation (2.3)).

i	N	Lower bound	Upper bound
$\varepsilon=-5.0$			
2	2	−24.8	−6.9
2	3	−16.4	−10.7
2	4	−14.3	−12.4
2	5	−13.6	−13.0
2	6	−13.39	−13.2
2	7	−13.321	−13.265
4	2	−14.1	−12.3
4	3	−13.6	−13.0
4	4	−13.36	−13.22
4	5	−13.32	−13.27
4	6	−13.299	−13.285
4	7	−13.298	−13.290
$\varepsilon=-0.1$			
2	2	−14.1	−12.6
2	3	−13.4	−13.19
2	4	−13.33	−13.27
3	3	−13.4	−13.2
4	2	−13.5	−13.1
4	3	−13.32	−13.26
4	4	−13.30	−13.284
$\varepsilon=0.1$			
2	2	−14.0	−12.7
2	3	−13.4	−13.2
2	4	−13.31	−13.28
3	2	−13.7	−13.0
3	3	−13.34	−13.25
3	4	−13.30	−13.28
3	2	−13.5	−13.1
4	3	−13.32	−13.27

Note that a sufficiently small ε parameter is introduced in accordance with the discussion in section 2.

For Hamiltonian operators with parity invariant polynomial potentials, one can transform (3.1) into a moment problem equivalent involving the two-dimensional Stieltjes moments:

$$u(p,q)=\int_0^{+\infty} \mathrm{d}y \int_0^{+\infty} \mathrm{d}t\, y^p t^q \Psi(\sqrt{y}, t)/\sqrt{y}. \tag{3.2}$$

The Stieltjes moment equation counterpart to (3.1) is

$$mu(p+1, q) = -\delta_{q,0} v(p) + \varepsilon u(p, q) - q u(p, q-1) + 2p(2p-1) u(p-1, q) \tag{3.3}$$

where $v(p)$ is the Stieltjes moment for the initial configuration at $t = 0$,

$$v(p) = \int_0^\infty \mathrm{d}y\, y^p \Psi(\sqrt{y}, 0)/\sqrt{y}. \tag{3.4}$$

The moment variables (missing moments) for this problem are $\{v(p) | p \geq 0\}$ and the set $\{u(0, q) | q \geq 0\}$. Once these are specified, all other moments may be generated through (3.3). It is immediate to see that for the finite set of missing moment variables $\{v(p) | 0 \leq p \leq \mathbf{H}-1\}$ and $\{u(0, q) | 0 \leq q \leq V\}$ the moments $\{u(p, q) | 0 \leq q \leq V, 0 \leq p \leq \mathbf{H}+q\}$ can be generated. The linear dependence of the $u(p, q)$ moments on the missing moments can be represented as follows:

$$u(p, q) = \sum_{j=0}^{\mathbf{V}} M_1(p, q; j) u(0, j) + \sum_{i=0}^{\mathbf{H}-1} M_2(p, q; i) v(i) \tag{3.5}$$

where $q = 0, \ldots, V$ and $p = 0, \ldots, \mathbf{H}+q$. The M-coefficients satisfy

$$mM_1(p+1, q; j) = \varepsilon M_1(p, q; j) - q M_1(p, q-1; j) + 2p(2p-1) M_1(p-1, q; j) \tag{3.6}$$

$$\begin{aligned} mM_2(p+1, q; i) &= -\delta_{q,0}\delta_{p,i} + \varepsilon M_2(p, q; i) - q M_2(p, q-1; i) \\ &\quad + 2p(2p-1) M_2(p-1, q; i) \end{aligned} \tag{3.7}$$

together with the initialization conditions

$$M_1(0, q; j) = \delta_{q,j}, \qquad \text{for } 0 \leq q, j \leq \mathbf{V} \tag{3.8}$$

and

$$M_2(0, q; i) = 0 \qquad \text{for } 0 \leq q \leq \mathbf{V} \qquad \text{and } 0 \leq i \leq \mathbf{H}-1.$$

It is a well known theorem that the bosonic ground state wavefunction must be of uniform signature, which can be taken to be positive (Handy and Bessis 1985). Our objective then is to quantize the above system by requiring that the missing moment variables be constrained to correspond to a solution that is asymptotically bounded (therefore having finite two-dimensional Stieltjes moments in space and time) and positive for all time. All of the basic formalism and discussion in the previous section applies here too. Accordingly, we will only specify the specific form of the necessary relations pertinent to the harmonic oscillator case.

We will adopt the normalization

$$\sum_{j=0}^{\mathbf{V}} u(0, j) + \sum_{i=0}^{\mathbf{H}-1} v(i) = 1. \tag{3.9}$$

Eliminating $u(0, 0)$ we can express the linear dependence of the $u(p, q)$s on the unconstrained missing moments as follows:

$$\begin{aligned} u(p, q) &= M_1(p, q; 0) + \sum_{j=1}^{\mathbf{V}} [M_1(p, q; j) - M_1(p, q; 0)] u(0, j) \\ &\quad + \sum_{i=0}^{\mathbf{H}-1} [M_2(p, q; i) - M_1(p, q; 0)] v(i). \end{aligned} \tag{3.10}$$

As in the finite dimensional case in section 2, we will be working with the functions (note that the true ground state energy moment values, $\vartheta(p)$, satisfy $-2p(2p-1)\vartheta(p-1)+m\vartheta(p+1)=E_g\vartheta(p)$, for $p\geq 0$)

$$R_i[v]=[-2i(2i-1)v(i-1)+mv(i+1)]/v(i). \tag{3.11}$$

For simplicity, we shall restrict ourselves to the case $i=0$, or $R_0[v]=mv(1)/v(0)$. Treating the latter as a parameter and eliminating $v(1)$ we obtain the final linear relation required:

$$u(p,q)=\sum_{j=0}^{\mathbf{H}+\mathbf{V}-1}\mathbf{N}_s(p,q;j)x_j \tag{3.12}$$

where $x_0=1$, $x_1=v(0)$, $x_{2\leq j\leq \mathbf{H}-1}=v(j)$, and $x_{\mathbf{H}\leq j\leq \mathbf{H}+\mathbf{V}-1}=u(0;j-\mathbf{H}+1)$; also

$$\mathbf{N}_s(j)=\begin{cases} M_1(p,q;0) & \text{if } j=0\\ M_2(p,q;0)+(R_0/m)M_2(p,q;1)-M_1(p,q;0)[(R_0/m)+1] & \text{if } j=1\\ M_2(p,q;j)-M_1(p,q;0) & \text{if } 2\leq j\leq \mathbf{H}-1\\ M_1(p,q;j-\mathbf{H}+1)-M_1(p,q;0) & \text{if } \mathbf{H}\leq j\leq \mathbf{H}+\mathbf{V}-1. \end{cases}$$

Instead of working with the two-dimensional analogues of the Hankel–Hadamard determinants, it is more effective to work with the two-dimensional formulation of the linear relations in (2.28). The only modifications are that one must define an appropriate coordinate pair sequence ordering $\{(i,j)_n|n=1,\ldots,\}$ and there are three sets of inequalities:

$$\sum_{n_1,n_2=1}^{N}C_{n_1}u(m_1+i_{n_1}+i_{n_2},m_2+j_{n_1}+j_{n_2})C_{n_2}>0 \tag{3.13}$$

for arbitrary Cs and for $(m_1,m_2)=(0,0)$, $(1,0)$, and $(0,1)$ and $N=0,1,\ldots,\infty$. The adopted sequence ordering proceeds as follows. Define the set of coordinate pairs (i,j) where $j=0,1,\ldots,\mathrm{J}$ and $i=0,\ldots,\mathrm{I}+j$, for given I and J. Let $(0,0)$ be the first coordinate sequence element and vary 'i' while holding 'j' fixed within the prescribed limits; thereby resulting in $(0,0)_1$, $(1,0)_2$, $(2,0)_3,\ldots,(\mathrm{I},0)_{\mathrm{I}+1}$, $(0,1)_{\mathrm{I}+2}$, $(1,1)_{\mathrm{I}+3},\ldots$. For given I and J, the total number of sequence elements is $D_{\mathrm{I},\mathrm{J}}=(2\mathrm{I}+\mathrm{J}+2)(\mathrm{J}+1)/2$. Note that for given I and J, the set

$$\{(m_1+i_{n_1}+i_{n_2},m_2+j_{n_1}+j_{n_2})|(m_1,m_2)=(0,0),(1,0),(0,1);\text{ and } 1\leq n_1,n_2\leq D_{\mathrm{I},\mathrm{J}}\} \tag{3.14}$$

defines all the coordinates for which the moments in (3.2) must be defined. They in turn define the number, $\mathbf{m}_s$, of constrained missing-moment variables required, which will usually be $\{v(i)|0\leq i\leq \mathbf{H}=2\mathrm{I}+1\}$ and $\{u(0,j)|0\leq j\leq \mathbf{V}=2\mathrm{J}+1\}$. Of course, the normalization constraint, combined with using R_0 as a parameter (and eliminating $v(1)$) produces $\mathbf{m}_s-2$ unconstrained missing moments.

Inserting (3.12) into (3.13) defines the necessary formalism for implementing the cutting method.

On the basis of the preceding formalism we were able to generate the bounds quoted in table 4. Note that the convergence rate is slow. Nevertheless, the results are consistent with the ET-EMM theory.

Table 4. Results for quantum harmonic oscillator problem. The I, J and $D_{I,J}$ parameters are explained in the context of equation (3.14). Actual ground state energy value for $m = 1$ is $E_g = 1$.

ε	I,	J,	$D_{I,J}$	Lower bound	Upper bound
3	2	2	12	0.66	1.25
10	2	2	12	0.94	1.21
10	3	3	22	0.97	1.03

4. Conclusion

We have developed a Euclidean time formulation of the basic eigenvalue moment method which has none of the theoretical and practical limitations of the time-independent EMM formulations (as discussed in the introduction). Because of the large number of missing-moment variables, one does not expect a rapid rate of convergence for the generated bounds; however, the analysis presented and the supporting numerical examples do confirm the correctness of the ET-EMM formulation. In addition, this work is another application of the basic principles identified in the work of Handy and Lee (1991) concerning the necessary and sufficient conditions required for the basic EMM theory to apply; specifically, that the associated configuration space (Schrödinger) equation admits a unique solution which is simultaneously bounded (with finite power moments) and positive.

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