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2006 J. Phys. A: Math. Gen. 39 3425

(http://iopscience.iop.org/0305-4470/39/13/019)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 3425–3446 doi:10.1088/0305-4470/39/13/019

(Quasi)-convexification of Barta's (multi-extrema) bounding theorem: $\mathrm{Inf}_x(\frac{H\Phi(x)}{\Phi(x)}) \leqslant E_{\mathrm{gr}} \leqslant \mathrm{Sup}_x(\frac{H\Phi(x)}{\Phi(x)})$

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Received 18 October 2005, in final form 14 February 2006
Published 15 March 2006
Online at stacks.iop.org/JPhysA/39/3425

Abstract

There has been renewed interest in the exploitation of Barta's *configuration space* theorem (BCST) (Barta 1937 *C. R. Acad. Sci. Paris* **204** 472) which bounds the ground-state energy, $\mathrm{Inf}_x\left(\frac{H\Phi(x)}{\Phi(x)}\right) \leqslant E_{\mathrm{gr}} \leqslant \mathrm{Sup}_x\left(\frac{H\Phi(x)}{\Phi(x)}\right)$, by using any Φ lying within the space of positive, bounded, and sufficiently smooth functions, $\mathcal{C}$. Mouchet's (Mouchet 2005 *J. Phys. A: Math. Gen.* **38** 1039) BCST analysis is based on gradient optimization (GO). However, it overlooks significant difficulties: (i) appearance of multi-extrema; (ii) inefficiency of GO for stiff (singular perturbation/strong coupling) problems; (iii) the nonexistence of a systematic procedure for arbitrarily improving the bounds within $\mathcal{C}$. These deficiencies can be corrected by transforming BCST into a moments' representation equivalent, and exploiting a generalization of the eigenvalue moment method (EMM), within the context of the well-known generalized eigenvalue problem (GEP), as developed here. EMM is an alternative eigenenergy bounding, variational procedure, overlooked by Mouchet, which also exploits the positivity of the desired physical solution. Furthermore, it is applicable to Hermitian and non-Hermitian systems with complex-number quantization parameters (Handy and Bessis 1985 *Phys. Rev. Lett.* **55** 931, Handy *et al* 1988 *Phys. Rev. Lett.* **60** 253, Handy 2001 *J. Phys. A: Math. Gen.* **34** 5065, Handy *et al* 2002 *J. Phys. A: Math. Gen.* **35** 6359). Our analysis exploits various quasi-convexity/concavity theorems common to the GEP representation. We outline the general theory, and present some illustrative examples.

PACS numbers: 03.65.Ca, 03.65.Ta, 03.65.Vf

1. Introduction

1.1. Deficiencies of Barta's configuration space formulation

The recent work by Mouchet (2005) develops gradient optimization strategies for implementing Barta's (Barta 1937) eigenenergy bounding procedure for the (bosonic)

ground-state energy, $E_{\rm gr}$. In particular, for any strictly positive trial function, $\Psi > 0$, within the set of positive, twice differentiable, and bounded functions, $\mathcal{C}$, the infimum and supremum, as defined below, generate lower and upper bounds to the ground-state energy:

$$\mathrm{Inf}_x \left(\frac{H\Psi(x)}{\Psi(x)} \right) \leqslant E_{\rm gr} \leqslant \mathrm{Sup}_x \left(\frac{H\Psi(x)}{\Psi(x)} \right). \tag{1}$$

The restriction to the ground state is because of the well-known theorem that in configuration space, the ground-state wavefunction is positive, $\Psi_{\rm gr} > 0$.

Mouchet's analysis assumes that one is working with closed form expressions for the trial wavefunction. Although this approach is quite flexible, it is an incomplete resolution of an important, well known, deficiency of Barta's formalism (i.e. 'Barta's deficiency'). Specifically, given bounds generated from an initial trial function, how does one systematically improve upon this, to arbitrary tightness of the bounds, within the set $\mathcal{C}$? This is particularly important since the selection of suitable trial functions is not an intuitive process. To begin to answer this within configuration space requires infinite parameter representations for all of $\mathcal{C}$. This is not possible.

Besides this limitation, Barta's configuration space formulation also presents significant multi-extrema complications in sampling the ratio $\frac{H\Psi(x)}{\Psi(x)}$ over all x values. Clearly, any alternate approach that convexifies this problem (or its equivalent), thereby requiring the determination of one global extremum, would be a tremendous improvement. There are many important problems in physics where the appearance of multi-minima, and strategies for circumventing these, is a major concern. One important class of methods for doing this is simulated annealing (Kirkpatrick *et al* 1983). Related methods such as *iterative annealing* have impacted more contemporary research such as those studying the protein folding problem (Thirumalai and Hyeon 2005).

An additional difficulty with gradient approaches is that they may not be the ideal strategy for dealing with stiff systems (such as those associated with singular perturbation/strong coupling interactions) for which very small integration steps may slow the global search for the infimum and supremum. (By way of contrast, the approach presented here does not require a gradient search. Instead a linear programming-based bisection approach proves highly effective.)

1.2. A remedy to Barta's deficiencies: the eigenvalue moment method

In the 1980s, these deficiencies were well known to D Bessis and his group at Saclay, particularly as a consequence of Barnsley's (Barnsley 1978) earlier studies on Barta's theorem. Their objective was to develop tight (converging) bounds for the notoriously difficult quadratic Zeeman effect for hydrogenic atoms in superstrong magnetic fields (QZE). In particular, Le Guillou and Zinn-Justin (1983) emphasized an intricate order dependent, hypervirial, conformal analysis which gave numerical predictions for the QZE ground-state binding energy. The QZE is an example of a singular perturbation/strong coupling problem (Bender and Orszag 1978), for which different methods (i.e. variational, numerical, analytical, etc) can yield widely varying results. Bessis was interested in developing positivity based alternatives to Barta's theorem by which to asses the accuracy of Le Guillou and Zinn-Justin's results.

Independent of these concerns, Handy (1984) discovered that certain well-known theorems within the classic mathematical literature known, collectively, as the *moment problem* (Shohat and Tamarkin 1963) could be used to quantize physical systems through the generation of (geometrically) converging, lower and upper bounds, to the ground-state energy. The *moment problem* is concerned with the necessary and sufficient conditions the power moments of a positive function, $\mu_p = \int \mathrm{d}x\, x^p \Psi(x)$, must satisfy in order to determine that function.

More generally, Handy's interest in moments' quantization formulations originated from earlier studies that suggested their effectiveness in studying the multiscale dynamics of certain singular perturbation-strong coupling problems in field theory (Handy 1981). That is, a moments representation implicitly defined a multiscale hierarchy of sensitivity to smaller and smaller scale structures. This was a precursor to wavelet theory (Grossmann and Morlet 1984, Daubechies 1988), and was used, more recently, to incorporate continuous wavelet transform theory into quantum mechanics (Handy and Murenzi 1997, 1998, 1999).

Handy's eigenenergy bounding procedure exploited the confluence of several, hitherto, separate results. These were as follows: (i) the (multidimensional) Schrödinger equation with rational fraction potential could be readily transformed into a *moment equation* recursion relation for the power moments of the wavefunction, $\mu_p = \int_{\mathcal{D}} \mathrm{d}x\, x^p \Psi(x)$, involving the energy as a parameter, E; (ii) the (multidimensional) bosonic ground-state wavefunction must be positive, $\Psi_{\mathrm{gr}} > 0$; (iii) the *moment problem* positivity theorems define an infinite hierarchy of constraints on the power moments, and in turn, on E. The particular positivity theorem used by Handy (1984) was the well-known nesting constraints for the (diagonal and off-diagonal) Pade approximants (generated from the μ_p's) of the associated Stieltjes integral for Ψ_{gr} (Baker 1975). (For future reference, as discussed in the appendix, if the support space defining the moments correspond to $\mathcal{D} = \Re$, or $\Re^+$, the moments are referred to as Hamburger or Stieltjes, respectively.)

In their first collaboration, Handy and Bessis (1985) recognized that the Stieltjes–Pade theorems would not be extendable to multidimensions (in anticipation of applying the underlying moment problem quantization philosophy to the QZE problem). They proposed to exploit the *moment problem* positivity theorems based on the nonlinear, Hankel–Hadamard (HH) determinantal inequalities. These could be extended, in principle, to multidimensions (Devinatz 1957); however, this proved too costly. In a subsequent breakthrough (Handy *et al* 1988), they realized that the HH nonlinear formulation could be transformed into an equivalent linearized version, which was then amenable to linear programming analysis (Chvatal 1983). Handy devised an efficient (bi-section) method referred to as the *cutting algorithm*, which led to the generation of tight, converging, bounds to the QZE problem, confirming the results of Le Guillou and Zinn-Justin (Handy *et al* 1988). The entire procedure is referred to as the eigenvalue moment method (EMM).

Thus, historically, the EMM approach was specifically invented to bypass all of the unattractive features of Barta's configuration space theorem. Mouchet overlooks this in his review of variational (bounding) methods, despite the fact that the EMM procedure is an *affine map invariant, variational procedure* (Handy and Murenzi 1998). That is, the EMM bounds automatically sample over all affine map transformations (translations, scalings, rotations, etc) of the trial functions (i.e. polynomials). Affine maps are at the heart of fractals (Barnsley 1988) and wavelet transform theory (Grossman and Morlet 1984, Daubechies 1988). Fractals and wavelets represent important representations for dealing with systems with significant multiscale structures. For this same reason, the EMM bounds are very good for dealing with (stiff) singular perturbation type systems with significant multiscale dynamics.

1.3. Moment problem reformulation of Barta's theorem: the generalized eigenvalue problem

Despite the successes of the EMM procedure, Mouchet's work has inspired the author to develop a *moment problem* counterpart to Barta's configuration space theorem. Several new results ensue from this. The first is that the new formulation does not require the introduction of a *moment equation*. Instead, we are able to generalize the underlying EMM philosophy

in a manner more in keeping with operator (matrix) theory. Whereas the moments in the EMM formulation are constrained by the moment equation relations, in the new formulation, all of the moments are unconstrained relative to one another. The energy parameter does not explicitly appear. Instead, one studies the extremal eigenvalues of the corresponding *generalized eigenvalue problem* (GEP) (Boyd and Vandenberghe 2004) defined according to $\mathbf{H}\overrightarrow{V} = \lambda\mathbf{U}\overrightarrow{V}$, where $\mathbf{H}$ represents the moment representation operator (matrix) for the Hamiltonian, and $\mathbf{U}$ represents a positive definite matrix operator (the Hankel moment matrix). We are not interested in the generalized eigenvectors , $\overrightarrow{V}$, but make reference to them for clarity. Instead, it is the extremal eigenvalues, $\lambda_{\min} \leqslant \lambda \leqslant \lambda_{\max}$, that are of interest, since these will directly relate to the infimum and supremum expressions in Barta's configuration space theorem.

We will investigate two different versions of the above GEP system. In the first case, we will assume that the moments, μ_p, used in defining the $(\mathbf{H}, \mathbf{U})$ operator pair, correspond to a positive trial function (i.e. either we have a closed form for the function, Ψ, and its power moments, μ_p; or we only know the μ_p's, but have no closed form expression for Ψ). We can then generate monotonically converging sequences to both the infimum and supremum: $\mathrm{Inf}_x\left(\frac{H\Psi}{\Psi}\right) < \cdots < \lambda_{\min;n} < \cdots < \lambda_{\min;1}$ and $\lambda_{\max;1} < \cdots < \lambda_{\max;n} < \cdots < \mathrm{Sup}_x\left(\frac{H\Psi}{\Psi}\right)$. In principle, this already defines one clear advantage, since any multi-extrema features of the ratio $\frac{H\Psi}{\Psi}$ are circumvented by our ability to generate monotonically converging sequences.

The $(\mathbf{H}, \mathbf{U})$ matrix operator pair, although of infinite dimension, can be studied in terms of their finite-dimensional, upper left hand, submatrices. For each of these submatrices, we can define a finite-dimensional, convex moment variable space, $\mathcal{U}_n$. In our second study of the GEP formulation, we will determine the optimal values, over $\mathcal{U}_n$, for each of the extremal GEP eigenvalues (i.e. $\mathrm{Sup}_{\mu\in\mathcal{U}_n}(\lambda_{\min;n}(\mu))$ and $\mathrm{Inf}_{\mu\in\mathcal{U}_n}(\lambda_{\max;n}(\mu))$). These will generate converging bounds to the ground-state energy: $\mathrm{Inf}_{\mu\in\mathcal{U}_n}(\lambda_{\max;n}(\mu)) < E_{\mathrm{gr}} < \mathrm{Sup}_{\mu\in\mathcal{U}_n}(\lambda_{\min;n}(\mu))$. The EMM formalism plays an important role in proving the last result.

Readers not familiar with the EMM formalism should consult appendix A for a review which also clarifies the notation adopted in the rest of this work. For those familiar with the EMM formulation, they will recall that the moment equation representation leads to relations of the form $\mu_p = \hat{M}_E(p, 0) + \sum_{\ell=1}^{m_s} \hat{M}_E(p, \ell)\mu_\ell$, where the $\hat{M}_E(p, \ell)$ coefficients are known functions of the energy parameter, E. These moment constraints divide the infinite set of moments into two sets: the unconstrained moments (referred to as either the *initialization* or *missing* moments); and the constrained moments. For one-dimensional systems, the first set corresponds, after imposing a normalization, to $m_s < \infty$ (problem dependent) variables. For multidimensional systems, both sets are infinite in number; although they define an infinite hierarchy of finite-dimensional subspaces within which the EMM analysis leads to exact (non-truncated) results. All the moments, and (unknown) energy (for the ground state), must then satisfy the Hankel–Hadamard determinantal constraints, denoted by $\Delta_{m,n}(\mu) > 0$, as defined in appendix A. Within each finite-dimensional subspace (indexed by the parameter Q), the computational focus is to determine those E values for which there exist moment solutions to the HH inequalities. The set of admissible energies correspond to an interval whose endpoints bound the true ground-state energy, $E_{\mathrm{gr}} \in \left(E_Q^L, E_Q^U\right)$.

2. Moment problem reformulation of Barta's theorem as a generalized eigenvalue problem

In this work, we directly transform Barta's configuration space theorem into a moment problem representation. By so doing, we obtain a theoretically complete formalism that addresses and solves Barta's configuration space deficiencies. Our analysis is limited to Hamiltonian

systems with rational fraction potentials, since in such cases, the Schrödinger equation can be transformed into a moment equation representation. This is not a serious limitation, since such Hamiltonians (and others that can be transformed into differential representations with rational fraction coefficients) correspond to a large, and important, class of physical systems.

In contrast to the EMM approach which restricts itself to the set of moments satisfying the physical moment equation, the new formalism makes no such restriction.

The review of the EMM formalism, given in appendix A defines $\mathcal{U}_Q$ as a subset within the domain of initialization moments (i.e. the subset of initialization moment values whose moment equation generated moments, up to moment order Q, satisfy the HH positivity constraints). Within the present generalized eigenvalue problem (GEP) representation, where the moments are no longer constrained by a moment equation, this same notation will be appropriately modified as given below.

Definition (as implemented within the EMM formulation, for moments constrained by a moment equation)**.**

$$\mathcal{U}_Q = \left\{ (\mu_1, \ldots, \mu_{m_s}) \middle| \mu_p = \hat{M}_E(p,0) + \sum_{\ell=1}^{m_s} \hat{M}_E(p,\ell)\mu_\ell,\ 0 \leqslant p \leqslant Q, \right.$$
$$\left. \text{and } \Delta_{0,n}(\mu) > 0, 0 \leqslant n \leqslant \frac{Q}{2}, \right\} \subset (-1,1)^{m_s}.$$

Note that the elements of $\mathcal{U}_Q$ implicitly must satisfy some, physically motivated, normalization prescription. The $\Delta_{0,n}(\mu)$'s are the Hankel–Hadamard (HH) determinants and the $\hat{M}_E(p,\ell)$'s are the coefficients of the EMM moment equation recursion relation (refer to equation (A.1), and equations (A.3)–(A.6), in appendix A).

The GEP modification of this same notation will be

Definition (modification within the GEP formalism)**.**

$$\mathcal{U}_Q = \left\{ (\mu_0, \ldots, \mu_Q) \middle| \text{ where } \Delta_{0,n}(\mu) > 0, 0 \leqslant n \leqslant \frac{Q}{2} \right\}.$$

That is, $\mathcal{U}_Q$ refers to the domain of Hamburger moments, up to moment order, Q, satisfying all the corresponding HH positivity constraints (and not constrained to satisfy any moment equation). In either case, Q is implicitly an even number.

It is also implicitly assumed that the elements of $\mathcal{U}_Q$ must satisfy some physically motivated normalization prescription.

Within each of the finite-dimensional subsets, $\mathcal{U}_Q$, Barta's relations manifest themselves in terms of a *generalized eigenvalue problem* (GEP) (Watkins 2002)

$$\mathbf{H}|\vec{V}\rangle = \lambda \mathbf{U}|\vec{V}\rangle, \tag{2}$$

where $\mathbf{H}$ and $\mathbf{U}$ correspond to finite, real and symmetric matrices, to be defined in the appendices. The matrix elements will be linear in the moments. Because of the restriction to $\mathcal{U}_Q$ the $\mathbf{U}$-Hankel matrix is positive definite. The matrices $(\mathbf{H}, \mathbf{U})$ are designated as a *symmetric* pair. As will be seen by the explicit example discussed below, whereas all of the moment variables in $\mathcal{U}_Q$ contribute to the structure of $\mathbf{H}$, a reduced number of these contribute to $\mathbf{U}$; however, this reduced number still guarantee the positive definiteness of $\mathbf{U}$.

Through a Cholesky decomposition (Watkins 2002), $\mathbf{U} = \mathbf{R}^t\mathbf{R}$, the GEP is transformed into a standard, symmetric matrix, eigenvalue problem,

$$\mathbf{R}^{-t}\mathbf{H}\mathbf{R}^{-1}|\vec{W}\rangle = \lambda|\vec{W}\rangle. \tag{3}$$

The extremal eigenvalues $\lambda_{\min} \leqslant \lambda \leqslant \lambda_{\max}$, satisfying the above, or alternatively $\mathrm{Det}(\mathbf{H} - \lambda\mathbf{U}) = 0$, are defined by

$$\lambda_{\min}(\mu) = \mathrm{Inf}_{\overrightarrow{C}} \frac{\langle \overrightarrow{C} |\mathbf{H}(\mu)| \overrightarrow{C} \rangle}{\langle \overrightarrow{C} |\mathbf{U}(\mu)| \overrightarrow{C} \rangle}, \quad \{\mu\} \in \mathcal{U}_Q; \tag{4}$$

and

$$\lambda_{\max}(\mu) = \mathrm{Sup}_{\overrightarrow{C}} \frac{\langle \overrightarrow{C} |\mathbf{H}(\mu)| \overrightarrow{C} \rangle}{\langle \overrightarrow{C} |\mathbf{U}(\mu)| \overrightarrow{C} \rangle}, \quad \{\mu\} \in \mathcal{U}_Q, \tag{5}$$

where $\overrightarrow{C} \neq \overrightarrow{0}$. Of course, we also have $\lambda_{\min}(\mu) = -\mathrm{Sup}_{\overrightarrow{C}} \frac{\langle \overrightarrow{C} |-\mathbf{H}(\mu)| \overrightarrow{C} \rangle}{\langle \overrightarrow{C} |\mathbf{U}(\mu)| \overrightarrow{C} \rangle}$.

The above ratios can also be written in terms of $\frac{\frac{\langle \overrightarrow{C} |\mathbf{H}(\mu)| \overrightarrow{C} \rangle}{\langle \overrightarrow{C} | \overrightarrow{C} \rangle}}{\frac{\langle \overrightarrow{C} |\mathbf{U}(\mu)| \overrightarrow{C} \rangle}{\langle \overrightarrow{C} | \overrightarrow{C} \rangle}}$. Let $\lambda_{\mathbf{H},\mathbf{U}}^{\min,max}(\mu)$ denote the extremal eigenvalues of the $\mathbf{H}$ and $\mathbf{U}$ matrices, respectively. Since $\lambda_{\mathbf{U}}^{\min}(\mu) > 0$, if we also assume that $\lambda_{\mathbf{H}}^{\min}(\mu) > 0$ (for simplicity), then $\frac{\lambda_{\mathbf{H}}^{\min}(\mu)}{\lambda_{\mathbf{U}}^{\max}(\mu)} \leqslant \lambda_{\min}(\mu) \leqslant \lambda_{\max}(\mu) \leqslant \frac{\lambda_{\mathbf{H}}^{\max}(\mu)}{\lambda_{\mathbf{U}}^{\min}(\mu)}$. However, if $\lambda_{\mathbf{H}}^{\min}(\mu) < 0$, then $\frac{\lambda_{\mathbf{H}}^{\min}(\mu)}{\lambda_{\mathbf{U}}^{\min}(\mu)} \leqslant \lambda_{\min}(\mu)$. These expressions will prove important later on.

Physicists refer to any function which, locally, lies below the tangent plane as a *convex function*. Mathematicians define a function, $f(x)$, as convex if the set $\{(x, y)|y \geqslant f(x)\}$ is convex. Thus, what a physicist would regard as a concaved function, is referred to as a convex function by mathematicians. Throughout this work we will use the physicist's definition, except in a few cases where we cite the actual theorems (placing quotation marks around them), as they appear in the literature.

Definition.

$$\begin{pmatrix}\text{Concaved}\\ \text{Convex}\end{pmatrix} \text{Function}_{[\text{physicists}]} \equiv \begin{pmatrix}\text{`Convex'}\\ \text{`Concaved'}\end{pmatrix} \text{Function}_{[\text{mathematicians}]}.$$

It is a well-known theorem that the smallest eigenvalue of a symmetric matrix is a convex function with regards to the matrix elements as variables. This led to various alternative algorithmic strategies (i.e. gradient methods) for implementing EMM (Handy *et al* 1991, 1996).

The smallest eigenvalue of the generalized eigenvalue problem is not convex as such, but it shares the good fortune that it does not have any multi-maxima or saddle points. That is, there can be regions of relative flatness. Thus, although there can only be one global maximum value, the points in $\mathcal{U}_Q$ corresponding to the global maximum may not be unique. These properties are what the mathematicians refer to as *quasi-'concaved'*.

Despite this, in the infinite limit (all of moment space) the physical problem strongly suggests that the point, in the moment variables space, corresponding to a global maximum for $\lambda_{\min}(\mu)$, is unique. This is because there can only be one physical ground state (the ground-state energy can only be associated with one point in $\mathcal{U}_\infty$). Since we are only interested in obtaining tight bounds for E_{gr} these issues do not affect this objective.

We now revert to the mathematics nomenclature which is the opposite to the physicist's intuitive interpretation, as previously noted.

Definition. *A function,* $f(\overrightarrow{\mu}) : \mathcal{U} \to \Re$, *is quasi-'concaved' if*

$$f(s\overrightarrow{\mu}_1 + (1-s)\overrightarrow{\mu}_2) \geqslant \min\{f(\overrightarrow{\mu}_1), f(\overrightarrow{\mu}_2)\}, \qquad 0 \leqslant s \leqslant 1, \quad \overrightarrow{\mu}_{1,2} \in \mathcal{U}. \tag{6}$$

Actually, this is an 'if only if' statement. The usual definition is that a function, $f(x)$, is 'quasiconcaved' if the superlevel sets $S_a \equiv \{x | f(x) \geqslant a\}$ are convex.

It therefore follows that for a quasi-'concaved' function there can be flat regions where the function stays constant. However, along the one-dimensional path defined by $0 < s < 1$, there can be no local minimum. If the function is strictly 'concaved', then any local differential search will always yield a path which leads to the global maximum. However, for quasi-'concaved' functions, within regions of flatness, more effort may be required to find a path that leads to a global maximum.

We have the following important theorem (mathematical nomenclature).

Theorem 1. $\lambda_{\max}(\mu)$ *is a* **quasi-'convex'** *function of the matrix elements (**H**, **U**), which are linear in the moments* (Boyd and Vandenberghe 2004).

Similarly, $\lambda_{\min}(\mu)$ (being the negative of a quasi-'convex' function, refer to discussion following equation (5)) is a **quasi-'concaved'** function.

From the definition of the extremal eigenvalues one has that $\lambda_{\min}(\mu) \leqslant \lambda_{\max}(\mu)$. However, there will be moment elements in $\mathcal{U}_Q$ for which the extremal eigenvalues coincide. This will be the case for those satisfying the moment equation, up to moment order Q (i.e. those moments that also satisfy the EMM moment equation).

Definition. *Denote by* $\overrightarrow{\mu}_E = \{\mu_0, \mu_1, \ldots, \mu_Q\} \in \mathcal{U}_Q$, *an element of* $\mathcal{U}_Q$ *that also satisfies the moment equation (equation (A.1), in appendix A), for the given E value. Such a point, by definition, automatically satisfies the EMM positivity constraints. This is only possible if* $E \in \left(E_Q^L, E_Q^U\right)$. *That is, it must lie within the EMM eigenenergy bounds. Now use it to generate the* (**H**, **U**) *symmetric pair matrices, as defined in the appendices. In appendix B appears the proof of*

Theorem 2.

$$\lambda_{\min}(\mu_E) = E = \lambda_{\max}(\mu_E). \tag{7}$$

We shall denote by $\mathcal{U}_{Q;EMM} \subset \mathcal{U}_Q$, the subset of points satisfying the EMM conditions (i.e. satisfies the moment equation up to order Q, and the positivity conditions, for an E value that must lie within the EMM bounds).

Let us explicitly distinguish the extremal GEP eigenvalues for each $\mathcal{U}_n$ of dimension $n+1$ by the notation: $\lambda_{\max/\min;n}(\mu)$. Also, let $\mathcal{C}$ denote the set of functions that are positive, bounded (exponentially decreasing), and continuously differentiable up to the second order. In appendix B it is established that if $\Psi \in \mathcal{C}$, and $\mu_p = \int \mathrm{d}x\, x^p \Psi(x)$, $p < \infty$ are its moments, then

Theorem 3.

$$\mathrm{Inf}_x \left(\frac{H\Psi(x)}{\Psi(x)} \right) \leqslant \lambda_{\min;n+1}(\mu) \leqslant \lambda_{\min;n}(\mu), \tag{8}$$

$$\lambda_{\max;n}(\mu) \leqslant \lambda_{\max;n+1}(\mu) \leqslant \mathrm{Sup}_x \left(\frac{H\Psi(x)}{\Psi(x)} \right), \tag{9}$$

and

$$\lim_{n\to\infty} \begin{pmatrix} \lambda_{\min;n}(\mu) \\ \lambda_{\max;n}(\mu) \end{pmatrix} = \begin{pmatrix} \mathrm{Inf}_x \left(\frac{H\Psi(x)}{\Psi(x)} \right) \\ \mathrm{Sup}_x \left(\frac{H\Psi(x)}{\Psi(x)} \right) \end{pmatrix}, \tag{10}$$

for each $\Psi \in \mathcal{C}$.

This is an interesting result, particularly when combined with sequence acceleration methods, since it allows one to determine Barta's lower and upper bounds for a function whose moments are known, even when the function is not given in closed form. Also, the monotonic nature of the results may prove useful in circumventing potential multi-extrema features of the $\frac{H\Psi}{\Psi}$ ratio, when evaluated in terms of Barta's configuration space formulation.

Let us now define the Sup and Inf of the extremal eigenvalues over their finite-dimensional convex domain, $\mathcal{U}_n$:

$$\begin{pmatrix} \lambda^{\text{Sup}}_{\text{min};n} \\ \lambda^{\text{Inf}}_{\text{max};n} \end{pmatrix} \equiv \begin{pmatrix} \text{Sup}_{\mu\in\mathcal{U}_n}(\lambda_{\text{min};n}(\mu)) \\ \text{Inf}_{\mu\in\mathcal{U}_n}(\lambda_{\text{max};n}(\mu)) \end{pmatrix}. \tag{11}$$

From equation (7), since $\mathcal{U}_{n;EMM} \subset \mathcal{U}_n$, we must have that $\lambda^{\text{Sup}}_{\text{min};n} \geqslant E^U_n$, the EMM upper bound. Similarly, $\lambda^{\text{Inf}}_{\text{max};n} \leqslant E^L_n$, the EMM lower bound:

Theorem 4.

$$\lambda^{\text{Inf}}_{\text{max};n} \leqslant E^{\text{EMM-lowerbound}}_n \leqslant E_{\text{gr}} \leqslant E^{\text{EMM-upperbound}}_n \leqslant \lambda^{\text{Sup}}_{\text{min};n}, \tag{12}$$

and, in the infinite limit, $n \to \infty$:

$$\lambda^{\text{Inf}}_{\text{max};n} \leqslant \lambda^{\text{Inf}}_{\text{max};n+1} \leqslant E_{\text{gr}} \leqslant \lambda^{\text{Sup}}_{\text{min};n+1} \leqslant \lambda^{\text{Sup}}_{\text{min};n}. \tag{13}$$

This is also proved in appendix B.

2.1. Important assumption/condition

Although $\mathcal{U}_n$ will be a bounded convex set through the normalization conditions used, it is also important that its boundary ($\delta\mathcal{U}$) does not include points at which the positive definiteness is lost. That is, if $\overrightarrow{\mu_b} \in \delta\mathcal{U}$, we do not want $\Delta_{0,j\leqslant n}(\overrightarrow{\mu_b}) = 0$, or $\lambda^{\min}_{\mathbf{U}}(\overrightarrow{\mu_b}) = 0$, using the notation in the discussion following equation (5). If this is were to happen, then the $\lambda^{\text{Sup}}_{\text{min};n}$, as well as $\lambda^{\text{Inf}}_{\text{max};n}$, could become singular (i.e. $+\infty$, $-\infty$, respectively). In the present application, we can insure the above by simply imposing additional moment inequality constraints associated with any (rough) upper bound to the ground-state energy. This will be clarified in the next section, where we implement the numerical analysis on a specific problem.

3. Some numerical results

We will use the quartic potential, $V(x) = x^4$, to illustrate, numerically, most of the previous results. The ground-state energy is $E_{\text{gr}} = 1.060\,362\,090\,484$.

3.1. Equations (8)–(10), using $\Psi(x) = \mathcal{N}\,\mathrm{e}^{-x^2}$

This is a trivial example. One has $\frac{H\Psi(x)}{\Psi(x)} = 2 - 4x^2 + x^4$. The infimum is $\text{Inf}(2 - 4x^2 + x^4) = -2$. The even order, Gaussian function power moments, satisfy the recursion relation $\mu_{p+2} = \left(\frac{1+p}{2}\right)\mu_p$, $p \geqslant 0$. Normalizing according to $\mu_0 \equiv 1$, determines the normalization factor $\mathcal{N}$.

Since the Gaussian function, $\Psi_g = \mathrm{e}^{-x^2}$ also satisfies $-\partial^2_x\Psi_g + 4x^2\Psi_g = 2\Psi_g$, an alternate recursion relation for the moments is $-p(p-1)\mu_{p-2} + 4\mu_{p+2} = 2\mu_p$. Using this, one can transform the matrix structure in equation (B.11) (i.e. $-p(p-1)\mu_{p-2} + \mu_{p+4} - \lambda\mu_p$) into $-4\mu_{p+2} + \mu_{p+4} - (\lambda - 2)\mu_p$. The generalized eigenvalue problem results, for this problem, are given in table 1. Note that the convergence is slow, but consistent with the various theorems. We also note the curious repetitive, non-repetitive, structure manifested by the eigenvalues (confirmed, to high precision, through *Mathematica*). No sequence acceleration analysis has been attempted.

Table 1. Quartic potential results using $\mathcal{N}e^{-x^2}$ trial function; Barta's lower bound is -2 (note that Dim $\equiv N+1$ and max moment order, Q, satisfy $Q = 4+2N$).

Dim(Q)	$\lambda_{\min:Q}$	Dim(Q)	$\lambda_{\min:Q}$	Dim(Q)	$\lambda_{\min:Q}$
1 (4)	0.750 00	34 (70)	−1.742 04	67 (136)	−1.863 61
2 (6)	−0.250 00	35 (72)	−1.751 51	68 (138)	−1.866 87
3 (8)	−0.250 00	36 (74)	−1.751 51	69 (140)	−1.866 87
4 (10*)	−0.458 10	37 (76*)	−1.753 80	70 (142)	−1.868 40
5 (12)	−0.825 22	38 (78)	−1.754 47	71 (144)	−1.868 40
6 (14)	−0.825 22	39 (80)	−1.754 47	72 (146)	−1.868 800 4
7 (16)	−1.062 61	40 (82)	−1.776 64	73 (148)	−1.868 800 4
8 (18)	−1.062 61	41 (84)	−1.776 64	74 (150*)	−1.868 801 3
9 (20*)	−1.067 05	42 (86)	−1.792 00	75 (152)	−1.875 13
10 (22)	−1.288 93	43 (88)	−1.792 00	76 (154)	−1.875 13
11 (24)	−1.288 93	44 (90)	−1.800 67	77 (156)	−1.880 65
12 (26)	−1.378 98	45 (92)	−1.800 67	78 (158)	−1.880 65
13 (28)	−1.378 98	46 (94)	−1.804 22	79 (160)	−1.884 75
14 (30*)	−1.386 56	47 (96)	−1.804 22	80 (162)	−1.884 75
15 (32)	−1.462 59	48 (98*)	−1.804 83	81 (164)	−1.887 46
16 (34)	−1.462 59	49 (100)	−1.809 20	82 (166)	−1.887 46
17 (36)	−1.541 81	50 (102)	−1.809 20	83 (168)	−1.888 94
18 (38)	−1.541 81	51 (104)	−1.822 58	84 (170)	−1.888 94
19 (40)	−1.566 36	52 (106)	−1.822 58	85 (172)	−1.889 53
20 (42)	−1.566 36	53 (108)	−1.832 19	86 (174)	−1.889 53
21 (44*)	−1.567 86	54 (110)	−1.832 19	87 (176*)	−1.889 62
22 (46)	−1.613 60	55 (112)	−1.838 02	88 (178)	−1.891 37
23 (48)	−1.613 60	56 (114)	−1.838 02	89 (180)	−1.891 37
24 (50)	−1.657 66	57 (116)	−1.840 77	90 (182)	−1.895 88
25 (52)	−1.657 66	58 (118)	−1.840 77	91 (184)	−1.895 88
26 (54)	−1.676 29	59 (120)	−1.841 515	92 (186)	−1.899 58
27 (56)	−1.676 29	60 (122)	−1.841 515	93 (188)	−1.899 58
28 (58*)	−1.680 12	61 (124*)	−1.841 519	94 (190)	−1.902 36
29 (60)	−1.686 37	62 (126)	−1.850 45	95 (192)	−1.902 36
30 (62)	−1.686 37	63 (128)	−1.850 45	96 (194)	−1.904 22
31 (64)	−1.721 07	64 (130)	−1.858 18	97 (196)	−1.904 22
32 (66)	−1.721 07	65 (132)	−1.858 18	98 (198)	−1.905 29
33 (68)	−1.742 04	66 (134)	−1.863 61	99 (200)	−1.905 29
				100 (202)	−1.905 76
				101 (204)	−1.905 76

∗ Except for these entries, all others appear in pairs, to 20 significant figures

3.2. Equations (8)–(10), using $\Psi(x) = |\Phi(x)|^2$, where $\Phi(x)$ satisfies the PT-invariant Schrödinger equation $-\partial_x^2\Phi - (\mathrm{i}x)^3\Phi = \mathcal{E}\Phi$

We now investigate the utility of the previous formalism when the positive trial function is not known, in closed form; although the moments are (numerically) known. For this exercise, we could take $\Psi(x)$ to be the (positive) ground state of any (solvable) Schrödinger potential problem, $-\partial_x^2\Psi_s + V_s(x)\Psi_s(x) = E_s\Psi_s(x)$. In such cases, one would determine the Inf/Sup of (i.e. $H_4 \equiv -\partial_x^2 + x^4$), $\frac{H_4\Psi_s}{\Psi_s} = -\frac{\partial_x^2\Psi_s}{\Psi_s} + x^4 = E_s - V_s(x) + x^4$. This would then be a trivial analysis.

Instead, we pursue a different class of problems whose differential structure does not lead to an easily calculable set of Barta bounds. Such is provided by the class of non-Hermitian systems that have received much attention in the context of PT-symmetry breaking systems

Table 2. Quartic potential results using as trial configuration the $|\Phi(x)|^2$ solution corresponding to PT-invariant, non-Hermitian, system $-\partial_x^2\Phi(x) - (\mathrm{i}x)^3\Phi(x) = \mathcal{E}\Phi(x)$, for $\mathcal{E} = 1.156\,267\,071\,988\,1133$. Barta's lower bound is *approximately* (-1.782), based upon Runge–Kutta integration.

Q	$\lambda_{\min:Q}$	Q	$\lambda_{\min:Q}$
4	0.765 183 031 6	30	−1.412 946 343
6	−0.370 149 731 6	32	−1.412 946 343
8	−0.579 749 584 2	34	−1.466 405 630
10	−0.579 749 584 2	36	−1.466 405 630
12	−0.917 569 994 9	38	−1.471 430 659
14	−1.025 936 484	40	−1.505 086 215
16	−1.025 936 484	42	−1.505 086 215
18	−1.202 683 806	44	−1.535 124 305
20	−1.202 683 806	46	−1.535 124 305
22	−1.202 840 090	48	−1.530 286 871
24	−1.349 131 584	50	−1.556 428 376
26	−1.349 131 584	52	−1.556 428 376
28	−1.369 576 335	54	−1.579 966 618
		56	−1.579 966 618 4
		58	−1.579 966 618 4
		60	−1.588 250 832 6

(Bender and Boettcher 1998). The simplest example of this is the well known $V(x) = -(\mathrm{i}x)^3$ system, which we write as $-\partial_x^2\Phi(x) - (\mathrm{i}x)^3\Phi(x) = \mathcal{E}\Phi(x)$. This system admits only real eigenenergies; however, its eigenstates are all complex functions. Nevertheless, the probability density, $\Psi(x) = |\Phi(x)|^2 \equiv S(x) > 0$, satisfies a linear, fourth-order differential equation (Handy 2001):

$$\partial_x\left(-\frac{1}{x^3}\partial_x^3 S(x) - 4\frac{\mathcal{E}}{x^3}\partial_x S(x)\right) + 4x^3 S(x) = 0. \tag{14}$$

Although all of the bound states of this system are positive, we shall work with the one corresponding to the smallest $\mathcal{E} = 1.156\,267\,071\,988\,1133$. The Hamburger moments of the even function, $S(x)$, satisfy a simple recursion relation (Handy 2001):

$$4\mu_{p+7} = (p+4)p(p-1)(p-2)\mu_{p-3} + 4\mathcal{E}p(p+4)\mu_{p-1}, \tag{15}$$

for $p \geqslant 0$. The GEP-moment analysis, given in table 2, tells us that $\mathrm{Inf}\left(\frac{H_4 S(x)}{S(x)}\right) < -1.57$. In order to verify this, we can implement a Runge–Kutta analysis on $S(x)$, in order to calculate $-\frac{S''}{S}$. If one is not too careful (i.e. implementation of a naive second order finite differencing), a significantly wrong answer is obtained (i.e. Barta's infimum is $O(.3)$). Instead, by using the relation

$$\left(\frac{H_4 S(x)}{S(x)}\right) = -\frac{\Phi\partial_x^2\Phi^* + \Phi^*\partial_x^2\Phi + 2\partial_x\Phi^*\partial_x\Phi}{\Phi^*\Phi} + x^4 = 2\mathcal{E} - 2\left|\frac{\partial_x\Phi}{\Phi}\right|^2 + x^4,$$

the resulting expression lends itself to a more accurate Runge–Kutta verification, yielding the (approximate) Barta *infimum* as -1.782. This is very consistent with the GEP generated results in table 2.

3.3. Generating converging bounds for quartic potential (theorem 4): the need for a rough upper bound to the energy

In this last example, we will not work with a fixed set of moments for a positive trial configuration. Instead, we will implement an optimization procedure for determining

$\mathrm{Sup}(\lambda_{\mathrm{min};\,Q}(\mu))$ and $\mathrm{Inf}(\lambda_{\mathrm{max};\,Q}(\mu))$, for $\mu \in \mathcal{U}_Q$. Contrary to the gradient analysis in Mouchet's (Mouchet 2005) work, we can determine these quantities by implementing a bisection type analysis within the λ-variable space, similar to that developed within the EMM, linear programming based, 'cutting-algorithm' (Handy *et al* 1988).

3.3.1. Defining $\mathcal{U}_Q$. The $\mathcal{U}_Q$ space is defined as the set of Hamburger moments, $\{(\mu_0, \ldots, \mu_Q)\}$, satisfying

$$\langle \overrightarrow{C}_1 | \mu_{n_1+n_2} | \overrightarrow{C}_1 \rangle > 0, \qquad \forall \overrightarrow{C}_1 \neq 0, \quad 0 \leqslant n_1 + n_2 \leqslant Q. \tag{16}$$

In addition, for the case of $\mathrm{Sup}(\lambda_{\mathrm{min};\,Q}(\mu))$, we are interested in the set of λ_l's satisfying (i.e. equation (B.11))

$$\langle \overrightarrow{C}_2 | -(n_1+n_2)(n_1+n_2-1)\mu_{n_1+n_2-2} + \mu_{n_1+n_2+4} - \lambda_l \mu_{n_1+n_2} | \overrightarrow{C}_2 \rangle > 0, \qquad \forall \overrightarrow{C}_2 \neq 0,$$
$$0 \leqslant n_1 + n_2 + 4 \leqslant Q. \tag{17}$$

Whereas, for the $\mathrm{Inf}(\lambda_{\mathrm{max};\,Q}(\mu))$, the latter set of inequalities are replaced by (i.e. equation (B.15))

$$\langle \overrightarrow{C}_2 | \lambda_u \mu_{n_1+n_2} + (n_1+n_2)(n_1+n_2-1)\mu_{n_1+n_2-2} - \mu_{n_1+n_2+4} | \overrightarrow{C}_2 \rangle > 0, \qquad \forall \overrightarrow{C}_2 \neq 0,$$
$$0 \leqslant n_1 + n_2 + 4 \leqslant Q. \tag{18}$$

3.3.2. Normalization prescription: bounding $\mathcal{U}_Q$. One must also impose some normalization condition. A choice that leads to a bounded $\mathcal{U}_Q$ set is

$$\mu_0 + \mu_{Q(\mathrm{even})} = 1. \tag{19}$$

To study the consequences of this, note that the physical moments for the ground-state wavefunction (i.e. assume $\Psi = \Psi_{\mathrm{gr}}$) satisfy

$$\mu_p = \int_{-1}^{+1} \mathrm{d}x\, x^p \Psi(x) + \int_{x \notin [-1,1]} \mathrm{d}x\, x^p \Psi(x). \tag{20}$$

The $p =$ even moments must be positive and satisfy

$$0 < \mu_{p=\mathrm{even}} = \int_{-1}^{+1} \mathrm{d}x\, x^p \Psi(x) + \int_{x \notin [-1,1]} \mathrm{d}x\, x^p \Psi(x) < \int_{-1}^{+1} \mathrm{d}x \Psi(x) + \int_{x \notin [-1,1]} \mathrm{d}x\, x^Q \Psi(x), \tag{21}$$

or

$$0 < \mu_{p=\mathrm{even}} < \mu_0 + \mu_Q = 1. \tag{22}$$

For the odd-order moments, a similar set of relations ensues for $|\mu_{p=\mathrm{odd}}| \leqslant \int_{-1}^{+1} \mathrm{d}x |x^p| \Psi(x) + \int_{x \notin [-1,1]} \mathrm{d}x |x^p| \Psi(x) < \mu_0 + \mu_Q = 1$. Thus, we have

$$-1 \leqslant \mu_{p=\mathrm{odd}} \leqslant +1. \tag{23}$$

3.3.3. Linear programming—bisection algorithm for determining $\lambda_{\mathrm{min}}^{\mathrm{Sup}}$ and $\lambda_{\mathrm{min}}^{\mathrm{Sup}}$. The following algorithm implicitly makes use of the quasi-convex nature of $\lambda_{\mathrm{min};\,Q}(\mu)$ and the quasi-concave structure of $\lambda_{\mathrm{max};\,Q}(\mu)$ for $\mu \in \mathcal{U}_Q$.

We outline the basic structure of our computational algorithm. Assume that for a trial positive solution, $(\mu_0^*, \ldots, \mu_Q^*)$, we have determined its corresponding extremal eigenvalue, $\lambda_{\mathrm{min};\,Q}(\mu_*)$. Within the interval $[\lambda_{\mathrm{min};\,Q}(\mu_*), \infty)$, we pick an arbitrary point, λ_a, and use the

EMM 'cutting-algorithm' to determine if there exists a point in $\mathcal{U}_Q$, satisfying the normalization conditions, as well as equation (17), for $\lambda_l = \lambda_a$. There are two possibilities:

(A) If there is such a point, then we repeat the entire procedure, but within the interval $[\lambda_a, +\infty)$.

(B) If there is no such point, then the entire procedure is repeated within the interval $[\lambda_{\min;Q}(\mu_*), \lambda_a]$.

The objective is to eventually generate a reducing sequence of intervals, $\left[\lambda_{a_1}, \lambda_{a_2}\right] \supset \cdots \supset \left[\lambda_{a_i}, \lambda_{a_{i+1}}\right]$, until an acceptably small interval is attained. The endpoints will tightly bound $\lambda^{\text{Sup}}_{\min;Q}$.

For the $\lambda^{\text{Inf}}_{\max;Q}$, a similar procedure is required. Thus, one would select a point within the interval $(-\infty, \lambda_{\max;Q}(\mu_*))$. Upon picking an arbitrary point within this interval, λ_a, one would then determine the existence, or non-existence of a μ-point lying within $\mathcal{U}_Q$, and satisfying the normalization conditions. Such a point must also satisfy equation (18), for $\lambda_u = \lambda_a$. If there is such a μ-point, then the entire procedure is repeated for the interval $(-\infty, \lambda_a)$. If there is no such point, then the updated interval is $(\lambda_a, \lambda_{\max;Q}(\mu_*))$.

3.3.4. The need for a rough upper bound. All of the above is contingent on making sure that the boundary of $\mathcal{U}_Q$ includes no points at which the $\mathbf{U}(\mu)$ matrix has zero eigenvalues. This was emphasized previously. The adopted choice of normalization, if not supplemented with additional linear constraints on the moments, includes such singular points. Specifically, because the $\mathbf{U}$ matrix only includes moments up to order μ_{2N}, while the $\mathbf{H}$ matrix includes the additional moments $\{\mu_{2N+1}, \ldots, \mu_{2N+4}\}$, one possible boundary point could be all of the first $2N + 4$ moments set to zero (i.e. $\mu_{0 \leqslant n \leqslant 2N+3} = 0$) and the last moment set to unity, $\mu_{2N+4} = 1$. To avoid these, and other such possibilities, any rough upper bound for E_{gr} will help in restricting $\mathcal{U}_Q$ to avoid such boundaries.

Let $E_{\text{pub}} \gg E_{\text{gr}}$ denote a *poor upper bound* to the ground-state energy. The true moment equation for the quartic problem is $E_{\text{gr}}\mu_p = -p(p-1)\mu_{p-2} + \mu_{p+4}$. Taking $p =$ even, we have

$$E_{\text{pub}}\mu_p + p(p-1)\mu_{p-2} > \mu_{p+4}, \qquad p = \text{even}. \tag{24}$$

Thus, these additional inequality relations will lead to proper $\mathcal{U}_Q$ sets. In table 3, we take $E_{\text{pub}} = 2$.

The results in table 3 confirm the previous theoretical results. Note that the EMM bounds will be, generally, tighter than those derived from a 'moment problem extension of Barta's theorem'. The calculations were done using the Stieltjes form for the moments (i.e. all odd-order Hamburger moments were set to zero, *ab initio*, $\mu_{\text{odd}} = 0$). The results in table 3 confirm that knowledge of a rough upper bound for the ground-state energy lead to converging bounds for the ground-state energy. This result is similar to that developed in a Euclidean time reformulation of the EMM philosophy, as applied to positive matrices (Handy and Ndow 1992).

4. Conclusion

We have outlined a theoretical procedure for transforming Barta's configuration space theorem into a moment problem equivalent. The advantages of the latter are that it leads to a (quasi)-convexity/concavity reformulation that avoids multi-extrema difficulties associated with the configuration space formulation. In addition, by so doing, we solve the problem of defining a

Table 3. Results of the quasi-convexity/concavity analysis (i.e. 'moment problem reformulation of Barta's theorem') applied to the quartic potential problem: $-\Psi''(x) + x^4\Psi(x) = E\Psi(x)$.

Moment order P^*	Theorem 4 bounds	EMM bounds
6	$.934 < E_{\rm gr} < 1.170$	$.934 < E_{\rm gr} < 1.150$
7	$1.021 < E_{\rm gr} < 1.168$	$1.028 < E_{\rm gr} < 1.153$
8	$1.027 < E_{\rm gr} < 1.080$	$1.028 < E_{\rm gr} < 1.067$
9	$1.050 < E_{\rm gr} < 1.068$	$1.059 < E_{\rm gr} < 1.067$
10	$1.055 < E_{\rm gr} < 1.063$	$1.059 < E_{\rm gr} < 1.062$
11	$1.055 < E_{\rm gr} < 1.062$	$1.059 < E_{\rm gr} < 1.061$
12	$1.0602 < E_{\rm gr} < 1.0613$	$1.0602 < E_{\rm gr} < 1.0610$

P^*: $\{\mu_{2\rho} | 0 \leqslant \rho \leqslant P\}$.

procedure for improving Barta's bounds, once an initial trial configuration is used. This was an outstanding, theoretical problem, within the configuration space formulation. We show that the eigenvalue moment method (EMM) is an integral part of this procedure, and allows us to prove theorem 4. In turn, the results presented here support ('prove') the empirically observed fact that the EMM feasibility energy values correspond to a continuous set (an interval) since it is bounded by the supremum and infimum of the extremal eigenvalues associated with the underlying generalized eigenvalue problem.

It should be emphasized that although the previous effort was focused on determining the eigenenergy, one can also generate converging bounds on the individual moments themselves, since these must lie in a bounded, convex, space. Thus, for example, in one dimension, one could ask, what are the moment values of the function, $\Psi(x) = \mathrm{e}^{(-x^4+x^2)}$. Given that this function satisfies $-\Psi''(x) + [-8x^2 - 16x^4 + 16x^6]\Psi = \lambda\Psi$, with $\lambda = -2$, and this differential system admits a, bounded, positive solution, one can apply all of the previous formalism to compute the moments through converging lower and upper bounds.

One of the reviewers posed an interesting question: Can the previous method(s) be applied to studying the Schwinger–Dyson equations? In statistical physics, and Euclidean formulations of field theory (i.e. path integral representations), all the various correlation functions may be regarded as moments of positive functionals. Thus, consider expressions of the type

$$\mu_{p_1,\ldots,p_N} \equiv \int \mathrm{d}x_1 \cdots \int \mathrm{d}x_N \prod_{i=1}^{N} x_i^{p_i} \exp(-F[x_1, \ldots, x_N]),$$

where the function, $F[\overrightarrow{x}]$, is assumed to be a polynomial-type function (i.e. of finite degree in each variable). The kernel $\exp(-F[x_1, \ldots, x_N])$ is assumed to be asymptotically vanishing. One can apply the previous formalism (including the EMM approach) to determining converging bounds on these moment expressions. To initiate this one first rewrites the kernel in terms of some convenient differential relation:

$$\partial_{x_n}^{q_n} \exp(-F[\overrightarrow{x}]) = \text{polynomial}_n([\overrightarrow{x}]) \exp(-F[\overrightarrow{x}]).$$

These differential relations, in turn, lead to a moment equation set of constraints on the $\mu_{p_1,\ldots,p_N}$ moments. Thus, in principle, one can also extend the previous approach to such systems, including those for $N \to \infty$, which would correspond to the field theoretic cases. The algorithmic details of this are under investigation. The author extends his appreciation to the reviewer for this question.

Acknowledgments

This work benefited from partial, visitation support extended to the author through NSF award NBTC-URG 47956-7824, involving Cornell University's Nanobiotechnology Center and Clark Atlanta University (CAU). The efforts, in this regard, of Dr Ishrat Khan are gratefully acknowledged. This work benefited from discussions with Dr Lois Pollack's group focusing on protein folding studies. Additional insights from discussions with Mr Harold Brooks, Professor Daniel Bessis, Dr Christopher J Tymczak, and Mr Siddharth Joshi (with much appreciation for assisting in understanding some of the mathematical convexity/concavity theorems), as well as the computing resources of CAU's Center for Theoretical Studies of Physical Systems, are gratefully acknowledged.

Appendix A. Technical preliminaries

In order to clarify the notation used in connection with the new contributions of this work, we develop them in the context of a short technical overview of the eigenvalue moment method (EMM). The EMM will also play an important role in proving some of the theorems introduced in this work; therefore, its review, here, will facilitate the overall understanding of our new results.

A.1. The moment equation

All of our results are predicated on being able to transform the Schrödinger equation into a *moment equation* representation. This is always possible for multidimensional systems with rational fraction potentials. For problems not of this type, it still may be possible to identify coordinate systems in which the transformed Schrödinger equation involves function coefficients that are of rational fraction form. This was the case for the quadratic Zeeman effect, as previously cited, for which parabolic coordinates led to the identification of a moment equation. Despite these limitations, these restrictions still define a large and important class of physics problems.

Because our intent is to develop the underlying theory, we have chosen to limit all discussions, and examples, to one-dimensional systems, for simplicity.

For one-dimensional systems, the moment equation corresponds to a recursive, linear, homogeneous, finite difference equation of order $1+m_s$, wherein all of the moments are linearly dependent on the first $1 + m_s$ moments $\{\mu_0, \ldots, \mu_{m_s}\}$. The latter will be referred to as the *initialization* moments, or the *missing moments*. Once any suitable normalization prescription is adopted, the moments can be written in terms of the unconstrained initialization moments. The form of the normalization prescription will vary, depending on the nature of the problem (i.e. Stieltjes, Hamburger, etc). In the Hamburger case, the even moments must be positive, the odd moments can have arbitrary signature. We want to choose a normalization prescription that automatically bounds the initialization moments. For the Hamburger case, one must have m_s = even, and we can take $\mu_0 + \mu_{m_s} = 1$. It then follows that $|\mu_\ell| \leqslant \mu_0 + \mu_{m_s} = 1$, for $0 \leqslant \ell \leqslant m_s$. Since $\mu_0 = 1 - \mu_{m_s}$, all of the remaining initialization moments are unconstrained. We can now write the moment equation as

$$\mu_p = \hat{M}_E(p, 0) + \sum_{\ell=1}^{m_s} \hat{M}_E(p, \ell)\mu_\ell, \qquad p \geqslant 0, \tag{A.1}$$

where the $\hat{M}_E(p, \ell)$ are known coefficients, nonlinearly dependent on the energy, E. We note that the (unconstrained) initialization moments must lie within the m_s dimensional cube: $\left(\mu_1, \ldots, \mu_{m_s}\right) \in (-1, 1)^{m_s}$.

A.2. Stieltjes–Pade positivity quantization

For parity invariant systems, the change of variables $x = \sqrt{y}, y \geqslant 0$, transforms the Hamburger moment problem (involving functions on the entire real axis, $\Re, \mu_p = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p \Psi(x)$) into a Stieltjes moment problem (functions restricted to the nonnegative real axis, $u_p = \int_0^{\infty} \mathrm{d}y\, y^p \Phi(y)$). For some of these systems, such as the harmonic oscillator problem (i.e. $\partial_x^2 \Psi + x^2 \Psi(x) = E\Psi(x)$), the moment equation's order becomes unity, or $m_s = 0$. In such cases, the even-order Hamburger moments of the wavefunction become Stieltjes moments of the modified wavefunction

$$\Phi(y) \equiv \frac{\Psi(\sqrt{y})}{\sqrt{y}} : \mu_{2\rho} = u_\rho = \int_0^{\infty} \mathrm{d}y y^\rho \Phi(y).$$

Because $m_s = 0$, the Stieltjes moments for the ground state become (known) nonlinear functions of E, the energy variable (i.e. $u_{\rho+1} = Eu_\rho + 2\rho(2\rho - 1)u_{\rho-1}, u_0 \equiv 1, u_1 = E, u_2 = 2 + E^2$, etc).

Since the Stieltjes moments for the Φ-ground state are known functions of E, these then also determine the Pade approximants (Baker 1975), $[M|N]_{(E;s)}$, for the associated Stieltjes integral, $I(s) = \int_0^{\infty} \mathrm{d}y \frac{\Phi(y)}{1+sy}$.

It is a well-known theorem that if a Stieltjes measure is positive, then the $[M|M]$ and $[M - 1|M]$ Pade approximants must satisfy a nested structure:

$$[M - 1|M]_{(E_g;s)} \leqslant [M|M + 1]_{(E_g;s)} \leqslant I(s) \leqslant [M + 1|M + 1]_{(E_g;s)} \leqslant [M|M]_{(E_g;s)} \tag{A.2}$$

Handy (1984) discovered that one could use this nested behaviour to quantize the ground-state energy, through converging lower and upper bounds. Thus, for arbitrary E, one generates the first Q Stieltjes moments (and all the Pade approximants that can be generated from them), and determines the energy interval, $\left(E_Q^L, E_Q^U\right)$, of feasible energy values that lead to Pade approximants satisfying the above nested structure. The endpoints of the feasibility energy interval become the numerically generated lower and upper bounds to the ground-state energy: $E_Q^L \leqslant E_{\mathrm{gr}} \leqslant E_Q^U$. The entire process is repeated at the next higher order ($Q \to Q{+}1$), resulting in a reduction of the feasibility energy interval. In this manner, geometrically converging, lower and upper bounds are obtained.

A.3. Hankel–Hadamard determinant positivity quantization

Since Pade approximants could not be easily extended to multidimensions, an alternate equivalent to the above moment problem quantization procedure was required. The standard moment problem positivity constraints, for a nonnegative function, $f(x) \geqslant 0$ (excluding distribution-type expressions with zero measure support), are generally expressed in terms of the Hankel–Hadamard (HH) determinantal, inequality constraints, given in equation (A.5). These are derived through the quadratic form integral expression

$$\int_{-\infty}^{+\infty} \mathrm{d}x \left(\sum_{n=0}^{N} C_n x^n\right)^2 f(x) > 0, \tag{A.3}$$

or

$$\langle \overrightarrow{C} | \begin{pmatrix} \mu_0, \mu_1, \ldots, \mu_N \\ \mu_1, \mu_2, \ldots, \mu_{N+1} \\ \cdots \\ \mu_N, \mu_{N+1}, \ldots, \mu_{2N} \end{pmatrix} | \overrightarrow{C} \rangle > 0, \qquad \forall \overrightarrow{C} \neq \overrightarrow{0}. \tag{A.4}$$

The real and symmetric Hankel moment matrix (defined in equation (A.4)) is therefore positive definite, with positive eigenvalues. Thus all of its subdeterminants of the following type, must be positive:

$$\Delta_{m,n}(\mu) > 0, m_{(\text{even})} \geqslant 0, \qquad n \geqslant 0, \tag{A.5}$$

where

$$\Delta_{m,n}(\mu) \equiv \text{Det} \begin{pmatrix} \mu_m, \mu_{m+1}, \ldots, \mu_{m+n} \\ \mu_{m+1}, \mu_{m+2}, \ldots, \mu_{m+n+1} \\ \cdots \\ \mu_{m+n}, \mu_{m+n+1}, \ldots, \mu_{m+2n} \end{pmatrix}. \tag{A.6}$$

For the Hamburger moment problem (i.e. the moment constraints leading to a positive function on $\Re$), it is sufficient to require that $\Delta_{m,n}(\mu) > 0$ for $m = 0, n \geqslant 0$ (Baker 1975).

It is clear that the HH inequalities are necessary conditions for any positive function. That they are sufficient for establishing the positivity of the underlying function can be motivated as follows. One can approximate the Gaussian, Dirac distribution, in terms of the quadratic form expansion. That is

$$\frac{1}{\beta\sqrt{\pi}} \mathrm{e}^{-\frac{(x-\tau)^2}{\beta}} = \frac{1}{\beta\sqrt{\pi}} \left(\mathrm{e}^{-\frac{(x-\tau)^2}{2\beta}} \right)^2 \approx \frac{1}{\beta\sqrt{\pi}} \left(\sum_{j=0}^{J} \frac{1}{j!} \left(-\frac{(x-\tau)^2}{2\beta} \right)^j \right)^2.$$

Thus, for sufficiently large J and small β values, the HH constraints are essentially sampling the local behaviour of a (bounded, asymptotically decaying) function, and requiring that it be positive.

The HH determinants can be extended to multidimensions, as developed in the work by Devinatz (1957).

The first use of the HH, moment problem (MP), positivity theorems to quantize the bosonic ground-state energy was published by Handy and Bessis (1985). We briefly outline the essentials of this work. Through the moment equation's structure, equation (A.1), the moments are explicitly dependent on the energy variable, E, and the (unconstrained) *initialization moments*, $\{\mu_1, \ldots, \mu_{m_s}\}$. So too are the HH determinants, $\Delta_{0,n}(\mu) = \Delta_{0,n}(\mu_1, \ldots, \mu_{m_s}; E)$, for $n < \infty$. Given an arbitrary E value, and (even number) moment expansion order, $Q < \infty$ (thus all the moments $\mu_{p \leqslant Q}$ are generated) one determines if there exists an m_s-dimensional, *initialization moment* solution set, $\mathcal{U}_{Q;E} \subset (-1, 1)^{m_s}$, satisfying all the corresponding HH inequalities $\left(\Delta_{0,0}(\mu) > 0, \Delta_{0,1}(\mu) > 0, \ldots, \Delta_{0,\frac{Q}{2}}(\mu) > 0\right)$. If this solution set exists ($\mathcal{U}_{Q;E} \neq \oslash$), then the associated E value is a possible physical ground-state value, to order Q. If not ($\mathcal{U}_{Q;E} = \oslash$), then the chosen E value is not a possible physical value for the ground-state energy. In this manner, a feasibility energy interval is determined, as before, in the Pade case. It can be shown that $\mathcal{U}_{Q;E}$ must be a convex set, if it exists $\left(E \in \left(E_Q^L, E_Q^U\right) \iff \mathcal{U}_{Q;E} \neq \oslash\right)$.

A.4. Variational-linear programming, moment problem quantization

Although the previous HH-MP procedure created greater flexibility in extending the underlying positivity quantization philosophy to more systems, its structure (i.e. the nonlinear dependence on the moments) made it too difficult for multidimensional systems.

Any bounded, convex, set (with nonlinear boundaries), such as the $\mathcal{U}_{Q;E}$'s can be represented as the intersection of infinitely many bounded polytopes (convex sets with hyperplanes as boundaries). One realizes that equation (A.4) defines this equivalent, alternative linear representation for the HH inequalities. That is, instead of working with a finite number of (large dimensioned) nonlinear inequality relations (i.e. the HH constraints), one can work with an equivalent set of infinitely many, linear, constraints. This provided the theoretical breakthrough in facilitating the implementation of moment problem positivity quantization strategy.

In order to capitalize on this linearized equivalent, one must devise an optimization strategy to essentially determine the optimal $\overrightarrow{C}$'s, or *cutting vectors* (refer to equation (A.4)). This required a clever combination of the moment equation formalism with linear programming theory (Chvatal 1983). Thus, through the ensuing *cutting algorithm*, devised by Handy, given an arbitrary E value, one rapidly 'cuts up' the starting (normalization) polytope (the hypercube, $(-1, 1)^{m_s}$) into either the null set (thereby establishing that $\mathcal{U}_{Q;E} = \oslash$ and E is unphysical), or into a polytope, $\mathcal{P} \supset \mathcal{U}_{Q;E}$, containing an *initialization point*, $\overrightarrow{\tilde{\mu}} = \left(\tilde{\mu}_1, \ldots, \tilde{\mu}_{m_s}\right)$ for which all the associated Hankel matrices are positive (concluding that $\overrightarrow{\tilde{\mu}} \in \mathcal{U}_{Q;E}$, hence $\mathcal{U}_{Q;E} \neq \oslash$, and that particular E is a possible value for the ground-state energy).

The above, entire, procedure is the eigenvalue moment method (EMM), which was used to solve the previously cited quadratic Zeeman problem.

Appendix B. Proof of theorems

We develop the basic relations and prove the various theorems previously quoted, with the exception of theorem 1 which is a standard result in the optimization theory, particularly in the context of mathematical economics. We will be limiting our discussion to the one-dimensional case, for simplicity.

Two crucial elements are required for deriving Barta's theorem in equation (1). The first is that in the configuration space representation, the bosonic ground-state wavefunction, $\Psi_{\rm gr}(x)$, must be of uniform signature, and thus can be taken to be positive, $\Psi_{\rm gr}(x) > 0$. Accordingly, given any trial function, Ψ, of arbitrary signature, and with a bounded and continuous second-order derivative, one obtains the zero identity for the scalar product: $\langle\Psi_{\rm gr}|(H - E_{\rm gr})|\Psi\rangle = 0$, where $E_{\rm gr}$ is the ground-state energy, and H is the Schrödinger equation Hamiltonian. Therefore, $H - E_{\rm gr}$, when applied to Ψ, must have a zero at some location

$$(H - E_{\rm gr})\Psi(x_0) = 0. \tag{B.1}$$

The second assumption is that if the trial function is strictly positive, $\Psi > 0$, then the range of the function $R(x) = \frac{H\Psi(x)}{\Psi(x)}$ must define a bounded subset of $\Re$ that contains $E_{\rm gr}$: $E_{\rm gr} \in \{R(x)|\forall x \in \Re\}$. This leads to equation (1) or $\mathrm{Inf}_x R(x) \leqslant E_{\rm gr} \leqslant \mathrm{Sup}_x R(x)$. Positivity is an important cornerstone of Barta's theorem.

Let $\mathcal{S}$ and $\mathcal{I}$ denote the supremum and infimum, respectively, for an arbitrary trial function, Ψ, lying within the set of functions, $\mathcal{C}$, which are positive, bounded (exponentially decaying), and have continuous, finite, second derivatives:

$$\mathcal{I} \equiv \mathrm{Inf}\left(\frac{H\Psi(x)}{\Psi(x)}\right), \tag{B.2}$$

$$\mathcal{S} \equiv \mathrm{Sup}\left(\frac{H\Psi(x)}{\Psi(x)}\right). \tag{B.3}$$

Define the configurations:

$$L_\Psi(x;\lambda_l) \equiv \frac{H\Psi(x)}{\Psi(x)} - \lambda_l \geqslant 0, \qquad \Longleftrightarrow \qquad \lambda_l \leqslant \mathcal{I}, \tag{B.4}$$

and

$$U_\Psi(x;\lambda_u) \equiv \lambda_u - \left(\frac{H\Psi(x)}{\Psi(x)}\right) \geqslant 0, \qquad \Longleftrightarrow \qquad \lambda_u \geqslant \mathcal{S}. \tag{B.5}$$

Although the trial functions must be positive (i.e. strictly positive) if they are to be easily used within Barta's procedure, the $\{U_\Psi(x), L_\Psi(x)\}$ functions can be nonnegative (provided the zeros correspond to sets of zero measure) and still generate strictly positive HH determinants. Accordingly,

$$(H - \lambda_l)\Psi(x) \geqslant 0, \qquad \Longleftrightarrow \qquad \lambda_l \leqslant \mathcal{I}, \tag{B.6}$$

and

$$(\lambda_u - H)\Psi(x) \geqslant 0, \qquad \Longleftrightarrow \qquad \lambda_u \geqslant \mathcal{S}. \tag{B.7}$$

Let us focus on the first relation:

$$\Phi_{\lambda_l}(x) = (H - \lambda_l)\Psi(x) \geqslant 0, \lambda_l \leqslant \mathcal{I}. \tag{B.8}$$

For any $\Psi(x) \in \mathcal{C}$, $\Phi_{\lambda_l}(x)$ must be integrable and positive almost everywhere (i.e. nonnegative). Thus, its power moments must satisfy the standard positivity relations of the *moment problem* (Shohat and Tamarkin 1963), as discussed in the Introduction.

We are restricting our analysis to Hamiltonians with rational fraction potentials, since these are those most easily transformable into a moment equation representation. For simplicity, the following discussion assumes that the potential is of (multidimensional) polynomial form. The generalization to singular potentials is straightforward, and briefly discussed below.

In order to make our analysis more transparent, we will consider the case of the quartic potential problem: $H = -\partial_x^2 + x^4$. Then $\Phi_{\lambda_l}(x) = \left(-\partial_x^2 + x^4 - \lambda_l\right)\Psi(x)$, and we can generate the power moments of the LHS, based on those of $\Psi(x)$.

Define the power moments of the trial function by $\mu_p \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p \Psi(x)$, $p \geqslant 0$. By assumption (i.e. $\Psi > 0$), these must satisfy the Hankel–Hadamard determinantal constraints for the Hamburger moment problem: $\Delta_{m,n}(\mu) > 0$, for $m = 0, n \geqslant 0$. These constraints are required for all positive (more generally, nonnegative) functions on the real axis.

The power moments of $\Phi_{\lambda_l}(x)$,

$$\nu_p \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p \Phi_{\lambda_l}(x), \qquad p \geqslant 0, \tag{B.9}$$

satisfy (i.e. upon substituting the Φ/Ψ relation and performing the necessary integration by parts)

$$\nu_p = -p(p-1)\mu_{p-2} + \mu_{p+4} - \lambda_l \mu_p, \qquad p \geqslant 0. \tag{B.10}$$

If $\lambda_l \leqslant \mathcal{I}$, then the ν moments generate the Hankel matrix that must satisfy the (HH) positivity constraints:

$$\Delta_{0,N}(\nu(\lambda_l)) = \mathrm{Det}\begin{pmatrix} \cdots \\ -(n_1+n_2)(n_1+n_2-1)\mu_{n_1+n_2-2} + \mu_{n_1+n_2+4} - \lambda_l \mu_{n_1+n_2} \\ \cdots \end{pmatrix} > 0, \tag{B.11}$$

for all $0 \leqslant n_1, n_2 \leqslant N < \infty$.

The form of the finite-dimensional Hankel matrix in equation (B.11) is symbolized by $\mathbf{H}$ -$\lambda_l\mathbf{U}$, with $\mathbf{U}$ the positive definite Hankel matrix for Ψ's moments.

We note that the $\{\nu_0, \ldots, \nu_{2N}\}$ moments, used to define the Hankel moment matrix for Φ_{λ_l}, depend on the $\{\mu_0, \ldots, \mu_{2N+4}\}$ moments of Ψ. Thus, we are working within the moment space $\mathcal{U}_Q$ where $Q = 2N+4$. Notational consistency would suggest that in the following discussion we make reference to $\lambda_{\min;\,Q_N}(\mu)$ where, $Q_N \equiv 2N+4$. To streamline the discussion, we will simply use the notation $\lambda_{\min;\,N}$.

Define by $\lambda_{\min;\,N}(\mu)$ the smallest zero satisfying (the μ dependence is not explicitly given, for greater clarity)

$$\Delta_{0,N}(\nu(\lambda_{\min;\,N})) = 0, \tag{B.12}$$

or

$$\mathrm{Det}(\mathbf{H}(\mu) - \lambda_{\min,N}\mathbf{U}(\mu)) = 0. \tag{B.13}$$

Accordingly, $(-\infty, \lambda_{\min;\,N}(\mu)) \supset (-\infty, \mathcal{I})$. This is because, so long as $\lambda_l \leqslant \mathcal{I}$, equation (B.11) must hold. Hence, any root in the λ-variable domain must be larger than $\mathcal{I}$.

We now show that the sequence $\{\lambda_{\min,N}(\mu)|N \geqslant 0\}$ must be nonincreasing, or $\lambda_{\min,N}(\mu) \geqslant \lambda_{\min,N+1}(\mu)$. The easiest way is to exploit the positive definiteness of $\mathbf{U}$, which leads to the Cholesky decomposition $\mathbf{U} = \mathbf{R}^t\mathbf{R}$, where $\mathbf{R}$ is the unique, upper triangular matrix, with positive diagonal entries. Its inverse is also of upper triangular form. Accordingly, $\lambda_{\min;\,N}$ is also the smallest zero for the equation

$$\mathrm{Det}\mathbf{R}^{-t}\mathbf{H}\mathbf{R}^{-1} - \lambda_{\min,N}\mathbf{1} = 0. \tag{B.14}$$

Of course, this is also the smallest eigenvalue of the indicated real, symmetric matrix, which, in turn, defines a nonincreasing sequence; thus proving the previous claim.

With regards to the λ_u's, an analogous result follows. Thus, if $\lambda_u \geqslant \mathcal{S}$, then

$$\Delta_{0,N}(-\nu(\lambda_u)) = \mathrm{Det}\begin{pmatrix} \cdots \\ \lambda_u\mu_{n_1+n_2} + (n_1+n_2)(n_1+n_2-1)\mu_{n_1+n_2-2} - \mu_{n_1+n_2+4} \\ \cdots \end{pmatrix} > 0, \tag{B.15}$$

for all $0 \leqslant n_1, n_2 \leqslant N < \infty$.

We now define $\lambda_{\max;\,N}(\mu)$ as the largest root satisfying

$$\Delta_{0,N}(-\nu(\lambda_{\max;\,N})) = 0, \tag{B.16}$$

or

$$\mathrm{Det}(\lambda_{\max,N}\mathbf{U}(\mu) - \mathbf{H}(\mu)) = 0. \tag{B.17}$$

(Note that $\lambda_{\max;\,N}$ is also the largest root of the generalized eigenvalue problem, $\mathrm{Det}(\mathbf{H}(\mu) - \lambda_{\max,N}\mathbf{U}(\mu)) = 0$.) It then follows that $(\lambda_{\max;\,N}, +\infty) \supset (\mathcal{S}, +\infty)$, and they form a nondecreasing sequence: $\lambda_{\max;\,N}(\mu) \leqslant \lambda_{\max;\,N+1}(\mu)$. This follows from the observation that $-\lambda_{\max;\,N}$ is the smallest root of

$$\mathrm{Det}(-\mathbf{H}(\mu) - (-\lambda_{\max,N})\mathbf{U}(\mu)) = 0,$$

and through the Cholesky decomposition of the positive $\mathbf{U}$ matrix, the $-\lambda_{\max;\,N}$ forms a nonincreasing sequence of smallest eigenvalues for the finite and symmetric matrix: $\mathbf{R}^{-t}(-\mathbf{H})\mathbf{R}^{-1}$.

B.1. Theorem 3

The first part of theorem 3 (equations (8) and (9)) follows from the previous results. The latter part of theorem 3 (equation (10)) results from the fact that the only λ_l values satisfying all of the HH positivity inequalities are those obeying $\lambda_l \leqslant \mathcal{I}$, similarly for λ_u: $\lim_{n\to\infty}\lambda_{\min;n}(\mu) = \mathcal{I}$, and $\lim_{n\to\infty}\lambda_{\max;n}(\mu) = \mathcal{S}$.

B.1.1. Alternative derivation. We include some additional remarks that provide a different perspective on all the above. We limit the discussion, for brevity, to the $\lambda_{\min;n}$ case.

The HH positivity theorems require that all of the HH determinants, for the ν-moments, be positive, as functions of λ_l. To simply investigate the positivity properties of one of these determinants is insufficient. Thus, we can either work with the quadratic form inequality in equation (A.4), adapted to the $\nu_p(\mu, \lambda_l)$ moments (equation (B.10)), for the $((N+1)\times(N+1))$-dimensional Hankel matrix, $\mathcal{H}_N(\nu)$:

$$\langle \overrightarrow{C} | \begin{pmatrix} \nu_0(\mu,\lambda_l), \nu_1(\mu,\lambda_l), \ldots, \nu_N(\mu,\lambda_l) \\ \nu_1(\mu,\lambda_l), \nu_2(\mu,\lambda_l), \ldots, \nu_{N+1}(\mu,\lambda_l) \\ \cdots \\ \nu_N(\mu,\lambda_l), \nu_{N+1}(\mu,\lambda_l), \ldots, \nu_{2N}(\mu,\lambda_l) \end{pmatrix} | \overrightarrow{C} \rangle > 0, \qquad \forall \overrightarrow{C} \neq \overrightarrow{0}, \tag{B.18}$$

or we can work with the $N+1$ HH determinants:

$$\Delta_{0,n}(\nu(\mu,\lambda_l)) > 0, \qquad n = 0, \ldots, N. \tag{B.19}$$

The set of λ_l values satisfying equation (B.18) must correspond to a convex set (Chvatal 1983) since it represents an infinite set of linear inequalities in the λ-variable. Thus, the feasibility λ set must be a semi-infinite interval. That is, if equation (B.18) is satisfied by the two values $\lambda_l = \lambda_l^{(\sigma_{1,2})}$,

$$\langle \overrightarrow{C} | -(n_1+n_2)(n_1+n_2-1)\mu_{n_1+n_2-2} + \mu_{n_1+n_2+4} - \lambda_l^{(\sigma_1)}\mu_{n_1+n_2} | \overrightarrow{C} \rangle > 0, \tag{B.20}$$

$$\langle \overrightarrow{C} | -(n_1+n_2)(n_1+n_2-1)\mu_{n_1+n_2-2} + \mu_{n_1+n_2+4} - \lambda_l^{(\sigma_2)}\mu_{n_1+n_2} | \overrightarrow{C} \rangle > 0, \tag{B.21}$$

then it must be satisfied by all $\lambda_l = s\lambda_l^{(\sigma_1)} + (1-s)\lambda_l^{(\sigma_2)}$, for $\leqslant s \leqslant 1$ (simply multiply each of the above two inequalities by $s \geqslant 0$ and $1-s \geqslant 0$, respectively, and add); thereby establishing the convex nature of the set of allowed λ_l values.

Since $\lambda_l \in (-\infty, \mathcal{I})$ satisfies equation (B.18) (from equation (B.6)), it follows that there exists a 'largest' semi-infinite interval $(-\infty, \lambda_{l;N})$, with $\mathcal{I} \leqslant \lambda_{l;N}$, satisfying all of equation (B.18). It is clear that $\lambda_{l;N+1} \leqslant \lambda_{l;N}$, since from equation (B.18), the quadratic form inequalities for the $\mathcal{H}_{N+1}(\nu)$ Hankel matrix include all of those corresponding to the $\mathcal{H}_N(\nu)$ case. The $\lambda_{l;N}$ value must then be the smallest root of the equation $\mathrm{Det}(\mathcal{H}_N(\nu(\mu,\lambda_l)) = 0$. That is, $\lambda_{l;N} = \lambda_{\min;N}$.

B.1.2. Extension to rational fraction (singular) potentials. The preceding, alternative, proof also shows us how to extend our results to the case of rational fraction type potentials. Consider the perturbed quartic potential $V(x) = x^4 + \frac{1}{x^2+2}$. Limiting ourselves to the 'infimum' case, for simplicity, we see that equation (B.8) can be modified by multiplying both sides by the positive denominator polynomial, x^2+2:

$$(x^2+2)\Phi_{\lambda_l}(x) = (-(x^2+2)\partial_x^2 + (x^2+2)x^4 + 1 - \lambda_l(x^2+2))\Psi(x) > 0, \qquad \lambda_l \leqslant \mathcal{I}. \tag{B.22}$$

Thus, the RHS generates a positive (Hankel) matrix, and one can proceed to define the corresponding $\lambda_{\min;N}$, which satisfies all the relations described above.

Thus, in general, as long as one multiplies equation (B.8), or its multidimensional counterpart, by positive 'denominator' type polynomials, in order to achieve a Hankel matrix structure, then all of our results apply.

B.1.3. Additional remarks. Given that the function $\frac{H\Psi}{\Psi}$ can have multiple extrema, having a systematic method of computing the infimum/supremum (as opposed to searching over all local extrema) may make the above results very convenient. That is, one can determine the infimum ($\mathcal{I}(\mu)$) and supremum ($\mathcal{S}(\mu)$) by studying the asymptotic limits of the $\lambda_{\min;n}$ and $\lambda_{\max;n}$, combined with sequence acceleration techniques, where possible.

Another important aspect of the previous results is that we can now extend Barta's result to positive functions which may not be given in closed form, but whose moments may be known. We provide one example of this in section 3.

B.2. Theorem 2

We now prove theorem 2 by way of the quartic potential problem. Whereas in the previous proofs we were working with an infinite set of numbers, $\{\mu_p | p \geqslant 0\}$, known to be the moments of a positive function, we will now be working with a finite set of moments that satisfy the moment equation, as well as the corresponding positivity theorems.

Let us assume that the $\{\mu_p | 0 \leqslant p \leqslant P\}$ moments satisfy the moment equation,

$$-p(p-1)\mu_{p-2} + \mu_{p+4} - E\mu_p = 0, \qquad 0 \leqslant p \leqslant P-4. \tag{B.23}$$

Alternatively,

$$\mu_{p+4} = E\mu_p + p(p-1)\mu_{p-2}, \qquad 0 \leqslant p \leqslant P-4. \tag{B.24}$$

Clearly, this recursive relation separates into the even and odd order moments. There are more efficient ways of dealing with such relations, however, for our immediate purposes, the above is satisfactory. Also, we implicitly assume that some normalization has been chosen.

Let $P = 2M$. Again, we assume that the moments

$$\{\mu_0, \mu_1, \ldots, \mu_{P=2M}\} \in \mathcal{U}_{P=2M;EMM} \subset \mathcal{U}_{P=2M},$$

satisfy the moment equation and all the HH determinantal inequality conditions that can be generated from them, for some E value. Thus $\Delta_{0,n}(\mu) > 0$, for $\leqslant M$. From equation (B.11), we see that the **U** matrix involves all of the moments up to order μ_{2N}, where N is to be determined. The **H** matrix involves the highest order moment, μ_{2N+4}. Thus, we want $2N + 4 = 2M$. That is, the highest dimension generalized eigenvalue problem (GEP) is $N + 1 = M - 1$.

From equation (B.23), it follows that for the special set of moments being considered, we have $\mathbf{H} = E\mathbf{U}$. The corresponding GEP problem becomes

$$\mathrm{Det}(\mathbf{H} - \lambda\mathbf{U}) = \mathrm{Det}(E\mathbf{U} - \lambda\mathbf{U}) = (E-\lambda)^{N+1}\mathrm{Det}(\mathbf{U}), \tag{B.25}$$

where $\mathrm{Det}(\mathbf{U}) = \Delta_{0,N}(\mu)$, revealing its $(N+1)$ th-order degeneracy. Hence

$$\lambda_{\min;N}(\mu_E) = \lambda_{\max;N}(\mu_E). \tag{B.26}$$

In summary, the GEP problem becomes extremely degenerate for those moments satisfying the moment equation, as well as all of the corresponding HH positivity constraints. The allowable E values are those generated through the EMM procedure corresponding to moment order $P = 2M$.

B.3. Theorem 4

Define the supremum of the smallest GEP eigenvalue by $\lambda^{\sup}_{\min;Q} = \mathrm{Sup}_{\mu\in\mathcal{U}_Q}\lambda_{\min;Q}(\mu)$; and the infimum of the largest GEP eigenvalue by $\lambda^{\inf}_{\max;Q} = \mathrm{Inf}_{\mu\in\mathcal{U}_Q}\lambda_{\min;Q}(\mu)$. Since the EMM related set of moments satisfy $\mathcal{U}_{Q;EMM} \subset \mathcal{U}_Q$, and on $\mathcal{U}_{Q;EMM}$ the extremal eigenvalues are

degenerate, it follows that the EMM upper bound, must be a lower bound to $\lambda^{\sup}_{\min;\,Q}$. Likewise, the EMM lower bound, must be an upper bound to $\lambda^{\inf}_{\max;\,Q}$. This confirms equation (12).

In the $Q \to \infty$ limit, the entire moment space, for a given set of moments $\overrightarrow{\mu} = (\mu_0, \ldots, \mu_{j\to\infty})$, we must have that $\lambda_{\min;\infty}(\mu) < E_{\rm gr} < \lambda_{\max;\infty}(\mu)$, from equation (10). Clearly then $\lambda^{\sup}_{\min;\infty} = E_{\rm gr} = \lambda^{\inf}_{\max;\infty}$; confirming equation (13).

Again, we implicitly assumed that $\mathcal{U}_Q$ satisfies some physically motivated normalization prescription.

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