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Rapid wavefunction reconstruction through Hankel–Hadamard moments analysis

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Abstract. Recent studies by Handy and Bessis on the effectiveness of a Hankel-Hadamard determinant quantisation analysis are generalised to include wavefunction reconstruction. For a given bosonic ground-state wavefunction, $\Psi(x) = e^{S(x)}$, excellent pointwise convergence to dS/dx can be readily achieved with very few moments. Our approach also yields very good lower and upper bounds to dS/dx.

1. Introduction

In earlier works, Handy and Bessis (1985), Handy (1985a) and Bessis *et al* (1987) showed that the traditional 'moments problem' (Shohat and Tamarkin 1963) could be used to quantise various important physical systems. These were achieved through the generation of *exponentially* convergent lower and upper bounds to the physical eigenvalues. Very few moments were required. Of particular importance is that the underlying Hankel-Hadamard (HH) determinant analysis proved very effective for strongly coupled systems, which are not usually amenable to conventional perturbation analysis.

It is natural to ask if similar techniques may be used to reconstruct wavefunctions. As will be seen, one can generate rapidly convergent bounds to wavefunctions in a pointwise manner. More specifically, for bosonic ground states, $\Psi(x) = e^{S(x)}$, one can obtain narrow bounds for dS/dx at any x. Such information can be important in verifying analytical results generated from WKB theory (Bender and Orszag 1978), particularly near turning points. All this is consistent with work by Handy and Bessis (1985) and Handy (1981, 1985b) where it is argued that moments are relevant in understanding singular perturbation issues in quantum physics.

The formalism to be presented here is a new solution to the century old 'moments problem', first posed by Stieltjes in 1895. At an intuitive level, the issue of function moments reconstruction was addressed as follows. Let the desired wavefunction, $\Psi(x)$, be non-negative. This is true for bosonic ground states (Handy and Bessis 1985). Excited bosonic states can be reformulated in terms of non-negative configurations (Handy 1985a). The Stieltjes integral is defined by

$$I(s) = \int_0^\infty dx \frac{\Psi(x)}{1+sx}. \tag{1}$$

Clearly, if $\Psi(x)$ dies off sufficiently fast at infinity, then $I(s)$ will have a branch cut along the negative s axis. The discontinuity in $I(s)$ across this cut will yield information on $\Psi(x)$:

$$I(s+\mathrm{i}\varepsilon)-I(s-\mathrm{i}\varepsilon)=(2\pi\mathrm{i}/s)\Psi(-s^{-1}) \qquad \text{for } s<0. \tag{2}$$

The Stieltjes integral in equation (1) can be expressed in terms of a moments expansion $I(s)=\sum_{p=0}^{\infty}(-s)^p\mu(p)$. This expansion can in turn be approximated through Padé analysis (Baker 1975). The latter may then be incorporated into equation (2) yielding approximations to Ψ.

From the above discussion it is not surprising that traditional function moments reconstruction programmes can be slow, requiring many moments. As will be seen in the following, our moments formulation for wavefunction reconstruction is very efficient and can yield rapidly convergent pointwise bounds.

It is important also to take note of the general usefulness of Padé resummation techniques as applied to analytic expansions of the type $\Psi(x)=\sum_{n=0}^{\infty}c_nx^n$. Such applications of Padé analysis are made in order to analytically continue the series expansion beyond its domain of convergence. Our approach differs from such types of analysis in that

(i) we do not require that $\Psi(x)$ be anywhere analytic, and

(ii) our approach gives extremely good bounds to $S'(x)$, where $\Psi=\mathrm{e}^S$.

It is also important to stress that just as in the usual WKB analysis our formalism explicitly focuses on $S'(x)$. As such, one can see that a moments perspective greatly complements WKB theory.

2. The Hankel–Hadamard moment inequalities

The principal result of the 'moment problem' of concern to us is the Hamburger moments theorem (Baker 1975), as follows.

Let $\Psi(x)$ be a function on the real axis. Let $\mu(p)=\int_{-\infty}^{\infty}\mathrm{d}x\, x^p\Psi(x)$ be the pth Hamburger moment. Then the necessary and sufficient condition that $\Psi(x)\geqslant 0$ (non-negative) for all x is ($m=0$!)

$$\Delta_{m=0,n}\{\mu\}=\det\begin{pmatrix}\mu(m=0) & \mu(m+1) & \dots & \mu(m+n)\\ \mu(m+1) & \mu(m+2) & \dots & \mu(m+1+n)\\ \vdots & & & \vdots\\ \mu(m+n) & \mu(m+n+1) & \dots & \mu(m+2n)\end{pmatrix}>0$$

$$\text{for all } n\geqslant 0. \tag{3}$$

These relations are referred to as the Hankel-Hadamard inequalities (HH).

From equation (3) a variety of alternate formulations are possible. Assume that one is interested in $\tilde{\Psi}(x)$ restricted to the interval $[a, b]$. Accordingly, one may apply equation (3) to three related functions: $\tilde{\Psi}(x)$, $\Phi(x)=(x-a)\tilde{\Psi}(x)$ and $\Omega(x)=(b-x)\tilde{\Psi}(x)$. It would then follow that each of these must be non-negative throughout the entire real axis. This can only be if $\tilde{\Psi}(x)\geqslant 0$ on $[a, b]$ and zero elsewhere. We summarise all this below.

The necessary and sufficient conditions for $\tilde{\Psi}(x)$ to be non-negative on $[a, b]$ and zero elsewhere are

$$\Delta_{0,n}\{\mu_\psi\}>0 \qquad \Delta_{0,n}\{\mu_\Phi\}>0 \qquad \Delta_{0,n}\{\mu_\Omega\}>0 \qquad \text{for } n\geqslant 0. \tag{4}$$

The various moments μ_f (for $f = \psi, \phi, \Omega$) correspond to the Hamburger moments over the entire real axis, $\mu_f(p) = \int_{-\infty}^{\infty} \mathrm{d}x\, x^p F(x)$. Because $\tilde{\Psi}$ is zero on the complement of the closed interval $[a, b]$, it follows that these Hamburger moments are equivalent to the moments of $\Psi(x)$ restricted to the closed interval $[a, b]$. Thus

$$\begin{aligned} \mu_\psi(p) &= \int_a^b \mathrm{d}x\, x^p \Psi(x) \equiv \mu(p) \\ \mu_\phi(p) &= \mu(p+1) - a\mu(p) \\ \mu_\Omega(p) &= b\mu(p) - \mu(p+1). \end{aligned} \tag{5}$$

If $a = 0$ and $b = \infty$, then upon ignoring the μ_Ω moments, one obtains the usual Stieltjes moment problem formulation (Baker 1975).

In the preceding discussion we have distinguished between $\tilde{\Psi}$ and Ψ. The latter is the physical wavefunction, not necessarily zero outside any interval $[a, b]$. The former is a truncated wavefunction corresponding to the physical one within the specified interval, and zero outside it. This distinction will become self-evident in the following discussion.

3. A simple example

In order to demonstrate our approach, consider the simple harmonic oscillator potential problem:

$$-\Psi'' + x^2\Psi = E\Psi. \tag{6}$$

The ground-state eigenvalue, $E = 1$, is first obtained through the methods of Handy and Bessis (1985). For this example the ground state is easy to determine. In general, once a Hankel-Hadamard moments determinant analysis has been implemented for finding the energy E, one may then focus on wavefunction reconstruction. For equation (6) we have

$$\Psi(x) = N \exp(S(x)) \qquad \text{where } S(x) = -\tfrac{1}{2}x^2. \tag{7}$$

The factor N represents an arbitrary normalisation.

Consider the interval $[0, \infty)$. It is known from the symmetry of Ψ (all references are to the ground state) that $\Psi'(0) = 0$. Accordingly, through an integration by parts, equation (6) can be made to yield a moment recursion relation. Firstly, for future reference,

$$\int_a^b \mathrm{d}x\, x^p \Psi'' = b^p \Psi'(b) - a^p \Psi'(a) - p\{b^{p-1}\Psi(b) - a^{p-1}\Psi(a)\} + p(p-1)\mu(p-2). \tag{8}$$

For the case $a = 0$, $b = \infty$, the expression a^p becomes the Kronecker delta $\delta_{0,p}$. Assuming

$$b^p\Psi(b) \xrightarrow[b\to\infty]{} 0 \qquad b^p\Psi'(b) \xrightarrow[b\to\infty]{} 0 \qquad \text{and} \qquad \Psi'(0) = 0$$

we have from equation (6)

$$-p\delta_{1,p}\Psi(0) - p(p-1)\mu(p-2) + \mu(p+2) = \mu(p). \tag{9}$$

Examining the odd-order moment relations, $p = 2q+1$, one has $(\mu(2q+1) \equiv u(q))$

$$u(q+1) = u(q) + (2q+1)2qu(q-1) + \delta_{0,q}\Psi(0). \tag{10}$$

If we choose the normalisation of Ψ so that $u(0) = 1$, then $\Psi(0)$ can be easily obtained. Firstly, note that the $u(q)$ correspond to

$$u(q) = \int_0^\infty \mathrm{d}y\, y^q \Psi(\sqrt{y})/2 \qquad y = x^2. \tag{11}$$

Clearly, the $u(q)$ are then the Stieltjes moments of the modified function measure $f(y) = \Psi/2$. We may thus apply the Stieltjes-HH inequalities formulation in order to determine $\Psi(0)$. Specifically, these are $\Delta_{0,n}\{u\} > 0$ and $\Delta_{1,n}\{u\} > 0$, for $n \geq 0$. From equation (10), it is evident that only one parameter, $\Psi(0)$, needs to be specified before all the moments are determined. Furthermore, from (10) it is also apparent that the linear dependence of each $u(q)$ upon $\Psi(0)$ makes each $\Delta^0_{1,n}$ determinant a polynomial in $\Psi(0)$. Thus, given an arbitrary number N_m, it is simple to determine the common domain in $\Psi(0)$ space satisfying the Stieltjes-HH inequalities $(n \leq N_m - 1)$. Thus, rapidly convergent bounds to the true value $\Psi(0) = 1$ can be generated. The results are given in table 1.

Table 1. Application of the HH inequalities in determining bounds to $\Psi(0)$ for the harmonic oscillator potential $(u(0) = 1)$.

$\Psi_-(0)$	$\Psi_+(0)$	Maximum HH dimension
0.45	2.0	1
0.91	1.17	2
0.98	1.03	3
0.998	1.004	4
0.999 78	1.000 53	5

Let us now work on the finite interval $[0, r]$. Again $\Psi'(0) = 0$ and $E = 1$. Let $\Psi(r) \equiv \alpha$, and $\Psi'(r) \equiv \beta$, and we have

$$\mu_r(p) \equiv \int_0^r \mathrm{d}x\, x^p \Psi(x) \tag{12}$$

and

$$\mu_r(p+2) = \mu_r(p) + \beta r^p - p\alpha r^{p-1} + \delta_{p,1}\Psi(0) + p(p-1)\mu_r(p-2). \tag{13}$$

The odd-order moments α and β satisfy an inhomogeneous difference equation. The odd-order moments depend upon $\mu_r(1)$, α and β for their complete determination. On the other hand, the even-order moments α and β satisfy a homogeneous difference equation. Because of this and the fact that moments remain moments if they are renormalised by the same factor $(\mu_r(p\text{-} \rightarrow \mu_r(p)/\alpha)$, we have that the even-order moments are effectively determined upon specifying $\chi \equiv \mu_r(0)/\alpha$ and $\zeta \equiv \beta/\alpha$. Note also that α is a positive quantity. The reduction in the number of undetermined parameters afforded by the even-order moments makes them easier to work with, with regards to an HH analysis. Despite these practical concerns, application of a method to be discussed in § 5 would allow us to reduce the number of undetermined parameters in the odd-order moment case, enabling us, in principle, to work with $\mu_r(0)$ and α only.

Working with the even-order moments in equations (12) and (13), renormalised by a uniform factor of $1/\alpha$, we have

$$u_r(q) \equiv \int_0^{r^2} \mathrm{d}y\, y^q \frac{\Psi(\sqrt{y})/\Psi(r)}{2\sqrt{y}} \qquad y = x^2 \tag{14}$$

$$u_r(q+1) = u_r(q) + \zeta r^{2q} - 2qr^{2q-1} + 2q(2q-1)u_r(q-1). \tag{15}$$

It is clear that the function measure in equation (14) is non-negative, although singular at the y origin. Regardless of the latter, the HH inequalities for the interval $[0, r^2]$ become (note the change in notation)

$$\Delta_n^{(0)} \equiv \begin{vmatrix} u_r(0) & \dots & u_r(n) \\ \vdots & & \vdots \\ u_r(n) & \dots & u_r(2n) \end{vmatrix} > 0 \qquad \Delta_n^{(1)} \equiv \begin{vmatrix} u_r(1) & \dots & u_r(1+n) \\ \vdots & & \vdots \\ u_r(1+n) & \dots & u_r(1+2n) \end{vmatrix} > 0 \tag{16a}$$

$$\Delta_n^{(01)} \equiv \begin{vmatrix} \{r^2u_r(0) - u_r(1)\} & \dots & \{r^2u_r(n) - u_r(1+n)\} \\ \vdots & & \vdots \\ \{r^2u_r(n) - u_r(1+n)\} & \dots & \{r^2u_r(2n) - u_r(1+2n)\} \end{vmatrix} > 0. \tag{16b}$$

The above determinants are two-dimensional polynomials in $\zeta \equiv \mathrm{d}\ln(\Psi)/\mathrm{d}r$ and $\chi \equiv u_r(0)$. The closed algebraic expressions for the HH determinants of dimensionality no more than two are given below. For higher dimensionality we numerically determined the polynomial coefficients in ζ for fixed χ. More specifically, χ was varied in small increments within some arbitrarily chosen interval. At each such χ value, the above-mentioned polynomial coefficients (with respect to the ζ variable) were numerically determined. On the basis of this, at each fixed χ value, one could determine the common domain in ζ space for which the HH inequalities are satisfied. For many χ values, no ζ space domain existed. Accordingly, one would then say that for that specific χ value there could not exist a physical solution. In this manner the HH inequalities rapidly determine smaller and smaller physically allowed two-dimensional domains in χ-ζ space.

The numerical results for the harmonic oscillator are as follows. The correct physical results are $\chi = (\pi/2)^{1/2}\,\mathrm{erf}(r/2)\exp(r^2/2)$, $\zeta = -r$ (see Abramowitz and Stegun (1972) for the 'error function', $\mathrm{erf}(z)$). If $r > 1$ it is best to rescale the u_r moments so as not to incur too large numbers through the recursive moment relations. Thus, denoting $v_r(q) = u_r(q)/r^{2q}$, the new moment recusion relation is

$$v_r(q+1) = \frac{v_r(q)}{r^2} + \frac{\zeta}{r^2} - \frac{2q}{r^3} + \frac{2q(2q-1)}{r^4}\, v_r(q-1). \tag{17}$$

In addition, the HH inequalities in equation (16) remain the same with respect to the v_r, with the one exception that no r^2 factor appears in the counterpart to equation (16*b*)! It is also more efficient to take into account explicitly the linear difference equation nature of the moment recursion relation. Thus

$$u_r(q) = \chi A(q) + \zeta B(q) + D(q) \qquad A(0) = 1,\ B(0) = 0,\ D(0) = 0. \tag{18}$$

Each of the A, B and D coefficients satisfies a linear difference equation:

$$\begin{aligned} A(q+1) &= A(q)+2q(2q-1)A(q-1) \\ B(q+1) &= B(q)+2q(2q-1)B(q-1)+r^{2q} \\ D(q+1) &= D(q)+2q(2q-1)D(q-1)-2qr^{2q-1}. \end{aligned} \tag{19}$$

The HH inequalities for the u_r of dimension at most two (involving moments of maximum order three) are

$$\begin{aligned} &\Delta_0^{(0)}=\chi>0 \qquad \Delta_0^{(1)}=\chi+\zeta>0 \qquad \Delta_0^{(01)}=(r^2-1)\chi-\zeta>0 \\ &\Delta_1^{(0)}=Q_{12}(\chi)\zeta^2+Q_{11}(\chi)\zeta+Q_{10}(\chi)>0 \qquad \Delta_1^{(1)}=Q_{22}(\chi)\zeta^2+Q_{21}(\chi)\zeta+Q_{20}(\chi)>0 \\ &\tfrac{1}{2}\Delta_1^{(01)}=Q_{32}(\chi)\zeta^2+Q_{31}(\chi)\zeta+Q_{30}(\chi)>0. \end{aligned} \tag{20}$$

The Q functions are

$$\begin{aligned} &Q_{12}(\chi)=-1 \qquad Q_{11}(\chi)=-\chi+\chi r^2 \qquad Q_{10}(\chi)=2\chi^2-2\chi r \\ &Q_{22}(\chi)=12-r^2 \qquad Q_{21}(\chi)=22\chi+2r-5\chi r^2+\chi r^4 \\ &Q_{20}(\chi)=-4\chi r^3-4r^2+10r\chi+6\chi^2 \qquad Q_{32}(\chi)=6 \\ &Q_{31}(\chi)=-r^3-7\chi r^2+r+11\chi \qquad Q_{30}(\chi)=\chi r^5+\chi^2r^4-2\chi r^3-6(r\chi)^2-2r^2+5r\chi+3\chi^2. \end{aligned} \tag{21}$$

The results of solving the inequalities in equation (20) are given in table 2. Only three points are specified, for simplicity. These are sufficient to demonstrate the nature of our method. A more comprehensive analysis is tabulated in table 3. Note that the Δ_0 determinant inequalities yield $\chi>0$ and $-\chi<\zeta<\chi(r^2-1)$.

Table 2. Bounds for $\zeta\equiv \mathrm{d}\ln(\Psi(r))/\mathrm{d}r$ and $\chi\equiv u_r(0)$ (harmonic oscillator) using HH determinants of dimension at most two.

r	ζ_-	ζ_+	Actual	χ_-	χ_+	Actual
0.1	−0.100 000 8046	−0.099 999 5383	−0.1	0.100 3335	0.100 3348	0.100 334 0010
1	−1.141 666 127	−0.917 214 1378	−1	1.31	1.58	1.410 686 135
1.5	−11.319 708 59	−0.630 784 0671	−1.5	1	20	3.344 663 685

Table 3. Bounds for ζ and χ obtained through higher-order HH analysis for the harmonic oscillator.

r	Maximum order of moments used	ζ_-	ζ_+	χ_-	χ_+
1	4	−1.141 666 127	−0.996 244 5566	1.41	1.57
1	5	−1.000 204 533	−0.999 821 3984	1.4105	1.4109
1	6	−1.000 203 598	−0.999 992 1677	1.410 681	1.410 899
1.5	4	−11.625 000 00	−1.280 118 314	3.11	19.50
1.5	5	−1.516 928 940	−1.489 996 285	3.33	3.37
1.5	6	−1.516 928 940	−1.498 690 557	3.3432	3.37
1.5	7	−1.500 025 742	−1.499 956 408	3.3446	3.3447

Table 4. Bounds for $\zeta \equiv \mathrm{d}\ln(F(R))/\mathrm{d}R$ and $\chi \equiv u_R(0)$ for the spherical Zeeman hydrogenic atom ($Z=1$, $\lambda=1$, $g=0$, $R=1$).

E	Maximum order of moments used	ζ_-	ζ_+	χ_-	χ_+
0.593 7714	5	−2.430 197	−2.383 500	1.44	1.60
0.593 7714	6	−2.430 690	−2.398 333	1.47	1.60
0.593 7714	7	−2.396 200	−2.395 036	1.479	1.485
0.593 7714	8	−2.396 140	−2.395 560	1.481 07	1.485 00
0.593 7717	8	−2.396 141	−2.395 561	1.481 07	1.485 00
0.593 7711	8	−2.396 140	−2.395 560	1.481 07	1.485 00

4. A second example

A more interesting example is afforded by the three-dimensional system corresponding to a perturbed hydrogenic atom with a Hamiltonian of the form

$$H = -\tfrac{1}{2}\nabla^2 - Z/r + gr + \lambda r^2. \tag{22}$$

If $g=0$, equation (22) defines the spherically symmetric Zeeman problem (Handy and Bessis 1985). If $\lambda=0$, one has the spherical Stark effect (Bessis *et al* 1987). The composite system is a zero missing moment problem (Handy and Bessis 1985), similar in structure to the harmonic oscillator problem when viewed from an HH perspective. As explained in the above references, it is best to represent the s-wave ground-state wavefunction, $\Psi(r)$, in terms of an alternative representation

$$F(r) = r\exp(-ar^2 - br)\Psi(r) \qquad a = \sqrt{\lambda/2} \qquad b = g/\sqrt{2\lambda}. \tag{23}$$

The function $F(r)$ will also be non-negative for the physical solution. Thus all the previous analysis is relevant to $F(r)$ as well. Its differential equation is

$$rF'' + 2(2ar^2 + br)F' + [(b^2 + 2a + 2E)r + 2Z]F = 0. \tag{24}$$

As mentioned in the previous section, the energy E is first determined through the appropriate HH analysis. For simplicity we limit the following numerical analysis to the case $g=0$ and $\lambda=1$. It is then straightforward to show that $0.593\,7711 < E < 0.593\,7717$. Taking $u_R(q) = \int_0^R \mathrm{d}r\, r^q F(r)/F(R)$, a simple integration by parts along the interval $[0, R]$ yields (note that $F(0)=0$!)

$$u_R(q+1) = \frac{2u_R(q) + q(q+1)u_R(q-1) + R^{q+1}\zeta - (q+1)R^q + 4aR^{2+q}}{2(3a + 2aq - E)}. \tag{25}$$

As before, $\zeta \equiv F'(R)/F(R)$ and $\chi \equiv u_R(0)$. The application of the HH inequalities proceeds as before. The results are quoted in table 4. Because the energy is bounded from below and above, we examined the numerical stability of our method by applying the HH inequalities to equation (25) for three different energy estimates. All are consistent. The non-monotonic behaviours of the ζ bounds are due to too coarse an x partitioning.

5. The quartic anharmonic oscillator

We may apply the preceding HH analysis to the quartic anharmonic oscillator problem

$$-\Psi'' + (mx^2 + x^4)\Psi = E\Psi. \tag{26}$$

As explained by Handy and Bessis (1985) and Handy (1986), the cases $m=0$ and $m\neq 0$ are similar. Because the former is explicitly solved in the references cited, we shall continue our discussion for this case only.

Once again, the counterpart to equation (15) is

$$u_r(q+2)=Eu_r(q)+\zeta r^{2q}-2qr^{2q-1}+2q(2q-1)u_r(q-1). \tag{27}$$

Unlike equation (15), the moments of equation (27) are completely determined once $u_r(0)\equiv\chi$, $u_r(1)\equiv\eta$ and $\zeta\equiv\Psi'(r)/\Psi(r)$ are specified (having first determined $E=1.060\,362\,09$). We call this a 'three missing parameter problem', in keeping with the definition of the 'n missing moment problem' of Handy and Bessis (1985). It is possible, in principle, to apply the HH inequalities to the system defined above in equation (27) and obtain a succession of smaller and smaller three-dimensional subregions corresponding to the allowed physical values. Clearly this approach can be time consuming. Alternatively, one can apply the methods of Handy (1986) and eliminate some of the 'missing parameters'. We briefly outline this approach below.

We may transform the quartic anharmonic system into many representation spaces in which the ground-state wavefunction configuration is non-negative and the moments are finite. Thus consider

$$\Phi(x)=\left|\sum_{i=0}^{I} c_i x^{2i}\right|^2\Psi(x) \tag{28}$$

where the c_i can be complex. Taking $u_\Phi(q)=\int_0^r \mathrm{d}x\, x^{2q}\Phi(x)$, we have

$$u_\Phi(q)=\sum_{i,j=0}^{I} c_i^* c_j u_r(q+i+j). \tag{29}$$

As in the previous section we may explicitly make manifest the inhomogeneous linear difference equation nature of equation (27) in terms of the dependence of the moments on the three missing parameters (note that $A(0)=B(1)=1$, $A(1)=B(0)=D_{0,1}(0)=D_{0,1}(1)=0$):

$$u_r(q)=A(q)\chi+B(q)\eta+D_0(q)+D_1(q)\zeta. \tag{30}$$

We shall denote the sum of the last two terms by $D(q)$. Substituting in equation (29) gives

$$u_\Phi(q)=\chi\sum_{i,j=0}^{I} c_i^* c_j A(q+i+j)+\eta\sum_{i,j=0}^{I} c_i^* c_j B(q+i+j)+\sum_{i,j=0}^{I} c_i^* c_j D(q+i+j). \tag{31}$$

As shown by Handy (1986) it is possible to solve for c_i which make the η-series coefficient zero for $0\leq q\leq Q$, Q being arbitrary. Although the above process is inductive

Table 5. Bounds for ζ and χ using the missing parameter eliminator algorithm ($I=7$, $Q=5$, $E=1.060\,362\,09$). Note that M_χ (maximum order of moments used) cannot exceed Q!

r	M_χ	ζ_-	ζ_+	χ_-	χ_+
0.5	3	−0.577 015 3471	−0.574 986 0018	0.544	0.557
0.5	4	−0.577 015 3471	−0.575 794 3158	0.5491	0.5570
0.5	5	−0.575 804 0671	−0.575 803 9718	0.549 1656	0.549 1662
1	3	−1.479 898 601	−1.371 182 189	1.39	2.06
1	4	−1.479 898 601	−1.398 395 126	1.55	2.06
1	5	−1.400 489 122	−1.400 373 482	1.550 60	1.5514

Table 6. Bounds for ζ, χ and η from an HH analysis of equation (27).

Maximum order of moments used	r	ζ_-	ζ_+	χ_-	χ_+	η_-	η_+
3	0.5	−0.578 7426	−0.574 7501	0.549 1655	0.549 1661	0.043	0.045
4	0.5	−0.576 7856	−0.571 4360	0.549 1656	0.549 1661	0.044 1	0.044 5
5	0.5	−0.575 8040	−0.575 8034	0.549 1656	0.549 1661	0.044 10	0.044 12

and can be used to eliminate the χ coefficient as well, we will not do so here. Thus, as in the previous examples, we shall be working within a two-dimensional parameter space with respect to solving for the HH inequalities. Note that the c are E dependent only! Since E is calculated first, it follows that the HH analysis which ensues involves fixed c coefficients. However, in solving for the c_i it is best to avoid large numbers by rescaling the moments and c_i as follows: $\hat{u}_\Phi(q) = u_\Phi(q)/g^q$, $\hat{c}_i = c_i g^i$, $\hat{A}(q) = A(q)/g^q$, etc. The missing parameters ζ and χ are not rescaled. Note that the HH determinant expressions stay the same with respect to the $\hat{u}_\Phi$ dependence with the exception that the counterpart to equation (16*b*) involves $r^2\hat{u}_\Phi(q) - g\hat{u}_\Phi(1+q)$!

Table 5 gives the results of the preceding analysis for two points. In table 6 we corroborate the results of table 5 by implementing a three missing parameter HH search analysis on equation (27). For the latter, two parameters (χ and η) were varied within some arbitrarily chosen two-dimensional rectangular domain. At each such point the ζ-polynomial coefficients were numerically determined, followed by a determination of ζ subregions satisfying the HH inequalities, up to some given order. As in the previous examples, rapid convergence to a small three-dimensional physically allowed subregion was observed.

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