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Positivity and the energy quantization of physical systems: the C-shift moment method

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Abstract. The eigenvalue moment method (EMM) of Handy and Bessis is reformulated with special emphasis on the importance of positivity as a general quantization criterion; thereby making EMM theory relevant in the analysis of manifestly non-positive systems such as those corresponding to multi-dimensional excited bosonic states.

1. Introduction

The eigenvalue moment method (EMM) (Handy and Bessis 1985, Handy *et al* 1988a, b) has been shown to be an effective theory for generating converging bounds to the eigenenergies of bosonic quantum states, provided the associated wavefunctions can be 'uniquely' represented in terms of bounded non-negative configurations. These restrictions have, for the most part, limited the applicability of the EMM theory to multi-dimensional bosonic ground states (inlcuding the lowest energy states within each symmetry class). An important exception is the case of the one-dimensional Schrödinger operator. In this case, the EMM formalism can be directly applied to the modulus-squared of the wavefunction, $|\Psi|^2$; thereby permitting the quantization of all states (Handy 1987a, b).

Despite these apparent limitations, a careful examination of the underlying principles inherent to EMM theory leads to an alternate formulation capable of addressing multi-dimensional excited bosonic states. In this work we present the essential theoretical structure of the 'C-shift' reformulation and apply it to various one- and two-dimensional systems. In particular, besides the pedagogic consideration of the harmonic oscillator problem, we also apply the C-shift formalism to the quartic potential problem, $V(x)=x^4$, and to the important two-dimensional system defined by the potential function $V(x, y)=x^2+y^2+\lambda(xy)^2$. The latter problem has received much attention in the recent literature because of the non-separability of the associated Hamiltonian and its consequences with respect to chaotic behaviour in quantum systems (Killingbeck and Jones 1986, Vrscay and Handy 1989).

The C-shift formalism to be presented effectively allows us to use positivity (or more precisely, non-negativity) as a general quantization condition. To this extent it is in keeping with the general philosopy underlying 'density functional theory methods' (Parr and Yang 1989).

In order to make this work as complete as possible we give an overview of the essentials of the EMM theory. This will also facilitate the subsequent discussion on the 'C-shift' formalism.

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Consider the sextic anharmonic oscillator problem

$$-\Psi''(x)+mx^2\Psi(x)+gx^6\Psi(x)=E\Psi(x). \tag{1.1}$$

The ground state configuration is symmetric and non-negative:

$$\Psi(-x)=\Psi(x) \tag{1.2}$$

$$\Psi(x)\geqslant 0. \tag{1.3}$$

The physical solutions to (1.1) correspond to bounded configurations with finite Hamburger moments $\mu(q)$ defined by

$$\mu(q)=\int_{-\infty}^{\infty} \mathrm{d}x\, x^q\Psi(x) \tag{1.4}$$

and satisfying

$$\mu(q)<\infty. \tag{1.5}$$

Integrating (1.1) on both sides with respects to $\int \mathrm{d}x\, x^q$ one obtains the Hamburger moment equation

$$g\mu(q+6)=-m\mu(q+2)+E\mu(q)+q(q-1)\mu(q-2). \tag{1.6}$$

Because of the inherent symmetry of the desired solution, the odd-order Hamburger moments are zero. Through a simple change of variables, $x=\sqrt{y}$, the even-order Hamburger moments can be shown to be equivalent to the Stieltjes moments, $u(p)$, of the non-negative configuration $\Psi(\sqrt{y})/\sqrt{y}$, defined over the non-negative half-real axis:

$$u(p)=\int_0^{\infty} \mathrm{d}y\, y^p\Psi(\sqrt{y})/\sqrt{y}. \tag{1.7}$$

The corresponding Stieltjes moment equation is ($\mu(2p)=u(p)$)

$$gu(p+3)=-mu(p+1)+Eu(p)+2p(2p-1)u(p-1) \tag{1.8}$$

for $p\geqslant 0$.

The Stieltjes moment equation, (1.8), corresponds to a homogeneous linear finite difference equation of order three. As such, the 'missing moments' $u(0)$, $u(1)$, and $u(2)$ must be specified, in addition to the energy E (which appears as a parameter), before all the other moments can be generated. We may represent this succinctly by the linear relation

$$u(p)=\sum_{j=0}^{2} M(E;p,j)u(j) \tag{1.9}$$

where the E-dependent $M(\ )$ coefficients satisfy (1.8):

$$\begin{aligned} gM(E;p+3,j) &= -mM(E;p+1,j)+EM(E;p,j) \\ &\quad +2p(2p-1)M(E;p-1,j) \qquad p\geqslant 0 \end{aligned} \tag{1.10}$$

as well as the 'initialization conditions':

$$M(E; i, j) = \delta_{i,j} \qquad 0 \leqslant i, j \leqslant 2. \tag{1.11}$$

The homogeneous nature of (1.8) suggests that some suitable normalization condition must be chosen. One convenient choice is (bearing in mind the non-negativity of the ground state)

$$\sum_{i=0}^{2} u(i) = 1. \tag{1.12}$$

Eliminating $u(0)$ and inserting into (1.9) we arrive at the final linear expression relating the moments to the unconstrained missing moments ($u(1)$ and $u(2)$):

$$u(p) = \hat{M}(E; p, 0) + \hat{M}(E; p, 1)u(1) + \hat{M}(E; p, 2)u(2) \tag{1.13}$$

where

$$\hat{M}(E; p, j) = \begin{cases} M(E; p, 0) & \text{if } j = 0 \\ M(E; p, j) - M(E; p, 0) & j = 1, 2. \end{cases} \tag{1.14}$$

Restricting ourselves to the ground state, the normalization prescription in (1.12) restricts the missing moments $u(1)$ and $u(2)$ to the unit square in the positive quadrant of the $u(1) \times u(2)$ domain.

The quantization of the ground state energy, E, is achieved by imposing upon (1.13) the necessary and sufficient constraints for the Stieltjes moments to correspond to a non-negative measure. These constraints are usually expressed in the form of Hankel-Hadamard (HH) determinental inequalities (Shohat and Tamarkin 1963); however, Handy *et al* (1988a, b) reformulated them in terms of an equivalent set of linear inequality constraints suitable for application of linear programming theory (Chvatal 1983). Specifically, in one dimension, the necessary and sufficient conditions for a given set of Stieltjes moments, $\{u(p)\}$, to correspond to a non-negative function are

$$\sum_{i,j=0}^{I} C(i)u(s+i+j)C(j) \geqslant 0 \tag{1.15}$$

for $I \geqslant 0$, $s = 0, 1$, and arbitrary C.

Inserting (1.13) into (1.15) there follows an uncountably infinite number of linear inequality constraints on the missing moments $u(1)$ and $u(2)$:

$$\sum_{k=1}^{2} A(E; C; k)u(k) < B(E; C) \tag{1.16}$$

where

$$B(E; C) = -A(E; C; 0) \tag{1.17a}$$

$$A(E; C; k) = -\sum_{i,j=0}^{I} C(i)\hat{M}(E; s+i+j, k)C(j) \tag{1.17b}$$

for $k = 0, 1, 2$.

For completeness we take note of the fact that the quadratic form structure of (1.15) may be transformed into an equivalent nonlinear theory corresponding to the

HH determinental inequalities:

$$\Delta_{s,I}[u] = \det(u(s+i+j)) \geq 0 \tag{1.18}$$

for all $I \geq 0$, $s = 0, 1$. The implied u matrix (the argument of the determinant functional) is of dimension $I+1$, corresponding to $0 \leq i, j \leq I$. In addition, most of the data cited in the tables refer to the maximum moment order used, $P_{\max}$, in the corresponding calculation. In terms of I, this means $2I+1 \leq P_{\max}$.

If there exists a $u(1) \times u(2)$ solution set to (1.16), U, then it must be convex (Chvatal 1983). The quantization of the ground state energy involves determining the existence or non-existence of U, for given E and I. This in turn can be ascertained quickly by implementing a linear programming 'cutting procedure' within the unit square domain in $u(1) \times u(2)$ (Handy *et al* 1988a, b).

Given I and a conveniently partitioned energy interval one then procedes to determine the existence of U for each energy value within the partition. If U does not exist, then the associated energy is non-physical. If U does exist, then the associated energy is physically possible, up to order I. In this manner converging bounds to the true ground state energy are obtained. The result of this analysis, as applied to the sextic anharmonic problem, are summarized in table 1.

Table 1. Eigenenergy bounds for the sextic anharmonic oscillator with $m = g = 1$.

Max moment order, $P_{\max}$	Eigenenergy bounds
8	$1.41 < E < 1.47$
10	$1.423 < E < 1.438$
12	$1.4352 < E < 1.4364$
14	$1.4355 < E < 1.4357$

It is important to stress that if the potential were asymmetric then we would have worked with Hamburger moments directly. Analogous constraints to those in (1.15) can be formulated in this case (i.e. $s = 0$ only). For multi-dimensional problems an analogous formalism also applies (Handy *et al* 1988a, b).

Three important factors contribute to the implementability of the EMM:

(I) All the physical solutions to the Schrödinger equation have finite power moments; whereas the non-physical solutions have infinite power moments.

(II) A linear moment equation can be generated from the associated configuration space physical system (i.e. the Schrödinger equation).

(III) The desired solution is uniquely associated with an asymptotically bounded (i.e. asymptotically zero) and non-negative configuration enabling the imposition of moment constraints derived from the theory of the 'moment problem' (Shohat and Tamarkin 1963). These in turn, through a linear programming based cutting method (Handy *et al* 1988a, b), generate converging lower and upper bounds to the desired eigenenergy.

Conditions I and II are valid for many quantum systems. Condition III would seem specialized and not always realizable; however, this is not the case. Indeed, any bounded (i.e. locally finite and asymptotically zero) physical wavefunction configuration can be transformed into a non-negative and bounded representation. If the wavefunction is not locally finite, but the nature and location of its singularity known,

analogous transformations exist. In section 2 we show how we can always transform a quantum problem into a representation satisfying all three criteria (i.e. I–III).

2. The '*C*-shift' method

Consider the one-dimensional Schrödinger equation for arbitrary potential, $V(x)$,

$$-\Psi''(x)+V(x)\Psi(x)=E\Psi(x). \tag{2.1}$$

The physical solutions are associated with exponentially bounded configurations satisfying

$$\lim_{x\to\pm\infty}\Psi(x)=0. \tag{2.2}$$

The non-physical solutions diverge asymptotically (Agmon 1983). In addition, it is well known that while the bosonic ground state wavefunction can be taken to be non-negative, all excited states are of non-uniform signature (Bender and Orzag 1978). As indicated in the preceding section, the EMM theory requires that the associated wavefunction configuration be non-negative; therefore it cannot be applied directly to the excited states.

Our objective is to find a suitable representation satisfying the three conditions necessary for implementing the EMM theory, as stipulated at the end of section 1 (hereafter referred to as conditions I–III).

The boundedness property of each physical configuration, as expressed by (2.2), suggests that there is a smallest non-negative constant, 'C', satisfying

$$\Psi(x)+C\geqslant 0 \qquad \text{for all } x. \tag{2.3}$$

The determination of C will be discussed shortly.

This non-negative configuration will not have finite power moments. This requires the introduction of an additional non-negative regulating functional-factor, $R(x)$, so that the composite physical configuration has finite Hamburger moments:

$$\Phi(x)=(\Psi(x)+C)R(x) \tag{2.4}$$

$$\int_{-\infty}^{\infty}\mathrm{d}x\,x^p\Phi(x)<\infty \qquad \text{for } \Phi \text{ physical.} \tag{2.5}$$

We will refer to $\Phi(x)$ as a (non)physical configuration if its associated $\Psi(x)$ representation is (non)physical (i.e. bounded (unbounded)).

In order to satisfy condition I, the regulating function must satisfy (2.5) for physical configurations and yield infinite Hamburger power moments for unphysical configurations. To this extent, approximate knowledge of the asymptotic behaviour of the Schrödinger equation solutions are required. For one-dimensional problems, this is readily provided by a zeroth-order JWKB analysis (Bender and Orzag 1978). For this case we have:

$$\Psi(x)\simeq\exp\left(\pm\int\mathrm{d}x\,\sqrt{V(x)}\right) \tag{2.6}$$

where + and − are associated with the non-physical and physical configurations, respectively. In terms of the above, $R(x)$ must satisfy the following conditions for all

integer p values:

$$\int_{-\infty}^{\infty} \mathrm{d}x\, x^p R(x) < \infty \tag{2.7a}$$

$$\int_{-\infty}^{\infty} \mathrm{d}x\, x^p R(x) \exp\left(-\int^{x} \mathrm{d}y \sqrt{V(y)}\right) < \infty \tag{2.7b}$$

and

$$\int_{-\infty}^{\infty} \mathrm{d}x\, x^p R(x) \exp\left(+\int^{x} \mathrm{d}y \sqrt{V(y)}\right) = \infty. \tag{2.7c}$$

It is clear that these conditions are required so that in the Φ-representation the physical solutions are the unique configurations with finite moments. If condition (2.7*c*) is not satisfied then non-physical Ψ configurations (those having infinite power moments) will transform into Φ-configurations with finite power moments; thereby possibly enlarging the set of Φ configurations consistent with the moment problem constraints. The latter would then prevent the generated bounds from convering to a particular eigenenergy; that is, most likely the generated bounds will be slowly converging, crude and uninteresting. An example of this is provided in table 3 as will be discussed in section 3.1.

Nevertheless, the preceding remarks are important because, for multi-dimensional problems, the approximate determination of the asymptotics for the Schrödinger equation solutions can be difficult. As such, one may adopt an empirical attitude and 'guess' at some suitable regulating function. The behaviour of the generated bounds would then indicate the appropriateness of the chosen regulating function. We will adopt this approach when we discuss the two-dimensional problem in section 3.3.

Condition II can usually be easily satisfied depending on the nature of the potential function and chosen $R(x)$. At worst a change of variables (or equivalently, a 'generalized moment formulation') may be required in order to generate a moment equation representation for the Φ configuration space problem.

Assuming (2.7*a*, *b*, *c*) are satisfied (that is condition I is satisfied), as well as condition II, then the identification of a suitable C value satisfying (2.3) will satisfy condition III. Usually, knowledge of a suitable C value is not known *a priori*. Our approach will be to guess at a suitable large C value. If this guess is too large, then it will simply mean that the convergence rate of the eigenenergy bounds will be reduced. If the guess is too small, then no energy bounds will be observed, at some suitably high moment order. These issues will become clearer through the examples presented in section 3.

In addition to the formalism previously presented, two important points arise which are critical to the implementation of the 'C-shift' theory. The first is the implicit assumption that the regulating function, $R(x)$, is not orthogonal to the desired physical configuration, $\Psi(x)$. Usually, this can be anticipated and an appropriate functional form adopted. Most of the preceding discussion is relevant because $R(x)$ will normally be chosen of even parity. Odd-parity states can be obtained by an analogous consideration of the expression $(x\Psi(x)+C)R(x)$.

The second important point is that an appropriate normalization within the Φ-representation must be adopted. Care must be taken to exclude the trivial zero solution, $\Psi(x)=0$, from appearing as a non-trivial $\Phi(x)=CR(x)$ solution. We must develop a normalization prescription that effectively 'projects out' this trivial solution; otherwise no converging bounds will be observed.

Finally, in the event that the physical wavefunction is locally infinite at a point, $\Psi(x_s)=\pm\infty$, one can always introduce an additional regulating factor, $S(x)$, which transforms the physical configuration Ψ into a bounded configuration (locally finite and asymptotically zero) amenable to the C-shift formalism: $(S(x)\Psi(x)+C)R(x)$. The determination of an appropriate $S(x)$ consistent with criteria I–III is made on the basis of the Ψ's singular behaviour at x_s, both of which are assumed known. The multi-dimensional generalization is immediate.

3. Examples

3.1. The harmonic oscillator

Consider the harmonic oscillator problem

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

A JWKB analysis results in the asymptotic behaviours $\exp(\pm x^2/2)$ for the non-physical and physical solutions, respectively. We may take $R(x)=\exp(-ax^2)$, where $a>0$ and in addition (from (2.7*a*, *b*, *c*))

$$-a-\tfrac{1}{2}<0 \tag{3.2a}$$

and

$$-a+\tfrac{1}{2}\geqslant 0. \tag{3.2b}$$

Combining these: $0<a\leqslant\frac{1}{2}$ ($a>0$ from (2.7*a*)).

Taking $\Phi(x)=(\Psi+c)R(x)$, the ensuing Φ-space equation is

$$-[\Phi''+4ax\Phi']+[x^2(1-4a^2)-2a-E]\Phi=C[x^2-E]\exp(-ax^2). \tag{3.3}$$

The symmetric nature of $R(x)$ makes the preceding formulation relevant only for symmetric solutions. Odd-parity solutions can be obtained by working with $(x\Psi+C)R(x)$ instead. For simplicity we limit all discussion to even-parity states only. The generalization is immediate.

As in the introduction, a Stieltjes moment formulation is possible for the symmetric states of (3.3):

$$\begin{aligned}[1-4a^2]u(p+1)&=-[4a(2p+1)-2a-E]u(p)+2p(2p-1)u(p-1)\\&\quad+C[v(p+1)-Ev(p)]\end{aligned} \tag{3.4}$$

where the v-moments are defined by

$$v(p)=\int_{-\infty}^{\infty}dx\,x^{2p}\exp(-ax^2) \tag{3.5a}$$

and satisfy the recursion relation

$$v(p+1)=(2p+1)v(p)/2a \qquad p\geqslant 0 \tag{3.5b}$$

$$v(0)=\sqrt{(\pi/a)}. \tag{3.5c}$$

The inhomogeneous linear finite difference equation in (3.4) admits the general solution

$$u(p)=M(E,a;p,0)u(0)+M(E,a;p,1)C \tag{3.6}$$

where the M-coefficients satisfy (3.4) and the initialization conditions

$$M(E, a; 0, 0) = 1 \tag{3.7a}$$

$$M(E, a; 0, 1) = 0. \tag{3.7b}$$

A normalization prescription must be adopted that prohibits the trivial $\Psi(x) = 0$ solution from becoming a non-trivial solution of (3.3). That is, in general, for any E value, the bounded and non-negative configuration $\Phi(x) = CR(x)$, for any C, will be a solution to (3.3). This is unsatisfactory and must be projected out. If we stipulate that (recall $C \geqslant 0$)

$$u(0) = 1 + CV(0) \tag{3.8}$$

then we are requiring $\int dx\, \Psi(x) \exp(-ax^2)$ be unity (note that $u(0) = \int dx\, (\Psi(x) + C) \exp(-ax^2)$) thereby projecting out the trivial solution.

Inserting (3.8) into (3.6) results in the relation

$$u(p) = \hat{M}(E, a; p, 0) + \hat{M}(E, a; p, 1)C \tag{3.9a}$$

where

$$\hat{M}(E, a; p, 0) = M(E, a; p, 0) \tag{3.9b}$$

and

$$\hat{M}(E, a; p, 1) = M(E, a; p, 1) + v(0)M(E, a; p, 0). \tag{3.9c}$$

Comparing (3.9a) with the analogous structure in (1.13), for each E value within a partitioned energy interval we may apply linear programming methods to determine the existence or non-existence of a C-solution set satisfying the analogue of (1.16) and (1.17) as well as $0 \leqslant C \leqslant C_{\max}$, where $C_{\max}$ is arbitrarily large. The results are given in table 2. Note that if $C_{\max}$ is sufficiently large, then the true energy is bounded. As $C_{\max}$ increases, the convergence rate of the bounds decreases. If $C_{\max}$ is chosen too small, then at some order no energy bounds are generated; that is no energy value exists satisfying the relevant linear inequality constraints (Because $\Phi(x)$ has become negative). Thus, empirically, the behaivour of the bounds as $C_{\max}$ is increased suggests whether or not a true physical energy is being obtained.

It should be noted from (3.4) that choosing $a = \frac{1}{2}$ dramatically alters the order of the moment-finite difference recursion relation. In fact, one obtains $u(0) = Cv(0)$ (i.e. $v(1) = v(0)$ when $a = \frac{1}{2}$). Comparing with (3.8), it is clear that this case corresponds to the regulator being orthogonal to the states of interest; and is therefore inappropriate from the C-shift perspective.

It is interesting to note the behaviour of the ground state energy bounds when the regulator parameter, a, exceeds the constraint $a \leqslant \frac{1}{2}$. Table 3 gives these results. The results are as predicted in section 2.

3.2. The quartic potential

An analogous formulation to that presented previously is possible for the quartic case

$$-\Psi''(x) + x^4\Psi(x) = E\Psi(x). \tag{3.10}$$

Again we limit our discusssion to symmetric states. A simple application of JWKB theory tells us that the asymptotic behaviour of the non-physical and physical solutions is governed by $\exp(\pm|x^3|/3)$. As such, the same regulator $R(x) = \exp(-ax^2)$ may be

Table 2. C-shift formulation for the harmonic oscillator potential. $R(x)=\exp(-ax^2)$, $a=\frac{1}{4}$. Bounds in parentheses refer to higher C_{max} value.

c_{max}	P_{max}	Eigenenergy bounds for lowest three even parity states	
10	10	$0.9<E<1.1$	
		$4.8<E<5.5$	
		$8.0<E<9.7$	
10	12	$0.99<E<1.01$	
		$4.97<E<5.08$	
		$8.76<E<9.13$	
10	14	$0.998<E<1.001$	
		$4.995<E<5.012$	
		$8.948<E<9.023$	
10	16	$0.9998<E<1.0001$	
		$4.9993<E<5.0018$	
		$8.990<E<9.004$	
10	18	$0.999\,98<E<1.000\,01$	
		$4.999\,9<E<5.000\,3$	
		$8.998\,3<E<9.000\,7$	
$10(10^5)$	20	$0.999\,997<E<1.000\,001$	$(0.97<E<1.01)$
		$4.999\,98<E<5.000\,04$	$(4.8<E<5.5)$
		$8.999\,7<E<9.000\,1$	$(7.5<E<\infty)$
10^5	22	$0.997<E<1.001$	
		$4.9<E<5.1$	
		$8.6<E<9.2$	
10^5	24	$0.9996<E<1.0002$	
		$4.99<E<5.01$	
		$8.94<E<9.03$	
10^5	26	$0.999\,95<E<1.000\,02$	
		$4.999\,6<E<5.000\,9$	
		$8.991<E<9.004$	
10^5	28	$0.999\,995<E<1.000\,002$	
		$4.999\,96<E<5.000\,12$	
		$8.998\,82<E<9.000\,46$	
10^5	30	$0.999\,999\,5<E<1.000\,000\,2$	
		$4.999\,99<E<5.000\,02$	
		$8.999\,83<E<9.000\,07$	

used. Note that no restriction on the a-parameter is required, other than $a>0$. The corresponding inhomogeneous, linear, Stieltjes moment recursion relation is

$$u(p+2)=4a^2u(p+1)-[-E+8ap+2a]u(p)+2p(2p-1)u(p-1)$$
$$+C[v(p+2)-Ev(p)] \qquad \text{for } p\geq 0. \tag{3.11}$$

Once again, there results the relations (the E and a dependence is implicitly assumed)

$$u(p)=M(p,0)u(0)+M(p,1)u(1)+M(p,2)C \tag{3.12}$$

Table 3. C-shift formulation for harmonic oscillator. $R(x)=\exp(-ax^2)$, where converging bounds require $0<a\leq\frac{1}{2}$.

$C_{\max}$	$P_{\max}$	a	Ground-state energy bounds
1	6	0.40	$0.998\,9<E<1.000\,2$
1	6	0.45	$0.99997<E<1.000\,01$
1	6	0.51	$0<E<1.000\,000\,001$
1	6	0.55	$0<E<1.000\,000\,7$
1	6	0.60	$0<E<1.000\,04$

where

$$M(0,0)=1 \qquad M(0,1)=0 \qquad M(0,2)=0$$

and

$$M(1,0)=0 \qquad M(1,1)=1 \qquad M(1,2)=0.$$

We may adopt the normalization condition

$$u(0)+u(1)=1+C(v(0)+v(1)) \tag{3.13}$$

which corresponds to taking $\int dx(1+x^2)\Psi(x)R(x)=1$.

Inserting (3.13) into (3.12) (i.e. eliminating $u(0)$) results in

$$u(p)=\hat{M}(p,0)+\hat{M}(p,1)u(1)+\hat{M}(p,2)C \tag{3.14a}$$

where

$$\begin{aligned}\hat{M}(p,0)&=M(p,0)\\ \hat{M}(p,1)&=M(p,1)-M(p,0)\\ \hat{M}(p,2)&=M(p,2)+(v(0)+v(1))M(p,0).\end{aligned} \tag{3.14b}$$

The generation of the representation in (3.14) allows us to preceed with the linear programming 'cutting method', referred to in section 1, to determine the existence or non-existence of a $u(1)\times C$ convex solution set to the relevant linear inequality constraints. Now, we require the additional constraints that $0\leq u(1)\leq 1+C_{\max}(v(0)+v(1))$ as well as $0\leq C\leq C_{\max}$.

The results of the ensuing analysis are presented in table 4. The results are consistent with the values reported in the literature (Hioe *et al* 1976).

3.3. A two-dimensional problem

An important two-dimensional problem which has appeared in the recent literature (Killingbeck and Jones 1986, Vrscay and Handy 1989) is that of the perturbed harmonic oscillator defined by

$$-\{\partial_x^2\Psi+\partial_y^2\Psi\}+[x^2+y^2+\lambda(xy)^2]\Psi=E\Psi. \tag{3.15}$$

An EMM analysis with respect to the ground state was given in the work of Vrscay and Handy (1989). It was found therein that an EMM formulation within the function space corresponding to $\Psi(x,y)\exp(-(x^2+y^2)/2)$ yielded satisfactory converging bounds. In keeping with this analysis we shall take $R(x,y)=\exp(-(x^2+y^2)/2)$.

Table 4. C-shift formulation for the quartic potential. $R(x)=\exp(-ax^2)$, $a=1$. Bounds in parentheses refer to higher C_{max} value.

C_{max}	P_{max}	Eigenenergy bounds for lowest two even-parity states
10	6	$0.5<E<3.9$ $5.8<E<\infty$
10	10	$1.0<E<1.2$ $7.3<E<7.6$
10	12	$1.05<E<1.09$ $7.44<E<7.48$
10	14	$1.056<E<1.063$ $7.447<E<7.459$
10	16	$1.0597<E<1.0606$ $7.4549<E<7.4564$
$10(10^5)$	18	$1.060\,26<E<1.060\,57$ $(0.1<E<2.7)$ $7.455\,5<E<7.456\,2$ $(6.6<E<\infty)$
$10(10^5)$	20	$1.060\,34<E<1.060\,39$ $(0.9<E<1.3)$ $7.455\,65<E<7.455\,74$ $(7.0<E<7.9)$
10^5	22	$0.9<E<1.2$ $7.2<E<7.6$
10^5	24	$1.04<E<1.07$ $7.43<E<7.49$
10^5	26	$1.057<E<1.067$ $7.451<E<7.469$
10^5	28	$1.059<E<1.062$ $7.454<E<7.458$
10^5	30	$1.0599<E<1.0606$ $7.4548<E<7.4560$
10^5	32	$1.060\,29<E<1.060\,39$ $7.455\,6<E<7.455\,8$

We will focus on the first excited state within the symmetry class corresponding to even parity with respects to the following three independent transformations: $x\leftrightarrow -x$, $y\leftrightarrow -y$, and $x\leftrightarrow y$. The true ground state is of even parity relative to all three transformations. The relevant C-shift configuration is $\Phi(x,y)=(\Psi(x,y)+C)R(x,y)$.

As in the one-dimensional case, we may define two-dimensional Stieltjes moments, $u(p,q)$ (generated from the associated two-dimensional Hamburger moments) satisfying the recursion relation

$$\begin{aligned}\lambda u(p+1,q+1)&=[2p(2p-1)u(p-1,q)+2q(2q-1)u(p,q-1)]\\&\quad+[E-2(2p+2q+1)]u(p,q)\\&\quad+[v(p+1,q)+v(p,q+1)+\lambda v(p+1,q+1)-Ev(p,q)]C\end{aligned}\tag{3.16}$$

where

$$v(p,q)=v(p)v(q).\tag{3.17}$$

Restricting ourselves to the aforementioned symmetry class, we have $u(p, q) = u(q, p)$. The ensuing missing moments correspond to the set $\{u(n, 0) | n \geq 0\}$. That is, once the missing moments corresponding to $n \leq N$ are specified, all the moments satisfying $0 \leq p, q \leq N$, are determined. However, the missing moment $u(N, 0) = u(0, N)$ does not contribute to any other $u(p, q)$ moment for $(p, q) \in [0, N] \times [0, N]$.

It is argued in the work of Handy *et al* (1988a, b), that the necessary and sufficient conditions for a given set of two-dimensional Stieltjes moments to correspond to a non-negative function-measure are given by linear inequality constraints analogous to those in (1.16) (for $x \leftrightarrow y$ symmetric configurations):

$$\sum_{l_1, l_2 = 1}^{D} C(i_{l1}, j_{l1}) u(s + i_{l1} + i_{l2}, j_{l1} + j_{l2}) C(i_{l2}, j_{l2}) \geq 0 \tag{3.18}$$

for $s = 0$, 1, arbitrary Cs, and arbitrary D (where $(i_l, j_l) = (i, j)_l$, $1 \leq l \leq D$, denotes a convenient coordinate pair sequence ordering for all non-negative integer pairs).

In the work by Vrscay and Handy the coordinate sequence ordering adopted is defined as follows. Consider the integer points within the square region $[0, I] \times [0, I]$. Starting with (0, 0) as the first sequence element, we proceed to enumeratre sequentially the coordinate pairs (i, j) by varying i first and then j: (0, 0), (1, 0), (2, 0), (3, 0), ..., $(I, 0), (0, 1), (1, 1), (2, 1), \ldots, (I, 1), \ldots, (0, I), (1, I), (2, I), \ldots, (I, I)$). Let us consider the first D sequence elements (i.e. $D \leq (1 + I)^2$). From the perspective of (3.18), the coordinates of the moments $u(s + i_{l1} + i_{l2}, j_{l1} + j_{l2})$ lie within the square $[0, 1 + 2I] \times [0, 1 + 2I]$. As such, one would take the associated missing moments to be, $\{u(n, 0)$, for $0 \leq n \leq N = 1 + 2I\}$ satisfying the possible normalization prescription:

$$\sum_{n=0}^{N} u(n, 0) = 1 + C \sum_{n=0}^{N} v(n, 0). \tag{3.19}$$

From (3.16) there follows the standard expansion (E dependences are implicitly assumed)

$$u(p, q) = \sum_{n=0}^{N} M(p, q; n) u(n, 0) + M_c(p, q) C \tag{3.20}$$

where $0 \leq p, q \leq N$, $0 \leq n \leq N$, and

$$M(p, 0; n) = \delta_{p,n} \qquad \text{for } 0 \leq p, n \leq N$$

$$M_C(p, 0) = 0 \qquad \text{for } 0 \leq p \leq N.$$

The M-coefficients satisfy the corresponding two-dimensional recursion relation in (3.16). In addition, $M(p, q; k) = M(q, p; k)$.

The incorrectness of taking (3.19) as our normalization now becomes apparent. Clearly, the solution

$$u(N, 0) = 1 + C\left[\sum_{n=0}^{N} v(n, 0)\right] \qquad \text{and} \qquad u(n, 0) = 0 \qquad \text{for } 0 \leq n \leq N - 1$$

is consistent with the normalization; thereby yielding

$$u^*(p, q) = M(p, q; N)\left\{1 + C\left[\sum_{n=0}^{N} v(n, 0)\right]\right\} + M_C(p, q) C.$$

The $M(p, q; N)$ coefficient is zero except for $(p, q) = (N, 0)$ and $(0, N)$ (provided (p, q) lies within the $[0, N] \times [0, N]$ region). As indicated in section 1, we may work

with (3.18) or its nonlinear counterpart defined by the appropriate two-dimenional HH determinants (Handy *et al* 1988a, b). In terms of the latter, it follows that

$$\det\{u^*(i_{l1}+i_{l2}, j_{l1}+j_{l2})\} = \det\{M_C(i_{l1}+i_{l2}, j_{l1}+j_{l2})C\} > 0 \tag{3.21a}$$

$$\det\{u^*(1+i_{l1}+i_{l2}, j_{l1}+j_{l2})\} > 0. \tag{3.21b}$$

Relation (3.21*a*) follows from noting that, in terms of the sequence ordering adopted by Vrscay and Handy, the matrix $M(i_{l1}+i_{l2}, j_{l1}+j_{l2}; N)$, corresponding to the case $s=0$, is identically zero. That is, none of the sequence elements $\{(i,j)_l\}$ $(1 \leq l \leq D = (1+I)^2)$ can combine to form $(N, 0)$ or $(0, N)$, where $N = 2I+1$ (i.e. $(i,j)_{l1}+(i,j)_{l2} \neq (2I+1, 0)$ or $(0, 2I+1)$).

The second relation, (3.21*b*) is slightly more difficult. The matrix $M(1+i_{l1}+i_{l2}, j_{l1}+j_{l2}; N)$ is non-zero only for $l1 = l2 = I+1$, and $l1 = l2 = I(I+1)+1$. Thus, for the $s=1$ case, $u^*(1+i_{l1}+i_{l2}, j_{l1}+j_{l2})$ consists of a positive diagonal matrix,

$$M(1+i_{l1}+i_{l2}, j_{l1}+j_{l2}; N)\left\{1+C\left[\sum_{n=0}^{N} v(n,0)\right]\right\}$$

added to the positve matrix $M_C(1+i_{l1}+i_{l2}, j_{l1}+j_{l2})c$. The latter has all its diagonal subdeterminants positive. From this follows (3.21*b*).

The preceding argument shows that the normalization in (3.19) is inadequate in projecting out the previous trivial unphysical moment solution. To remedy this, we must adopt a different coordinate pair sequence ordering. Again we focus on the non-negative integer pairs $(i,j) \in [0, I] \times [0, I]$, for given I. Again, we take $(0,0)$ as our first entry, and proceed as before in terms of ordering by first varying i then j; however, this time we exclude the points $(I, 0)$ and $(0, I)$! This then means that the maximum dimension is $D^* = (I+1)^2 - 2$. It then follows that the set of points $\{(s+i_{l1}+i_{l2}, j_{l1}+j_{l2})\}$ defined by this finite sequence ordering lie within the $[0, 2I+1] \times [0, 2I+1]$ square region, but exclude the points $(2I, 0)$, $(2I+1, 0)$, $(2I+1, 1)$ and the $x \leftrightarrow y$ counterparts. However, because the point $(2I+1, 2)$ is included, the missing moment $u(2I, 0)$ must be kept. That is, the generation of the moment $u(2I+1, 2)$ includes a $u(2I, 0)$ dependence. As such, the corresponding missing moment order for this coordinate pair sequencing is $N = 2I$. The corresponding normalization is then:

$$\sum_{n=0}^{2I} u(n,0) = 1 + \left(\sum_{n=0}^{2I} v(n,0)\right) C. \tag{3.22}$$

Table 5. *C*-shift formulation for the perturbed two-dimensional harmonic oscillator ($\lambda = 0.1$). I_d denotes the number of missing moments, $2I$, and the dimensionality $d \leq D^* = (I+1)^2 - 2$.

C	I_d	Bounds for the first excited state of even parity under $x \leftrightarrow -x$, $y \leftrightarrow -y$, and $x \leftrightarrow y$
0.5×10^{-2}	2_5	$6.12 < E < 6.19$
0.5×10^{-2}	2_7	$6.149 < E < 6.163$
10^{-4} [a]	3_{10}	$6.1578 < E < 6.1620$ [b]
10^{-4}	3_{12}	$6.1586 < E < 6.1600$
10^{-4}	3_{14}	$6.1591 < E < 6.1594$

[a] The change in C reflects an implicit change in normalization as I increases (refer to (3.22)). [b] Spurious narrow feasibility regions were encountered which subsequently disappeared at higher order.

The results of this analysis are given in table 5. For this problem we kept C fixed. The bounds quoted are consistent with the value given by Killingbeck and Jones (1986) of $E = 6.159\,2858$. Note that, contrary to one-dimensional systems with a fixed number of missing moments, multi-dimensional problems involve an infinite number of missing moments; although at any one time a finite number is required. As I increases, the wavefunction normalization implied by (3.22) also changes; accordingly, C must also change; that is, for a given excited state, its corresponding minimum C-value is I-dependent. This is reflected in the data in table 5.

4. Conclusion

We have presented the C-shift reformulation of the EMM for generating converging eigenenergy bounds. All of the numerical results required double precision arithmetic on the CRAY. It is our belief that better estimates for the asymptotic behaviour of the two-dimensional Schrödinger equation solutions should lead to a more suitable regulating function, $R(x)$, yielding improved bounds. This investigation is currently underway.

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