Multiscale reference function analysis of the $\mathcal{PT}$ symmetry breaking solutions for the $P^2 + iX^3 + i\alpha X$ Hamiltonian

2001 J. Phys. A: Math. Gen. 34 5593

(http://iopscience.iop.org/0305-4470/34/27/309)

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

J. Phys. A: Math. Gen. **34** (2001) 5593–5602 PII: S0305-4470(01)24386-8

Multiscale reference function analysis of the $\mathcal{PT}$ symmetry breaking solutions for the $P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$ Hamiltonian

C R Handy[1], D Khan[1], Xiao-Qian Wang[1] and C J Tymczak[2]

[1] Department of Physics & Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia 30314, USA
[2] Los Alamos National Laboratory T-14, Los Alamos, New Mexico 87545, USA

Received 20 April 2001
Published 29 June 2001
Online at stacks.iop.org/JPhysA/34/5593

Abstract

The recent work of Delabaere and Trinh (Delabaere E and Trinh D T 2000 *J. Phys. A: Math. Gen.* **33** 8771) discovered the existence of $\mathcal{PT}$ symmetry breaking, complex energy, L^2 solutions for the one-dimensional Hamiltonian, $P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$, in the asymptotic limit $\alpha \to -\infty$. Their asymptotic analysis produced questionable results for moderate values of α. We can easily confirm the existence of $\mathcal{PT}$ symmetry breaking solutions by explicitly computing the low-lying states for $|\alpha| < \mathrm{O}(10)$. Our analysis makes use of the multiscale reference function (MRF) approach, developed by Tymczak *et al* (Tymczak C J, Japaridze G S, Handy C R and Wang Xiao-Qian 1998a *Phys. Rev. Lett.* **80** 3678; 1998b *Phys. Rev.* A **58** 2708). The MRF results can be validated by comparing them with the converging eigenenergy bounds generated through the eigenvalue moment method, as recently argued by Handy (2001a, b). Given the reliability of the MRF analysis, its fast numerical implementation, high accuracy and theoretical simplicity, the present formalism defines an effective and efficient procedure for analysing many related problems that have appeared in the recent literature.

PACS numbers: 0230H, 0365, 0365G

1. Introduction

There has been much interest, recently, in understanding the symmetry breaking mechanism for $\mathcal{PT}$-invariant Hamiltonians of the type $P^2 + \sum_{j=0}^{J} C_J(\mathrm{i}X)^j$. The mathematical interest in these systems originated from a conjecture by Bessis, and WKB analysis confirmation by Bender and Boettcher (1998), that the class of potentials of the form $V(x) = (\mathrm{i}X)^n$ only allow for $\mathcal{PT}$-invariant solutions, and thus can only have real discrete spectra. The recent literature

testifies to the great interest in these problems, as can be found in the references cited by Bender *et al* (2001) and Mezincescu (2000, 2001).

An important work establishing that $\mathcal{PT}$ symmetry breaking systems do exist was the recent study by Delabaere and Trinh (2000) which used asymptotic methods to analyse the Hamiltonian $H_\alpha \equiv P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$. Their analysis has shown the existence of symmetry breaking solutions for large α values; however, for moderate values, their results were near the limits of their analytical validity. Despite this, they made certain questionable predictions for moderate α values.

Our immediate objective is to check the validity of the Delabaere and Trinh study, by explicitly computing the low-lying complex (and real) eigenenergies for moderate α values. We do this in two ways. The first makes use of the very efficient multiscale reference function (MRF) formalism of Tymczak *et al* (1998a, b). The results of this eigenenergy estimation analysis are then confirmed through application of a recently developed eigenenergy bounding theory proposed by Handy (2001a, b), which can generate converging bounds to the complex eigenenergies. This bounding approach, referred to as the eigenvalue moment method (EMM), is exact, although numerically slower in its implementation than the MRF procedure.

As a footnote to the above, we emphasize that the EMM theory generates an infinite hierarchy of closed, finite-dimensional, algebraic, eigenenergy constraints. These are then solved, numerically. In this regard, the EMM procedure is very different from other numerical schemes, such as numerical integration, which are intrinsically of an approximating nature, and cannot provide any fundamental theoretical insight into the underlying physical processes. The algebraic constraints generated through the EMM formalism can provide such insight; although such analysis has not been attempted to date. However, for the immediate purposes of this paper, we solely defer to EMM in order to check the validity of the MRF results.

In this paper, we provide the essentials of the MRF theoretical structure, as applied to the H_α Hamiltonian. The EMM theory is not discussed. Only the numerical bounds are quoted in the tables. This paper validates the relevance of MRF theory in the computation of complex eigenenergies, for the class of problems referenced above.

Both the MRF and EMM methods are dependent on a moments' representation for the given system. This in turn is readily realizable for any (multi-dimensional) rational fraction potential.

Any moment-based analysis is inherently multiscale in nature. That is, as the number of moments used increases, one is probing the system at successively smaller scales. Consistent with this, the MRF basis representation, particularly within configuration space, has important ties with (complex) turning point quantization (Handy *et al* (2000)), and wavelet analysis (Handy and Brooks (2001)).

We outline the basic MRF theory and its implementation, in the next section. The last section contains a detailed enumeration, and illustration, of the MRF results, which make precise the qualitative spectral structure conjectured by Delabaere and Trinh (2000).

2. The MRF representation

2.1. The moment equation

The starting point for the MRF analysis is the transformation of the Schrödinger equation into the Fourier representation, assuming that one is working with the physical, L^2, solutions. Thus, for the configuration space Schrödinger equation studied by Delabaere and Trinh (2000)

$$-\partial_x^2\Psi(x) + (\mathrm{i}x^3 + \mathrm{i}\alpha x)\Psi(x) = E\Psi(x) \tag{1}$$

its Fourier transform counterpart is (i.e. $x \to \mathrm{i}\partial_k$, $\partial_x \to \mathrm{i}k$)

$$k^2\hat{\Psi}(k) + (\partial_k^3 - \alpha\partial_k)\hat{\Psi}(k) = E\hat{\Psi}(k) \tag{2}$$

where

$$\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}\Psi(x). \tag{3}$$

It is important to note that, for the physical solutions, a simple application of WKB analysis (Bender and Boettcher (1998)) tells us that the asymptotic behaviour of the configuration space representation yields an entire Fourier transform. Because of this, the k-power series expansion is absolutely convergent, and defined in terms of the power moments:

$$\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}}\sum_{p=0}^{\infty}(-\mathrm{i}k)^p\frac{\mu_p}{p!} \tag{4}$$

where

$$\mu_p \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p\Psi(x) \tag{5}$$

define the Hamburger power moments.

We can generate the recursion relation for the μ_p from the standard power series expansion methods for linear differential equations (Bender and Orszag (1978)). Alternatively, we can apply $\int_{-\infty}^{+\infty}\mathrm{d}x\, x^p$ to both sides of equation (1), combined with integration by parts, and obtain the necessary *moment equation*:

$$\mu_{p+3} = -\alpha\mu_{p+1} - \mathrm{i}E\mu_p - \mathrm{i}p(p-1)\mu_{p-2} \tag{6}$$

for $p \geqslant 0$. This corresponds to a homogeneous, linear, finite difference equation, of effective order $1 + m_\mathrm{s} = 3$, since specification of the independent moments $\{\mu_0, \mu_1, \mu_2\}$, plus the (complex) energy parameter, E, generates all of the remaining moments. The independent moments are referred to as the *missing moments*.

The linear dependence of the moments, on the missing moments, can be expressed through the relation

$$\mu_p = \sum_{\ell=0}^{m_\mathrm{s}} M_{p,\ell}(E)\mu_\ell \tag{7}$$

where the energy-dependent coefficients satisfy the moment equation, with respect to the p-index, as well as the initial conditions $M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_1, \ell_2 \leqslant m_\mathrm{s}$.

2.2. *Defining an analytic basis in the Fourier space*

The physical solutions in the Fourier representation must also be L^2. One would like to find an appropriate basis into which to transform the Fourier power series expansion

$$\frac{1}{\sqrt{2\pi}}\sum_{p=0}^{\infty}(-\mathrm{i}k)^p\frac{\mu_p}{p!} = \frac{1}{\sqrt{2\pi}}\sum_{j=0}^{\infty}a_j\mathcal{B}_j(k). \tag{8}$$

The easiest choice, leading to a rapid, analytic generation of the a_j coefficients, is to take

$$\mathcal{B}_j(k) = (-\mathrm{i}k)^j\hat{R}(k) \tag{9}$$

where $\hat{R}$ is some arbitrary 'reference' function yielding a complete (if not orthogonal) basis. Thus, if $\frac{1}{\hat{R}(k)}$ is analytic, then one can generate the a_j by expanding $\frac{\hat{\Psi}(k)}{\hat{R}(k)}$. In particular, we can take $\hat{R}(k) = \mathrm{e}^{-\beta k^2}$, where $\beta > 0$, and otherwise arbitrary, yielding

$$A(k) \equiv \sum_{j=0}^{\infty}a_j(-\mathrm{i}k)^j = \mathrm{e}^{\beta k^2}\sum_{p=0}^{\infty}(-\mathrm{i}k)^p\frac{\mu_p}{p!}. \tag{10}$$

Table 1. E_1 branch for the discrete states of $P^2 + iX^3 + i\alpha X$.

α	$E_1^{(\mathrm{MRF})}(\alpha)$	EMM bounds: $E_R^{(L)} < E_R < E_R^{(U)}$ & $E_I^{(L)} < E_I < E_I^{(U)}$
−5.0	(1.343 3409, ±2.907 3602)	1.343 311[a] $< E_R <$ 1.343 354[a], 2.9073[a] $< E_I <$ 2.9075[a]
−4.5	(1.299 2519, ±2.312 4924)	1.299 242 $< E_R <$ 1.299 252, 2.3124 $< E_I <$ 2.3126
−4.0	(1.248 6637, ±1.761 7076)	1.248 637 $< E_R <$ 1.248 666, 1.761 688 $< E_I <$ 1.761 742
−3.5	(1.212 4399, ±1.260 9114)	1.212 421 $< E_R <$ 1.212 448, 1.260 88 $< E_I <$ 1.260 94
−3.0	(1.225 8438, ±0.760 0296)	1.225 837 $< E_R <$ 1.225 864, 0.760 00 $< E_I <$ 0.760 04
−2.5	(0.928 0136, 0)	0.927 999 80[b] $< E <$ 0.928 001 01[b]
−2.0	(0.620 9137, 0)	0.620 913 47 $< E <$ 0.620 913 86
−1.5	(0.596 4936, 0)	0.596 493 26 $< E <$ 0.596 493 51
−1.0	(0.699 9615, 0)	0.699 959 77 $< E <$ 0.699 959 78
−0.5	(0.892 6699, 0)	0.892 668 27 $< E <$ 0.892 668 49
0.0	(1.156 2673, 0)	1.156 266 95 $< E <$ 1.156 267 18
		1.156 267 071 988 113 24[c] $< E <$ 1.156 267 071 988 113 35[c]
0.5	(1.479 8519, 0)	1.479 851 79 $< E <$ 1.479 852 06
1.0	(1.856 1128, 0)	1.856 110 65 $< E <$ 1.856 111 08
1.5	(2.279 7563, 0)	2.279 751 85 $< E <$ 2.279 752 32
2.0	(2.746 7434, 0)	2.746 739 52 $< E <$ 2.746 740 23
2.5	(3.253 8767, 0)	3.253 875 96 $< E <$ 3.253 877 23
3.0	(3.798 5559, 0)	3.798 553 87 $< E <$ 3.798 553 95
3.5	(4.378 6140, 0)	4.378 596 45 $< E <$ 4.378 597 36
4.0	(4.992 1974, 0)	4.992 154 36 $< E <$ 4.992 155 04
4.5	(5.637 6822, 0)	5.637 631 49 $< E <$ 5.637 632 00
5.0	(6.313 6428, 0)	6.313 597 39 $< E <$ 6.313 606 65

[a] EMM analysis of Handy (2001b).
[b] EMM ($P_{\max}^{(S)} = 30$) analysis of Handy (2001a).
[c] EMM ($P_{\max}^{(S)} = 60$) analysis of Handy (2001a).

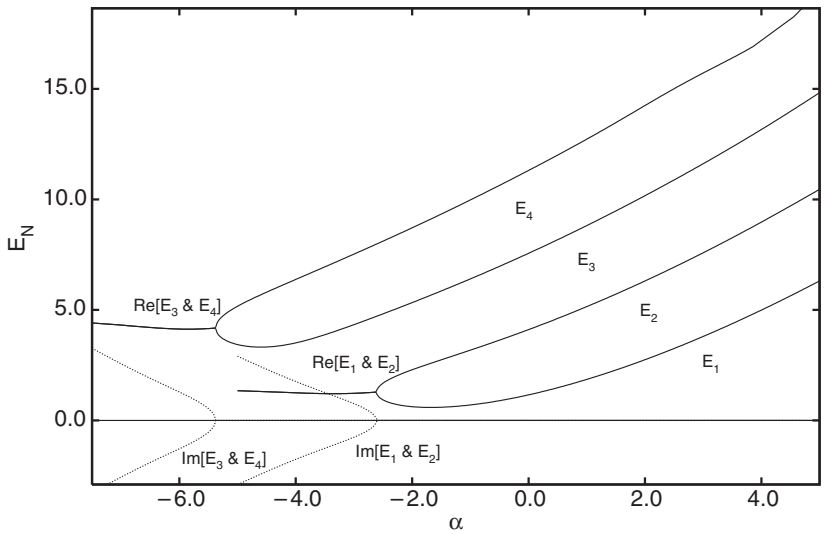

Figure 1. Eigenvalues E_N versus parameter α.

It is then clear that the a_j will become linear in the missing moments, $\{\mu_\ell | 0 \leqslant \ell \leqslant m_s\}$. Specifically,

$$a_j(E; \mu_0, \mu_1, \mu_2) = \sum_{p+2q=j} \frac{(-\beta)^q \mu_p}{q!p!} \tag{11}$$

Table 2. E_2 branch for the discrete states of $P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$.

α	$E_2^{(\mathrm{MRF})}(\alpha)$	EMM bounds: $E_R^{(L)} < E_R < E_R^{(U)}$ & $E_I^{(L)} < E_I < E_I^{(U)}$
−5.0	(1.343 3409, ±2.907 3602)	1.343 311[a] $< E_R <$ 1.343 354[a], 2.9073[a] $< E_I <$ 2.9075[a]
−4.5	(1.299 2519, ±2.312 4924)	1.299 243 $< E_R <$ 1.299 252, 2.3124 $< E_I <$ 2.3126
−4.0	(1.248 6637, ±1.761 7076)	1.248 637 $< E_R <$ 1.248 666, 1.761 688 $< E_I <$ 1.761 742
−3.5	(1.212 4399, ±1.260 9114)	1.212 421 $< E_R <$ 1.212 448, 1.260 88 $< E_I <$ 1.260 94
−3.0	(1.225 8438, ±0.760 0296)	1.225 837 $< E_R <$ 1.225 864, 0.760 00 $< E_I <$ 0.760 04
−2.5	(1.685 9358, 0)	1.685 977 65[b] $< E <$ 1.685 980 87[b]
−2.0	(2.292 2626, 0)	2.292 290 55 $< E <$ 2.292 293 33
−1.5	(2.742 5268, 0)	2.742 526 67 $< E <$ 2.742 530 34
−1.0	(3.179 7220, 0)	3.179 713 12 $< E <$ 3.179 717 50
−0.5	(3.632 0373, 0)	3.632 072 37 $< E <$ 3.632 077 67
0.0	(4.109 1279, 0)	4.109 227 04 $< E <$ 4.109 235 58
		4.109 228 752 806[c] $< E <$ 4.109 228 752 812[c]
0.5	(4.614 7402, 0)	4.614 833 91 $< E <$ 4.614 846 33
1.0	(5.150 1688, 0)	5.150 160 59 $< E <$ 5.150 176 40
1.5	(5.715 4576, 0)	5.715 384 38 $< E <$ 5.715 416 49
2.0	(6.310 0192, 0)	6.310 205 27 $< E <$ 6.310 252 82
2.5	(6.933 2376, 0)	6.934 054 53 $< E <$ 6.934 129 54
3.0	(7.585 0094, 0)	7.586 278 41 $< E <$ 7.586 380 28
3.5	(8.265 6580, 0)	8.266 130 65 $< E <$ 8.266 336 47
4.0	(8.974 5543, 0)	8.972 726 40[d] $< E <$ 8.973 328 36[d]
4.5	(9.707 7326, 0)	9.702 105 65[d] $< E <$ 9.707 894 36[d]
5.0	(10.457 5130, 0)	10.452 276 56[d] $< E <$ 10.480 068 75[d]

[a] EMM analysis of Handy (2001b).
[b] EMM ($P_{\max}^{(S)} = 30$) analysis of Handy (2001a).
[c] EMM ($P_{\max}^{(S)} = 50$) analysis of Handy (2001a).
[d] EMM ($P_{\max}^{(S)} < 30$) analysis of Handy (2001a).

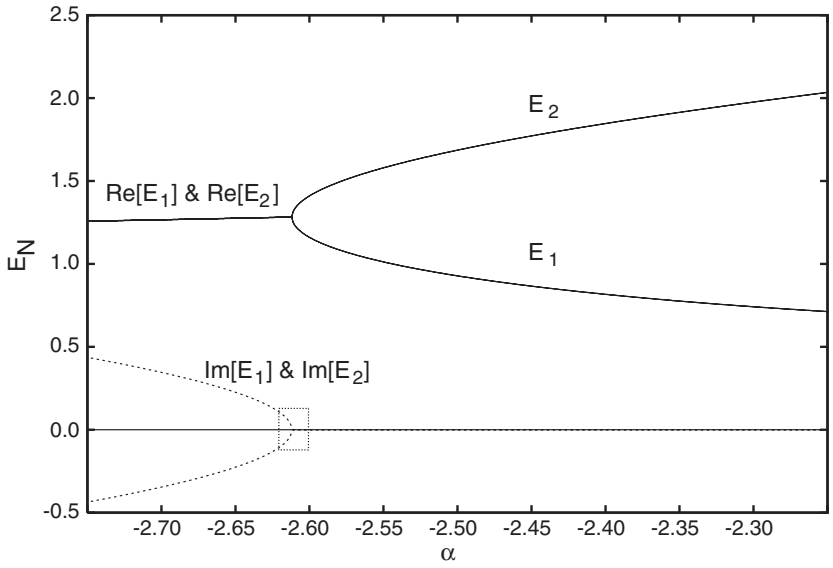

Figure 2. First and second eigenvalues versus α near the bifurcation.

Table 3. E_3 branch for the discrete states of $P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$.

α	$E_3^{(\mathrm{MRF})}(\alpha)$	EMM bounds: $E_R^{(L)} < E_R < E_R^{(U)}$ & $E_I^{(L)} < E_I < E_I^{(U)}$
−7.5	(4.410 3093, ±3.266 4292)	4.408 662[a] $< E_R <$ 4.411 426[a], 3.2645 $< E_I <$ 3.2700
−7.0	(4.312 0349, ±2.563 4751)	4.310 530 $< E_R <$ 4.313 107, 2.5618 $< E_I <$ 2.5674
−6.5	(4.205 6380, ±1.903 9658)	4.204 520 $< E_R <$ 4.206 360, 1.9026 $< E_I <$ 1.9074
−6.0	(4.134 3003, ±1.285 0914)	4.133 864 $< E_R <$ 4.134 534, 1.284 $< \pm E_I <$ 1.286
−5.5	(4.157 5135, ±0.531 3291)	4.155 648 $< E_R <$ 4.158 235, 0.5300 $< E_I <$ 0.5370
−5.0	(3.431 4015, 0)	3.431 367 41[b] $< E <$ 3.431 395 40[b]
−4.5	(3.323 2446, 0)	3.323 236 35 $< E <$ 3.323 250 18
−4.0	(3.508 7615, 0)	3.508 760 99 $< E <$ 3.508 775 44
−3.5	(3.877 6981, 0)	3.877 684 85 $< E <$ 3.877 701 78
−3.0	(4.333 4536, 0)	4.333 422 75 $< E <$ 4.333 446 54
−2.5	(4.822 9806, 0)	4.822 948 49 $< E <$ 4.822 984 27
−2.0	(5.331 3715, 0)	5.331 355 37 $< E <$ 5.331 403 11
−1.5	(5.857 6148, 0)	5.857 595 78 $< E <$ 5.857 665 76
−1.0	(6.403 6752, 0)	6.403 623 10 $< E <$ 6.403 728 94
−0.5	(6.971 4613, 0)	6.971 339 51 $< E <$ 6.971 527 63
0.0	(7.562 2889, 0)	7.562 159 01 $< E <$ 7.562 423 55
		7.562 273 8549[c] $< E <$ 7.562 273 8551[c]
0.5	(8.177 0143, 0)	8.176 872 01 $< E <$ 8.177 206 44
1.0	(8.816 2241, 0)	8.815 693 61 $< E <$ 8.816 443 75
1.5	(9.480 2011, 0)	9.479 135 94 $< E <$ 9.480 442 30
2.0	(10.168 6764, 0)	10.166 835 97 $< E <$ 10.169 075 46
2.5	(10.880 7993, 0)	10.878 961 80 $< E <$ 10.882 533 90
3.0	(11.615 9802, 0)	11.615 350 00 $< E <$ 11.620 750 00
3.5	(12.375 5952, 0)	12.370 900 00[d] $< E <$ 12.389 800 00[d]
4.0	(13.163 8132, 0)	13.161 600 00[d] $< E <$ 13.204 800 00[d]
4.5	(13.984 2043, 0)	13.860 000 00[d] $< E <$ 14.040 000 00[d]
5.0	(14.829 8186, 0)	14.720 000 00[d] $< E <$ 15.080 000 00[d]

[a] EMM analysis of Handy (2001b).
[b] EMM ($P_{\max}^{(S)} = 30$) analysis of Handy (2001a).
[c] EMM ($P_{\max}^{(S)} = 50$) analysis of Handy (2001a).
[d] EMM ($P_{\max}^{(S)} < 30$) analysis of Handy (2001a).

or

$$a_j(E;\mu_0,\mu_1,\mu_2) = \sum_{\ell=0}^{m_s=2}\left(\sum_{p+2q=j}\frac{(-\beta)^q M_{p,\ell}(E)}{q!p!}\right)\times\mu_\ell \tag{12}$$

for $j \geqslant 0$. Clearly, the maximum (Hamburger) moment order generated, $P_{\max}$, determines the maximum order of a_j generated, $0 \leqslant j \leqslant P_{\max}$.

2.3. The MRF quantization prescription

It has been argued by Tymczak *et al* (1998a, b) that the convergent zeros of the coefficient functions

$$a_j(E_n^{(j)}) = 0 \tag{13}$$

converge to the exact discrete state energies

$$\lim_{j\to\infty} E_n^{(j)} = E_n^{\mathrm{physical}}. \tag{14}$$

Table 4. E_4 branch for the discrete states of $P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$.

α	$E_4^{(\mathrm{MRF})}(\alpha)$	EMM bounds: $E_R^{(L)} < E_R < E_R^{(U)}$ & $E_I^{(L)} < E_I < E_I^{(U)}$
−7.5	(4.410 3093, ±3.266 4292)	4.408 662[a] $< E_R <$ 4.411 426[a], 3.2645 $< E_I <$ 3.2700
−7.0	(4.312 0349, ±2.563 4751)	4.310 530 $< E_R <$ 4.313 107, 2.5618 $< E_I <$ 2.5674
−6.5	(4.205 6380, ±1.903 9658)	4.204 520 $< E_R <$ 4.206 360, 1.9026 $< E_I <$ 1.9074
−6.0	(4.134 3003, ±1.285 0914)	4.133 864 $< E_R <$ 4.134 534, 1.284 $< \pm E_I <$ 1.286
−5.5	(4.157 5135, ±0.531 3291)	4.155 648 $< E_R <$ 4.158 235, 0.5300 $< E_I <$ 0.5370
−5.0	(5.167 8291, 0)	5.167 842 14[b] $< E <$ 5.167 981 49[b]
−4.5	(5.804 1737, 0)	5.804 279 00 $< E <$ 5.804 396 60
−4.0	(6.379 6826, 0)	6.379 699 97 $< E <$ 6.379 854 80
−3.5	(6.949 0904, 0)	6.948 808 80 $< E <$ 6.949 158 72
−3.0	(7.525 2398, 0)	7.524 895 39 $< E <$ 7.525 365 68
−2.5	(8.113 0836, 0)	8.113 024 13 $< E <$ 8.113 687 68
−2.0	(8.715 9047, 0)	8.716 316 57 $< E <$ 8.716 988 42
−1.5	(9.336 4444, 0)	9.336 585 47 $< E <$ 9.337 746 69
−1.0	(9.976 3275, 0)	9.975 528 96 $< E <$ 9.977 187 84
−0.5	(10.635 2870, 0)	10.633 430 56 $< E <$ 10.636 605 76
0.0	(11.312 0046, 0)	11.311 651 20 $< E <$ 11.315 884 80
		11.314 421 818[c] $< E <$ 11.314 421 824[c]
0.5	(12.007 2541, 0)	12.010 040 00 $< E <$ 12.016 760 00
1.0	(12.726 4921, 0)	12.724 736 00 $< E <$ 12.742 880 00
1.5	(13.476 1039, 0)	13.470 000 00 $< E <$ 13.515 000 00
2.0	(14.248 7931, 0)	14.210 000 00 $< E <$ 14.330 000 00
2.5	(15.008 8412, 0)	14.968 000 00 $< E <$ 15.220 000 00
3.0	(15.834 7839, 0)	15.712 500 00 $< E <$ 16.125 000 00
3.5	(16.402 0563, 0)	16.400 000 00 $< E <$ 17.000 000 00

[a] EMM analysis of Handy (2001b).
[b] EMM ($P_{\max}^{(S)} = 30$) analysis of Handy (2001a).
[c] EMM ($P_{\max}^{(S)} = 50$) analysis of Handy (2001a).

Table 5. MRF complex eigenenergy estimates for $P_{\max} = 100$.

α	E_1 & E_2	E_3 & E_4
−7.5		(4.410 244 3440, ±3.266 497 6653)
−7.0		(4.311 994 9171, ±2.563 558 4867)
−6.5		(4.205 598 3584, ±1.904 024 8046)
−6.0		(4.134 251 9473, ±1.285 122 7083)
−5.5		(4.157 475 0374, ±0.531 356 7960)
−5.0	(1.343 343 1987, ±2.907 390 6160)	
−4.5	(1.299 242 3296, ±2.312 515 4783)	
−4.0	(1.248 656 7335, ±1.761 719 3016)	
−3.5	(1.212 436 7296, ±1.260 909 9725)	
−3.0	(1.225 847 5767, ±0.760 022 4714)	

The above root equation must be adapted to the, $1+m_s$, linear, missing moment structure of the Hamiltonian in question. Thus, to any expansion order J, we impose that the last $1+m_s$, a_j-coefficients be zero (i.e. $a_{J-\ell} = 0$, for $0 \leqslant \ell \leqslant m_s$). This results in a $1+m_s = 3$-dimensional, determinantal equation for the energy:

$$\Delta_J(E) = 0 \tag{15}$$

Table 6. MRF real eigenenergy estimates for $P_{\max} = 100$.

α	E_1	E_2	E_3	E_4
−5.0			3.431 383 201 6	5.167 888 6857
−4.5			3.323 242 619 1	5.804 339 2228
−4.0			3.508 765 607 3	6.379 805 2063
−3.5			3.877 693 005 2	6.949 052 3010
−3.0			4.333 439 836 4	7.525 191 9556
−2.5	0.928 000 342 158	1.685 979 342 731	4.822 975 394 502	8.113 377 225
−2.0	0.620 913 574 064 8	2.292 292 501 9	5.331 383 401 0	8.716 619 963
−1.5	0.596 493 384 095 90	2.742 529 393 9422	5.857 622 001 9	9.337 028 976
−1.0	0.699 959 920 798 6	3.179 715 776 3716	6.403 645 104 9	9.976 132 38
−0.5	0.892 668 433 554 6	3.632 074 461 334	6.971 403 910 342	10.635 016 26
0	1.156 267 071 988 1	4.109 228 752 809	7.562 273 854 9	11.314 421 8
0.5	1.479 851 860 796 89	4.614 838 727 3616	8.177 082 531 6	12.014 824 35
1.0	1.856 110 766 056 6	5.150 168 955 614	8.816 245 171 7	12.736 497 38
1.5	2.279 752 047 593 0	5.715 408 707 15	9.479 889 209 56	13.479 563 2
2.0	2.746 739 980 856 0	6.310 238 361 05	10.167 947 849 9	14.244 031 9
2.5	3.253 876 926 368 9	6.934 096 040 540	10.880 225 999	15.029 831 15
3.0	3.798 554 700 716	7.586 310 988 692	11.616 445 659	15.836 828 4
3.5	4.378 596 945 623 65	8.266 172 869 0	12.376 276 93	16.664 848 1
4.0	4.992 154 082 578 6	8.972 968 434 7	13.159 359 16	17.513 684
4.5	5.637 630 445 616	9.706 000 860 0	13.965 315 33	18.383 109
5.0	6.313 632 040 368	1.046 459 957 615	14.793 761 8	19.272 882 3

where

$$\Delta_J(E) \equiv \mathrm{Det}\begin{pmatrix} \mathcal{M}^{(J)}_{0,0}(E,\beta), \mathcal{M}^{(J)}_{0,1}(E,\beta), \mathcal{M}^{(J)}_{0,2}(E,\beta) \\ \mathcal{M}^{(J)}_{1,0}(E,\beta), \mathcal{M}^{(J)}_{1,1}(E,\beta), \mathcal{M}^{(J)}_{1,2}(E,\beta) \\ \mathcal{M}^{(J)}_{2,0}(E,\beta), \mathcal{M}^{(J)}_{2,1}(E,\beta), \mathcal{M}^{(J)}_{2,2}(E,\beta) \end{pmatrix} \tag{16}$$

and

$$\mathcal{M}^{(J)}_{\ell_1,\ell_2}(E,\beta) \equiv \sum_{p+2q=J-\ell_1} \frac{(-\beta)^q M_{p,\ell_2}(E)}{q!p!} \tag{17}$$

for $0 \leqslant \ell_1, \ell_2 \leqslant m_s = 2$. In the tables, the $P_{\max}$ parameter corresponds to $J \equiv P_{\max}$.

3. Numerical implementation of MRF

The MRF analysis is implemented for $\beta = 0.5$. This value of the arbitrary parameter generates the fastest converging results.

In figure 1 we plot the $\mathcal{PT}$ symmetry breaking solutions ($\mathrm{Im}\,(E) \neq 0$), and the $\mathcal{PT}$ symmetry invariant solutions ($\mathrm{Im}\,(E) = 0$), for moderate α values at the limits of Delabaere and Trinh's asymptotic analysis. There are four branches depicted. In tables 1–4 we specify some of the points plotted and, in addition, compare the MRF eigenenergy estimates with the EMM bounds. The MRF results in these tables generally correspond to $J \leqslant 50$. The EMM results were calculated to the same moment order, $P_{\max} \leqslant 50$, for the complex energies. In those cases where the MRF method predicts a purely real eigenenergy, we used the faster EMM formalism corresponding to explicitly assuming that the underlying solutions are $\mathcal{PT}$ invariant (Handy (2001a)). For this case, the underlying problem is of Stieltjes character, and a Stieltjes moment order of $P^{(S)}_{\max} = 30$ corresponds to a Hamburger moment order of 60 (i.e. $P^{(S)}_{\max} = \frac{P_{\max}}{2}$). For this reason, in some cases the MRF estimates

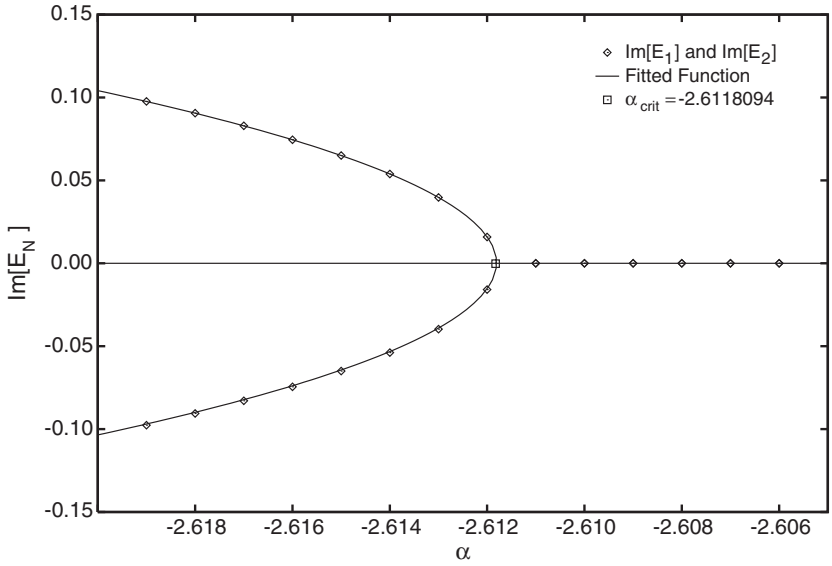

Figure 3. Imaginary part of the first and second eigenvalues near the bifurcation.

(computed at $J \leqslant 50$) lie outside of the EMM bounds. However, for some of the EMM bounds, numerical instability concerns required that $P_{\max}^{(S)} < 30$ (these were computed on a standard, double precision, IBM platform). Such cases are relatively few in number, and are explicitly identified. By working at a larger precision order, the corresponding bounds can be improved.

Note that for $\alpha = 0$ we quote the EMM bounds generated at higher Stieltjes moment order ($P_{\max}^{(S)} \leqslant 60$) given in the work by Handy (2001a). These bounds are very consistent with the corresponding entries in tables 5 and 6.

In tables 5 and 6 we quote the MRF results for $J = 100$ (using CRAY double precision). Only the stable digits are given (that is, tables 5 and 6 correspond to the (empirically determined) stable digits within the MRF generated sequence, for $0 \leqslant J \leqslant 100$).

The results are consistent: that is, the MRF results in tables 1–4, for the most part, lie within the bounds. This is definitely the case for tables 5 and 6. Note that in the tables we quote the imaginary parts of the energy as $\pm$: this is because we cannot tell which $\mathcal{PT}$ invariant branch continues into the $\mathcal{PT}$ breaking branch. For $\mathcal{PT}$ invariant Hamiltonians, complex energies come in conjugate pairs. Thus, if E is a solution, so too is E^*.

In figures 2 and 3 we narrow in on the smaller of the two critical α values, $\alpha_{\mathrm{cr}_{1,2}}$, as shown in figure 1. At these critical points, the energy goes from being real ($\mathcal{PT}$ invariant solutions) to complex ($\mathcal{PT}$ breaking solutions). They are

$$\alpha_{\mathrm{cr}_1} = -2.611\,809\,356 \tag{18}$$

corresponding to $E_{\mathrm{cr}_1} = 1.282\,773\,535\,62$, and

$$\alpha_{\mathrm{cr}_2} = -5.375\,879\,629 \tag{19}$$

corresponding to $E_{\mathrm{cr}_2} = 4.181\,388\,093$.

4. Conclusion

We have confirmed the asymptotic analysis prediction of Delabaerre and Trinh (DT) on the existence of symmetry breaking solutions for the H_α Hamiltonian. Our methods enable the precise analysis of the complex-real spectra, particularly for moderate α values at the limits of their DT asymptotic validity. The results of both an eigenenergy estimation method (MRF) and an eigenenergy bounding method (EMM) were presented. The algebraic simplicity and ease of computational implementability of the MRF method recommend it highly for application to similar problems. Through the use of readily available algebraic programming software, the MRF approach can be extended to arbitrary precision (indeed, Tymczak *et al* (1998b) were able to generate the quartic anharmonic oscillator ground state energy to more than 171 decimal places), making it a very powerful tool in these types of investigations. Recent (unpublished) extensions of the method have yielded an accuracy of 500 decimal places.

Acknowledgments

This work was supported through a grant from the National Science Foundation (HRD 9632844) through the Center for Theoretical Studies of Physical Systems (CTSPS). The author extends his appreciation to Professor D Bessis, Professor G Japaridze, Professor G A Mezincescu and Professor A Z Msezane for useful discussions.

References

Bender C M, Berry M, Meisinger P N, Savage V M and Simsek M 2001 *J. Phys. A: Math. Gen.* **34** L31
Bender C M and Boettcher S 1998 *Phys. Rev. Lett.* **80** 5243
Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)
Delabaere E and Trinh D T 2000 *J. Phys. A: Math. Gen.* **33** 8771
Handy C R and Brooks H 2001 *J. Phys. A: Math. Gen.* at press
Handy C R, Murenzi R, Bouyoucef K and Brooks H 2000 *J. Phys. A: Math. Gen.* **33** 2151
Handy C R 2001a *J. Phys. A: Math. Gen.* **34** L271
——2001b *J. Phys. A: Math. Gen.* **34** 5065
Mezincescu G A 2000 *J. Phys. A: Math. Gen.* **33** 4911
——2001 *J. Phys. A: Math. Gen.* **34** 3329
Tymczak C J, Japaridze G S, Handy C R and Wang Xiao-Qian 1998a *Phys. Rev. Lett.* **80** 3678
——1998b *Phys. Rev.* A **58** 2708