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Generating converging bounds to the (complex) discrete states of the $P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$ Hamiltonian

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Abstract

The eigenvalue moment method (EMM) is applied to the $H_\alpha \equiv P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$ Hamiltonian, enabling the algebraic/numerical generation of converging bounds to the complex energies of the L^2 states, as argued (through asymptotic methods) by Delabaere and Trinh. The robustness of the formalism, and its computational implementation, suggest that the present non-negativity formulation implicitly contains the key algebraic relations by which to prove Bessis' conjecture that the eigenenergies of the H_0 Hamiltonian are real. The required algebraic analysis of the EMM procedure pertaining to this problem will be presented in a forthcoming paper.

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1. Introduction

1.1. General overview

There has been much speculation on the mechanism responsible for symmetry breaking within a special class of $\mathcal{PT}$ invariant Hamiltonians. It has been argued by Bender and Boettcher (1998), based on a conjecture by Bessis, that the class of Hamiltonians of the form $P^2 + (\mathrm{i}X)^n$ admits bound states, within the complex plane, with real discrete spectra. Their arguments show that the $\mathcal{PT}$ invariance of the Hamiltonian is reflected in the wavefunction, $\Psi^*(-x) = \Psi(x)$, resulting in real spectra. However, Delabaere and Trinh (2000) have emphasized that $\mathcal{PT}$ invariance of the Hamiltonian is not sufficient to prevent symmetry breaking solutions. For instance, the Hamiltonian $P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$ admits bounded (L^2) solutions on the real axis, which can have complex energies for $\alpha < \alpha_{\mathrm{critical}} < 0$ (thereby breaking $\mathcal{PT}$ invariance), or real energies, for $\alpha > \alpha_{\mathrm{critical}}$.

An understanding of the underlying mechanism for symmetry breaking has remained elusive, despite numerous investigations on the above, and related problems, by Bender *et al* (1999a, b, 2000), Bender and Wang (2001), Caliceti (2000), Delabaere and Pham (1998), Handy (2001), Handy and Wang (2001), Levai and Znojil (2000), Mezincescu (2000, 2001), Shin (2000), and Znojil (2000), in addition to those already cited. However, the recent work by Dorey *et al* (2001) presents one possible explanation.

Our objective is to seek alternative (and less analytical) arguments that can possibly shed some light on this matter. In this regard, we have attempted to implement a novel 'positivity quantization' formalism based on the recent works by Handy (2001) and Handy and Wang (2001). These in turn make use of the eigenvalue moment method (EMM) originally developed by Handy and Bessis (1985) and Handy *et al* (1988a, b).

Our results, as communicated here, are very impressive. We are able to generate converging bounds for the (complex) discrete state energies, and arbitrary α. We are able to confirm the general results derived by Delabaere and Trinh, although our methods do not rely on asymptotic estimates, as theirs do.

It is important to emphasize that the EMM approach generates an infinite hierarchy of (closed) algebraic inequalities. We investigate the consequences of these relations from a numerical perspective. This is an important first step in identifying the algebraic relations responsible for symmetry breaking solutions within our formalism. Our results strongly suggest that a careful algebraic analysis of the underlying EMM relations will serve to identify the theoretical structure leading to a proof of Bessis' conjecture. This will be presented in a future paper. We emphasize that, unlike numerical integration schemes, which do not necessarily provide an understanding of the underlying theoretical structure of a problem, the algebraic/numerical structure of EMM can.

Beyond this, the ability to generate converging bounds to complex energy levels is a remarkable feat in its own right. This motivates the present communication. In a related work by Handy *et al* (HKWT, 2001a), they show how the *multiscale reference function* (MRF) formulation (Tymczak *et al* 1998a, b) can easily generate the (complex) discrete state energies for arbitrary α. Their estimation methods generate energies that fall within the bounds given here. As such, the present bounding theory provides a confidence test for the, numerically faster, MRF method. Because of this, we only generate energy bounds for important α values near the first complex-real bifurcation point, $\alpha_{\text{critical}} = -2.611\,8094$, as predicted by MRF.

1.2. Technical overview

The recent work by Handy (2001) introduced a new formalism that transforms the one-dimensional Schrödinger equation into a fourth-order, linear differential equation for $S(x) \equiv |\Psi(x)|^2$, regardless of the (complex) nature of the potential, $V(x) = V_R(x) + \mathrm{i}V_I(x)$:

$$\begin{aligned} -\frac{1}{V_I - E_I} S^{(4)} - \left(\frac{1}{V_I - E_I}\right)' S^{(3)} + 4\left(\frac{V_R - E_R}{V_I - E_I}\right) S^{(2)} \\ + \left(4\left(\frac{V_R - E_R}{V_I - E_I}\right)' + 2\left(\frac{V_R{}'}{V_I - E_I}\right)\right) S^{(1)} \\ + \left(4(V_I - E_I) + 2\left(\frac{V_R{}'}{V_I - E_I}\right)'\right) S = 0 \end{aligned} \tag{1}$$

where $S^{(n)}(x) \equiv \partial_x^n S(x)$, and $E = E_R + \mathrm{i}E_I$, etc. Through this fourth-order equation, one is able to transform the quantization problem into a non-negativity representation suitable for a moment problem (Shohat and Tamarkin 1963) based analysis, utilizing the Hamburger moments

$$u_p = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p S(x). \tag{2}$$

Such methods were originally developed by Handy and Bessis (1985) and Handy *et al* (1988a, b), and used to generate rapidly converging bounds to the bosonic ground state energy of singular perturbation/strong coupling (multi-dimensional) systems. This moment problem

based, 'positivity quantization', approach is generically referred to as the EMM. An efficient algorithmic implementation requires the use of linear programming (Chvatal 1983).

We emphasize that the only bounded (i.e. L^2 functions within the Ψ representation, or L^1, within the S-representation) and non-negative solutions to equation (1) are the physical solutions (Handy 2001). This is because, if $\Psi_{1;E}(x)$ and $\Psi_{2;E}(x)$ are independent solutions of the Schrödinger equation, for arbitrary E (and thus unbounded, except for the physical solutions), then $|\Psi_{1;E}(x)|^2$, $|\Psi_{2;E}(x)|^2$, $\Psi^*_{1;E}(x)\Psi_{2;E}(x)$, and $\Psi_{1;E}(x)\Psi^*_{2;E}(x)$, are the independent solutions to equation (1), assuming V is complex. If V is real, then all the solutions are real, and only the first three configurations are independent, leading to a third order linear differential equation for S (Handy 1987a, b). Thus, because of the uniqueness of non-negative and bounded solutions, application of EMM to the relevant moment equations (i.e. equations (47) and (51) for (1), or the alternate moment formulation discussed in section 2) will generate converging bounds to the physical energies (Handy and Bessis 1985, Handy *et al* 1988a, b).

Despite this, we discover that, for problems with complex energies, $E_I \neq 0$, the derivation of, as well as the actual, moment equation obtained from equation (1), are not the most efficient. A more efficient generation of the required u-moment equation can be derived by working within a broader framework involving three coupled differential equations for the probability density, $S(x)$, the kinetic energy density function, $P(x) \equiv |\Psi'(x)|^2$, and the probability current density, $J(x) = \frac{\Psi(x)\Psi'^*(x) - \Psi^*(x)\Psi'(x)}{2\mathrm{i}}$. The first two expressions are non-negative configurations. In particular cases, the probability current density will also be non-negative. This is discussed in section 2. However, this is not the immediate focus of this paper. Instead, it is to show how the realization of a non-negative, linear, differential representation for S leads to a very effective quantization procedure, capable of confirming the existence of symmetry breaking solutions.

Working within the coupled system of equations for $\{S, P, J\}$, one can generate many more moment constraints for the $E_I \neq 0$ case. It is in this sense that we say that the moment equation derived directly from equation (1) is 'incomplete', when $E_I \neq 0$. Generating as many moment constraints as possible speeds up the convergence rate of the bounds. However, as noted above, even if we work with the reduced set of moment constraints generated from equation (1), the bounds generated will converge to the unique physical answer, just more slowly.

Working directly with equation (1) leads to a complete set of moment equation constraints when $E_I = 0$. This is the case examined by Handy (2001), corresponding to the $P^2 + (\mathrm{i}X)^3$ problem (assuming real spectra, Handy (2001)). Application of EMM analysis in this case yielded impressive bounds for the first five energy levels (Handy 2001), as well as complex rotated versions of the Hamiltonian (Handy and Wang 2001).

The sensitivity of the EMM procedure, as evidenced by the excellent nature of these bounds, strongly suggest that Bessis' conjecture is more likely a consequence of some underlying algebraic identity than a more subtle analytic constraint.

Application of EMM to the more general case, $E_I \neq 0$, also yields very good bounds to the complex eigenenergies, as shown in this paper. We have implemented our bounding analysis up to a relatively low moment order. Our objective has been to affirm the S-EMM formalism's relevance as an effective bounding theory.

2. Derivation of the S-moment equation

We derive equation (1) in a manner different from that presented by Handy (2001). As noted previously, the present formalism is better suited for problems with $E_I \neq 0$.

Denote the Schrödinger equation by

$$H_x \Psi(x) = E\Psi(x) \tag{3}$$

where the normalized Hamiltonian is $H_x = -\epsilon\partial_x^2 + V(x)$, involving a complex potential, V, and complex energy, E. We make explicit the kinetic energy 'expansion' parameter, ϵ. As recognized by Handy (1981), within a moments representation, kinetic energy expansions become analytic. This will be an important component of the present theory. The following discussion assumes that ϵ is real and positive.

It is readily apparent that, if $V^*(-x) = V(x)$, and $\Psi(x)$ is a bound state with complex energy, E, then $\Psi^*(-x)$ is another bound state solution with energy E^*. Thus, complex roots come in complex conjugate pairs, for $\mathcal{PT}$ invariant Hamiltonians.

2.1. *The coupled differential equations for* $|\Psi(x)|^2$, $|\Psi'(x)|^2$, *and* $\frac{\Psi(x)\Psi'^*(x)-\Psi^*(x)\Psi'(x)}{2\mathrm{i}}$

Define the quantities $S(x) = |\Psi(x)|^2$, $P(x) = |\Psi'(x)|^2$, and $J(x) = \frac{\Psi(x)\Psi'^*(x)-\Psi^*(x)\Psi'(x)}{2\mathrm{i}}$. The expressions $\Sigma_1(x) \equiv \Psi^* H_x \Psi(x) + \text{c.c.}$, $\Delta_1(x) \equiv \Psi^* H_x \Psi(x) - \text{c.c.}$, and $\Sigma_2(x) \equiv \Psi'^* H_x \Psi(x) + \text{c.c.}$, satisfy (Handy and Wang 2001)

$$\Sigma_1(x) = \epsilon(2P(x) - S''(x)) + 2(V_R(x) - E_R)S(x) = 0 \tag{4}$$

$$\Sigma_2(x) = -\epsilon P'(x) + (V_R(x) - E_R)S'(x) - 2(V_I(x) - E_I)J(x) = 0 \tag{5}$$

and

$$-\frac{\mathrm{i}}{2}\Delta_1(x) = (V_I(x) - E_I)S(x) + \epsilon\partial_x J(x) = 0. \tag{6}$$

For the potential in question, $V(x) = \mathrm{i}x^3 + \mathrm{i}\alpha x$, if $S(x)$, $P(x)$, $J(x)$ form a solution set corresponding to energy (E_R, E_I), then $S(-x)$, $P(-x)$, $J(-x)$ is a solution set for energy $(E_R, -E_I)$.

In obtaining equation (1) (i.e. $\epsilon = 1$), we differentiate equation (4) and use equation (5) to substitute for P'. Upon dividing the resulting expression by $V_I - E_I$, and differentiating, we use equation (6) to substitute for J'. For future reference, we make this process explicit.

All of the physical configurations $\{S, P, J\}$ are implicitly assumed to be bounded and vanish at infinity. Thus

$$J(x) = -(\epsilon\partial_x)^{-1}\big((V_I(x) - E_I)S(x)\big) \tag{7}$$

where $\partial_x^{-1} \equiv \int_{-\infty}^{x} \mathrm{d}x_v$. In addition

$$P[S; x] = \frac{1}{2}S''(x) - \frac{1}{\epsilon}(V_R(x) - E_R)S(x). \tag{8}$$

We then obtain

$$-\epsilon^2\partial_x P[S(x); x] + \epsilon(V_R(x) - E_R)S'(x) + 2(V_I(x) - E_I)(\partial_x)^{-1}\big((V_I(x) - E_I)S(x)\big) = 0. \tag{9}$$

In order to transform this into equation (1), we simply apply the operator $\partial_x \frac{1}{V_I(x)-E_I}$, resulting in a fourth-order, linear, homogeneous, differential equation.

2.2. *The S-moment equation*

Let us denote by $\{u_p, v_p, w_p\}$ the Hamburger moments of the three functions S, P, J, respectively. Thus, $u_p \equiv \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p S(x)$, etc, for $p \geqslant 0$. For the present problem, $V_R = 0$,

and $V_I = x^3 + \alpha x$. Multiplying each of the three equations by x^p, and integrating by parts, yields

$$2\epsilon v_p - p(p-1)\epsilon u_{p-2} - 2E_R u_p = 0 \tag{10}$$

$$p\epsilon v_{p-1} + E_R p u_{p-1} - 2(w_{p+3} + \alpha w_{p+1} - E_I w_p) = 0 \tag{11}$$

and

$$(u_{p+3} + \alpha u_{p+1} - E_I u_p) - p\epsilon w_{p-1} = 0 \tag{12}$$

for $p \geqslant 0$. Note that from equation (10) (for $p = 0$) E_R must be positive.

We can convert this into a moment equation for the $\{u_p\}$ by using the first moment relation to solve for v_p in terms of the u. Likewise, taking $p \to p+1$ in the last moment relation determines w_p in terms of the u. Finally, substituting both relations in the second equation generates a moment equation for the u:

$$\begin{aligned}\epsilon^2\left(p - \frac{3p^2}{2} + \frac{p^3}{2}\right)u_{p-3} + 2p\epsilon E_R u_{(p-1)} - \frac{2E_I^2}{(p+1)}u_{p+1} + 2\alpha E_I\left(\frac{1}{p+1} + \frac{1}{p+2}\right)\\ \times u_{p+2} - \frac{2\alpha^2}{p+2}u_{p+3} + 2E_I\left(\frac{1}{p+1} + \frac{1}{p+4}\right)u_{p+4}\\ -2\alpha\left(\frac{1}{p+2} + \frac{1}{p+4}\right)u_{p+5} - \frac{2}{p+4}u_{p+7} = 0.\end{aligned} \tag{13}$$

This moment equation holds for all ϵ, including $\epsilon = 0$. In the latter case, upon multiplying the u-moment equation by $(p+1)(p+2)(p+4)$, the resulting relation (quadratic in p) incorporates the relation given in equation (12) for $\epsilon = 0$.

We note that the u-moment equation does not include one important additional moment constraint, that for the $p = 0$ relation in equation (12). This yields

$$u_3 + \alpha u_1 = E_I u_0. \tag{14}$$

Of course, this is the relation one obtains directly from the Schrödinger equation, upon multiplying it by $\Psi^*(x)$:

$$\int \mathrm{d}x\,(\epsilon P(x) + V(x)S(x)) = E\int \mathrm{d}x\,S(x) \tag{15}$$

and identifying the real and imaginary parts (the latter corresponding to equation (14)).

The recursive, linear, homogeneous, structure of the u-moment equation tells us that all of the moments are linearly dependent on the first seven moments $\{u_\ell | 0 \leqslant \ell \leqslant 6\}$. The additional constraint in equation (14) allows us to solve for u_3 in terms of u_0 and u_1. Thus, the reduced set of independent moments is $\{u_\ell | 0 \leqslant \ell \leqslant 2, 4 \leqslant \ell \leqslant 6\}$. These are referred to as the *missing moments*. In addition, we must impose a suitable normalization condition. The details are given in the next section.

There is an important theoretical point that must be stressed. The recursion relation in equation (13) is the moment equation resulting from integrating both sides of equation (9) by x^p. Both equations (9) and (1) are equivalent to each other, as explained above. However, the moment equation generated by equation (1) (refer to equations (47) and (51)) is different from equation (13), as explained in the appendix. It will involve one more degree of freedom (i.e. *missing moment* order) than equation (13). However, since equations (1) and (9) are equivalent, and Handy (2001) has argued that the only bounded and non-negative solutions are those corresponding to the physical configurations, application of EMM to either will result in converging bounds. Naturally, the moment equation involving fewer independent variables (i.e. *missing moments*) will yield faster converging bounds.

In addition, because equation (13) is the moment equation of equation (9), and similarly for equations (47), (51) and (1), any additional constraints, such as equation (14), are not required in order to generate converging bounds. Such constraints only improve the convergence rate of the bounds by reducing the number of independent, missing moment, variables.

From a different perspective, the manifest difference between equation (13) and equations (47) and (51) hinges on the fact that, in obtaining equation (1), we implicitly take $p \to p+1$ in equation (11). We note that this implies that equation (1) cannot generate the extra constraint $w_3 + \alpha w_1 - E_I w_0 = 0$, that is, the $p = 0$ relation from equation (13).

If $E_I = 0$, and the non-negative configurations $S(x)$ and $P(x)$ are symmetric, then these extra constraints (including equation (14)) are nonexistent. That is, equation (1) yields a complete set of moment constraints if $E_I = 0$.

The moment equations in equations (13) and (14) are the preferred relations (because they are easier to derive, and involve less missing moments), if $E_I \neq 0$.

We will work with the u-moment equation as given above, complemented by equation (14).

2.3. *The zeroth-order ϵ-contribution*

As previously noted, one of the most important reasons for working within a moments' representation is that it is analytic in ϵ.

If $\epsilon \neq 0$, there is equivalency between the sets of equations (10)–(12) and (13) and (14). When $\epsilon = 0$ (and thus $E_R = 0$), the w moments decouple from the u moments. We find that equations (13) and (14) include more solutions than those generated from equation (12). However, not all of these will be consistent with EMM quantization. One formal way of understanding this is to consider equation (9) when $\epsilon = 0$. We obtain

$$(V_I(x) - E_I)(\partial_x)^{-1}\big((V_I(x) - E_I)S^{(0)}(x)\big) = 0. \tag{16}$$

For real, bounded, configurations, $\{f(x), g(x)\}$, the integral $\int_{-\infty}^{+\infty} \mathrm{d}x\, f(x)(\partial_x)^{-1} g(x)$ becomes $\int_{-\infty}^{+\infty} \mathrm{d}x\, \big(((\partial_x)^{-1})^{\dagger} f(x)\big)\ g(x)$, where $((\partial_x)^{-1})^{\dagger} \equiv \int_x^{+\infty} \mathrm{d}x_v$. This follows from $\int_{-\infty}^{+\infty} \mathrm{d}x\, f(x) \int_{-\infty}^{x} \mathrm{d}x_v\, g(x_v) = \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{0} \mathrm{d}\xi\, f(x)\ g(\xi + x) = \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{0} \mathrm{d}\xi\, g(x) f(x-\xi) = \int_{-\infty}^{+\infty} \mathrm{d}x\, g(x) \int_x^{+\infty} \mathrm{d}x_v\, f(x_v)$.

Multiply equation (16) by $x^p R_\beta(x)$, where $R_\beta(x)$ is a regulating (bounded) function which reduces to unity when $\beta \to 0$. Integrating, and using $\big((\partial_x)^{-1}\big)^{\dagger}$, gives (i.e. in the $\beta \to 0$ limit)

$$((\partial_x)^{-1})^{\dagger}\big(x^{p+3} + \alpha x^{p+1} - E_I x^p\big) \to \frac{1}{p+4}x^{p+4} + \frac{\alpha}{p+2}x^{p+2} - \frac{E_I}{p+1}x^{p+1}. \tag{17}$$

This, in turn, upon multiplying by $(V_I(x) - E_I)S^{(0)}(x)$, and completing the x integration, gives the zeroth-order (in ϵ) moment relation in equation (13).

Therefore, the $\epsilon = 0$ moment equation in (13) (i.e. corresponding to equation (16)) tells us that

$$(V_I(x) - E_I)J^{(0)}(x) = 0. \tag{18}$$

This has the general, formal, solution $J^{(0)}(x) = \sum_\ell \mathcal{J}_\ell \delta(x - \tau_\ell)$, where the τ_ℓ are the turning points:

$$V_I(\tau_\ell(E)) = E_I. \tag{19}$$

The $\mathcal{J}_\ell$ are arbitrary. However, the $\epsilon = 0$ solution to equation (12) really corresponds to $J = 0$. We can (formally) argue this by applying $\partial_x (V_I(x) - E_I)^{-1}$ to equation (18), yielding

$$\partial_x J^{(0)}(x) = (V_I(x) - E_I)S^{(0)}(x) = 0 \tag{20}$$

which is the underlying configuration space relation corresponding to equation (12), for $\epsilon = 0$. The only possible, bounded, solution is $J = 0$.

Thus, the only solution to equation (13), for $\epsilon = 0$, consistent with the EMM quantization constraints (which demand boundedness and non-negativity), as discussed in the following section, should be that corresponding to $J^{(0)}(x) = 0$.

Consistent with the previous discussion, the $\epsilon = 0$ moment equations (10)–(12) yield $E_R = 0$:

$$w^{(0)}_{p+3} + \alpha w^{(0)}_{p+1} - E_I w^{(0)}_p = 0 \tag{21}$$

and

$$u^{(0)}_{p+3} + \alpha u^{(0)}_{p+1} - E_I u^{(0)}_p = 0 \tag{22}$$

for $p \geqslant 0$. The solution set to these are $u_p = \sum_\ell \mathcal{A}_\ell \tau_\ell^p$, and $w_p = \sum_\ell \mathcal{J}_\ell \tau_\ell^p$.

All of the (complex) turning points, for arbitrary E_I, contribute to the zeroth-order structure of $S(x)$.

2.4. The moment problem constraints

The moment problem conditions for non-negativity (Shohat and Tamarkin 1963) correspond to the inequalities

$$\int \mathrm{d}x \left(\sum_{n=0}^{N} C_n x^n \right)^2 S(x) \geqslant 0 \tag{23}$$

for $N < \infty$ and C_n arbitrary, real, variables. These are usually transformed into nonlinear (in the moments) Hankel–Hadamard (HH) determinantal inequalities, $\Delta_{0,N}(u) > 0$, where $\Delta_{0,N}(u) \equiv \mathrm{Det}\,(u_{i+j})$, and $0 \leqslant i, j \leqslant N$. However, we prefer their linear (in the moments) equivalent, corresponding to the quadratic form inequalities:

$$\sum_{n_1,n_2=0}^{N} C_{n_1} u_{n_1+n_2} C_{n_2} \geqslant 0. \tag{24}$$

These will be referred to as the linear HH non-negativity constraints.

The moment ('Hankel') matrix $u_{n_1+n_2}$ is linearly dependent on the *missing moments*, $\{u_0, u_1, u_2, u_4, u_5, u_6\}$, nonlinearly dependent on (E_R, E_I), and analytic with respect to ϵ. With respect to the following discussion, we note that, through an appropriate normalization prescription (as discussed in section 3), the missing moment variables will lie within a bounded, convex, domain.

The physical solution must satisfy all of the above constraints. To any finite order, N, if at a given energy value, $E = (E_R, E_I)$, there is a missing moment solution set, $\mathcal{U}_{N;E}$, then it must be convex. The EMM eigenenergy bounding procedure simply involves determining the energy subregions, $(E_R, E_I) \in \mathcal{R}_{N;j}$, for which $\mathcal{U}_{N;E}$ exists. The j-index enumerates the discrete states.

Based on the many applications of EMM over the last 16 years, one expects the $\mathcal{R}_{N;j}$ regions to be connected and bounded, although not necessarily convex. This is supported by our empirical results.

The boundary of the smallest rectangle containing $\mathcal{R}_{N;j}$ (i.e. $[E_R^{(L)}, E_R^{(U)}] \times [E_I^{(L)}, E_I^{(U)}] \supset \mathcal{R}_{N;j}$) defines the bounds for $(E_R, E_I) \in \mathcal{R}_{N;j}$. In practice, we numerically determine a slightly larger rectangle than this. Our numerical analysis will be based on the above relations. The following discussion addresses an interesting side issue that enhances our understanding of the above relations.

The numerically minded reader may wish to skip to section 3.

2.5. Simplification of the EMM constraints for non-negative $J(x)$

The HH inequalities are automatically satisfied by the atomic distribution $S(x) \to S^{(0)}(x) = \sum_\ell \mathcal{A}_\ell \delta(x - \tau_\ell)$, provided $\mathcal{A}_\ell \geqslant 0$. The zero equality is satisfied by polynomials, $P_{N;C}(x) \equiv \sum_{n=0}^{N} C_n x^n$ whose roots include all of the turning points, $P_{N;C}(x) = P_{N-3;\tilde{C}}(x) \times (V_I(x) - E_I)$.

For physical (non-atomic distribution) solutions, only the strict inequality can be satisfied. In this case, we can work with the relations

$$\int \mathrm{d}x \left(\sum_{j=0}^{N} \tilde{C}_n x^n \right)^2 (V_I(x) - E_I)^2 S(x) > 0. \tag{25}$$

Normally, one would prefer to work with such positive relations because they will not contain any zeroth-order ϵ dependence, thereby generating the positivity constraints that really contribute to quantization. However, in the present case, such inequalities are not independent of zeroth-order ϵ contributions.

Instead, as argued before, the zeroth-order structure of the moment equation in equation (13) is due to the probability current, J. However, we can only work with non-negativity constraints for the current, if it is non-negative.

If the probability current is non-negative, then

$$\int \mathrm{d}x \left(\sum_{j=0}^{N} C'_n x^n \right)^2 (V_I(x) - E_I)^2 J(x) \geqslant 0 \tag{26}$$

has no zeroth-order ϵ dependence. That is, from equation (18), all the zeroth-order terms are eliminated. This set of constraints is algebraically simpler than working with the analogue of equation (23), as applied to J, assuming $J \geqslant 0$.

2.6. Properties of the S, P, J equations and (minimal) conditions for J's positivity

We assume that $\epsilon > 0$, $E_R > 0$, and $V_R = 0$. The turning points satisfy $V_I(\tau_\ell) = E_I$. The following analysis is restricted to the real axis. We also assume that all of the configurations have analytic extensions into the complex x axis. Thus, $S(x) = \Psi(x)\Psi^*(x^*)$ is the analytic extension of $|\Psi(x)|^2$, etc. Since $V(x)$ is a regular function, the wavefunctions $\Psi(x)$ and $\Psi^*(x^*)$ are regular functions in the complex x plane; hence, so too are $S(x)$, $P(x)$, and $J(x)$.

Both S and P are non-negative. Because of their definitions, both S and P cannot be zero simultaneously, except at infinity (i.e. otherwise Ψ and Ψ' would be zero simultaneously, generating the trivial zero solution). When $S(x_o) = 0$, or $P(x_o) = 0$, then $\Psi(x_o) = 0$, or $\Psi'(x_o) = 0$, respectively; therefore, the probability current, J, is zero at all of the zeros of S and P.

It follows from the non-negativity of S that, if $S(x_o) = 0$, then these are extremal points, $S'(x_o) = 0$. The same holds for P.

Lemma 1. *If $S(x_o) = 0$, and $x_o \neq \tau$ (a real turning point), then J becomes negative in the neighbourhood of x_o.*

Since $S(x_o) = 0$, then $S'(x_o) = 0$, and $J(x_o) = 0$. From equation (6), $J'(x_o) = 0$. Differentiating equation (6) once, we obtain $J''(x_o) = 0$. Differentiating it a second time yields $-\epsilon J'''(x_o) = (V_I(x_o) - E_I)S''(x_o)$. From equation (4) $2P(x_o) = S''(x_o) \neq 0$. Thus, since $x_o \neq \tau$, it follows that $J'''(x_o) \neq 0$. That is, the local power series expansion for J becomes $J(x) = \frac{1}{6}J'''(x_o)(x - x_o)^3 + \mathrm{O}((x - x_o)^4)$.

Lemma 2. *If $J'(x_o) = 0$, and $x_o \neq \tau$, then J becomes negative in the neighbourhood of x_o.*

From equation (6) it follows that $S(x_o) = 0$ and lemma 1 applies.

Lemma 3. *If $(V_I(x) - E_I)$ is asymptotically monotonically increasing, with one real turning point, then $J(x) > 0$. $J(x)$ is strictly increasing for $x < \tau$, and strictly decreasing for $x > \tau$.*

By assumption, there is only one real turning point, τ. Also, $\lim_{x\to\pm\infty}(V_I(x)-E_I) = \pm\infty$. From equation (5) we have $(\epsilon P + E_R S)' = -2(V_I(x) - E_I)J(x)$; however, since S and P are asymptotically positive and decreasing to zero, we have $\lim_{x\to\pm\infty}(\epsilon P + E_R S)' = 0^{\mp}$. Accordingly, $\lim_{x\to\pm\infty} J(x) = 0^+$. It then follows that there must be two points (possibly the same), coming in from $-\infty$ and $+\infty$, where J has a positive local maximum. Denote these by $x_{o_1} \leqslant x_{o_2}$. At these points we have $J'(x_{o_{1,2}}) = 0$. If either of these points is not τ, then by lemma 2, we have a contradiction. Thus $x_{o_{1,2}} = \tau$, and $J(x)$ is strictly positive. Clearly, $J'(x) > 0$, for $x < \tau$, and $J'(x) < 0$, for $x > \tau$.

Lemma 4. *If $\alpha^3 + \frac{27}{4}E_I^2 > 0$, then $J(x) > 0$.*

Assume $V_I(x) = x^3 + \alpha x$. If $\alpha \geqslant 0$, then $V_I(x) - E_I$ satisfies the conditions of lemma 3. If $\alpha < 0$, then $V_I(x)$ will have a local maximum at $x_- = -(\frac{|\alpha|}{3})^{\frac{1}{2}}$, and a local minimum at $x_+ = -x_-$. At these locations, we have $V_I(x_-) = \frac{2}{3^{\frac{3}{2}}}|\alpha|^{\frac{3}{2}}$, and $V_I(x_+) = -V_I(x_-)$. If $E_I > V_I(x_-)$, or $E_I < V_I(x_+)$, then the conditions of lemma 3 are satisfied.

Lemma 5. *If $J(x) \geqslant 0$, then its local extrema must occur at the turning points.*

The local extrema correspond to $J'(x_o) = 0$. If $x_o \neq \tau$ (where there can be more than one real turning point), then according to lemma 2 we contradict the assumption that $J(x) \geqslant 0$. Thus, for non-negative J's, its zeros must coincide with the turning points.

Lemma 6. *$\epsilon P < E_R S$ within the local maxima regions of S, and $\epsilon P > E_R S$ within the local minima regions of S. They intersect at S's inflection points.*

This immediately follows from equation (4), $\epsilon P = E_R S + \frac{\epsilon}{2}S''$. We see that $\epsilon P(x)$ and $E_R S(x)$ intersect at the inflection points, $S''(x_i) = 0$. At infinity, since $\lim_{x\to\pm\infty} S''(x) = 0^+$, then $\lim_{x\to\pm\infty}(\epsilon P(x) - E_R S(x)) = 0^+$. Between any two successive extremas of $E_R S(x)$ there must be an intersection by $\epsilon P(x)$.

Lemma 7. *Let $(V_I - E_I)$ be asymptotically monotonically increasing, with one real turning point (τ). Let (x_1, x_2) be an interval whose endpoints correspond to successive extrema for S, where $S'(x_1) = S'(x_2) = 0$. If $(x_1, x_2) \subset (\tau, \infty)$, and $S(x)$ is increasing within the interval, then $P(x)$ must be monotonically decreasing within the interval, and vice versa (i.e. $S \leftrightarrow P$). When $(x_1, x_2) \subset (-\infty, \tau)$, then if S is decreasing within the interval, P must be monotonically increasing within the same interval, and vice versa.*

Under the conditions of the lemma, J is positive (by lemma 3); therefore, at any extremal value for S (i.e. $S'(x_o) = 0$), from equation (5), it follows that $\epsilon P'(x_o) = -2(V_I(x_o) - E_I)J(x_o)$. If $x_o > \tau$, then $(V_I(x_o) - E_I) > 0$, and we have that $P'(x_o) < 0$. Likewise, for S'. That is if $\tilde{x}_o > \tau$, and $P'(\tilde{x}_o) = 0$, then from equation (5) $E_R S'(\tilde{x}_o) = -2(V_I(\tilde{x}_o)-E_I)J(\tilde{x}_o) < 0$.

Let $\tau \leqslant x_1 < x_2$, and let (x_1, x_2) denote an open interval defined by two successive extremum points for S, within which S is increasing. It then follows that $P'(x)$ must be negative at each endpoint. However, P cannot have a local extremum within the interval, $P'(x_e) = 0$, since then $S'(x_e) < 0$, contradicting the assumptions made. Thus, P must be strictly decreasing within the closed interval $[x_1, x_2]$.

If $x_1 < x_2 \leqslant \tau$, then if (x_1, x_2) denotes an open interval on which S is decreasing ($x_{1,2}$ being two successive extremum points), then $P'(x)$ must be positive at each endpoint. P' must remain positive within the interval, otherwise at any internal extremum point, $S'(x_e) > 0$, contradicting the assumptions made.

From equation (5), under the conditions of lemma 3, then $\epsilon P(x) + E_R S(x)$ has only one extremum point, a global maximum, at the turning point.

Lemma 8. *If $P(x_o) = 0$, then $S(x)$ has a local maximum at x_o.*

If $P(x_o) = 0$, then $P'(x_o) = 0$ and $J(x_o) = 0$. From equation (5), $S'(x_o) = 0$. From equation (4) we have that $\epsilon S''(x_o) + 2E_R S(x_o) = 0$. This cannot be satisfied at any local minimum (since there, one has $S'' > 0$, and $S \geqslant 0$). We cannot have $S'' = 0$ and $S = 0$, since both S and P cannot be simultaneously 0. The only possibility is that x_o is a local maximum for S.

Lemma 9. *If $S(x_o) = 0$, then $P(x)$ has a local maximum at x_o.*

If $S(x_o) = 0$, then $S'(x_o) = 0$ and $J(x_o) = 0$. From equation (5), $P'(x_o) = 0$. From equation (6) $J'(x_o) = 0$. If we differentiate equation (5), $\epsilon P''(x_o) = -E_R S''(x_o)$. From equation (4), $2P(x_o) = S''(x_o) > 0$, therefore $P''(x_o) < 0$, corresponding to P having a local maximum at x_o.

The preceding lemmas do not shed any immediate resolution to the question as to when is $E_I = 0$. This is because they are mostly of a local nature and do not make use of the boundedness criteria, for physical solutions, other than lemmas 3 and 4. Nevertheless, these represent two important contributions.

A potentially significant question is, for what (α, E_R, E_I) values will the quantization of $J \geqslant 0$, through EMM, yield any results? The impact of J's non-negativity on the reality of E is presently under investigation.

For completeness, we note that, if $E_I = 0$, and V_I is asymptotically monotonic, with one zero point, then $J > 0$, as is evident from equation (6).

2.7. Additional properties

Let $V(x)$ be an arbitrary, $\mathcal{PT}$ invariant, potential: $V^*(-x) = V(x)$. For any bounded, complex, solution to the Schrödinger equation, $\Psi(x)$, with energy, E, the configuration $\Psi^*(-x)$ solves the same quantum problem but with eigenenergy E^*. This means that both $\{S(x), P(x), J(x)\}$ and $\{S(-x), P(-x), J(-x)\}$ solve equations (10)–(12) for (E_R, E_I) and $(E_R, -E_I)$, respectively. That is $\{u_p, v_p, w_p\} \leftrightarrow \{(-1)^p u_p, (-1)^p u_p, (-1)^p u_p\}$, satisfy the coupled moment equations (together with $(E_R, E_I) \leftrightarrow (E_R, -E_I)$).

There is another perspective on the above. The $\Psi^*(x)$ solves the equation

$$\epsilon \partial_x^2 \Psi^*(x) + V(x)\Psi^*(x) = -E^* \Psi^*(x). \tag{27}$$

Thus, we may regard $\Psi^*(x)$ as the solution to the Schrödinger equation upon taking $\epsilon \to -\epsilon$ (with eigenenergy $-E^*$). Similarly, $S(x), P(x), -J(x)$ solves equations (10)–(12) for $\epsilon \to -\epsilon$, $E_R \to -E_R$, and $E_I \to E_I$.

The EMM is an L^1 quantization theory which is analytic in ϵ. That is, bounded configurations are normalized according to L^1 integral relations (i.e. $\int \mathrm{d}x\, S(x) = 1$, etc) and not the usual L^2 conditions within the usual quantum mechanics Hilbert space formulation. In the present case, since we are working with $\{S, P, J\}$, our L^1 normalization coincides with the L^2 formulation of quantum mechanics, so long as $\epsilon \neq 0$. Within the usual quantum mechanical formalism, the eigenstates of the position operator (i.e. the translated Dirac delta function) are non-normalizable (within the L^2 norm). However, they are normalizable within the L^1 norm inherent to the EMM approach.

The final observation is that, upon performing the change of variables $y = \frac{x}{s}$, the Hamiltonian under consideration becomes

$$-\frac{\epsilon}{s^2}\partial_y^2 \Psi + \mathrm{i}(s^3 y^3 + \alpha s y)\Psi = E\Psi. \tag{28}$$

Dividing by s^3, we see that

$$E\left(\frac{\alpha}{s^2}, \frac{\epsilon}{s^5}\right) = \frac{E(\alpha, \epsilon)}{s^3}. \tag{29}$$

So it follows that, if $s = \epsilon^{\frac{1}{5}}$, then

$$E(\alpha, \epsilon) = \epsilon^{\frac{3}{5}} E\left(\frac{\alpha}{\epsilon^{\frac{2}{5}}}, 1\right). \tag{30}$$

3. EMM-numerical analysis of the $P^2 + \mathrm{i}X^3 + \alpha\mathrm{i}X$ Hamiltonian

The recursive, linear structure, of the u-moment equation in equation (13) can be written as (i.e. $\epsilon = 1$)

$$u_p = \sum_{\ell=0}^{6} \tilde{M}_{p,\ell}(E_R, E_I) u_\ell \tag{31}$$

for $p \geqslant 0$, where $\tilde{M}_{p,\ell}$ satisfies equation (13) with respect to the p index, as well as the initialization conditions $\tilde{M}_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_{1,2} \leqslant 6$.

These relations are supplemented by equation (14), written in the form $u_3 = E_I u_0 - \alpha u_1$. We can then substitute in the previous relation, obtaining

$$u_p = \sum_{\ell=0}^{6} M_{p,\ell} u_\ell \tag{32}$$

where

$$M_{p,\ell} = \begin{cases} \tilde{M}_{p,0} + E_I \tilde{M}_{p,3} & \ell = 0 \\ \tilde{M}_{p,1} - \alpha \tilde{M}_{p,3} & \ell = 1 \\ \tilde{M}_{p,2} & \ell = 2 \\ 0 & \ell = 3 \\ \tilde{M}_{p,\ell} & 4 \leqslant \ell \leqslant 6. \end{cases} \tag{33}$$

Since $M_{p,3} = 0$, we will work with the reduced set of independent moment variables $\nu_0 = u_0$, $\nu_1 = u_1$, $\nu_2 = u_2$, $\nu_3 = u_4$, $\nu_4 = u_5$ and $\nu_5 = u_6$. Thus

$$u_p = \sum_{\ell=0}^{5} \Omega_{p,\ell} \nu_\ell \tag{34}$$

where $\Omega_{p,\ell} = M_{p,\ell}$, for $0 \leqslant \ell \leqslant 2$, and $\Omega_{p,\ell} = M_{p,\ell+1}$, for $3 \leqslant \ell \leqslant 5$.

Finally, we define our normalization condition with respect to the even order u_p moments $\sum_{\ell=0}^{5} u_{2\ell} = 1$. Since each of these is positive, it ensures that the requisite linear programming analysis is done within the five-dimensional unit hypercube $[0, 1]^5$.

In order to impose this normalization condition, we invert the $\nu_\ell \leftrightarrow u_{2\ell}$ relation (i.e. $u_{2\ell} = \sum_{\ell_v=0}^{5} \Omega_{2\ell,\ell_v} \nu_{\ell_v}$, $0 \leqslant \ell \leqslant 5$):

$$\nu_\ell = \sum_{\ell_v=0}^{5} N_{\ell,\ell_v} u_{2\ell_v} \tag{35}$$

for $0 \leqslant \ell \leqslant 5$, and substitute into equation (34), $u_p = \sum_{\ell=0}^{5} \Omega_{p,\ell}\left(\sum_{\ell_v=0}^{5} N_{\ell,\ell_v} u_{2\ell_v}\right)$, obtaining

$$u_p = \sum_{\ell=0}^{5} \Gamma_{p,\ell} u_{2\ell} \tag{36}$$

Table 1. Bounds for the discrete states of $P^2 + \mathrm{i}X^3 + \mathrm{i}\alpha X$.

α	$P_{\max}$	$E_R^{(L)} < E_R < E_R^{(U)}$	$E_I^{(L)} < E_I < E_I^{(U)}$
-3	20	$0.7 < E_R < 1.7$	$0.4 < \pm E_I < 1.0$
-3	24	$1.10 < E_R < 1.45$	$0.5 < \pm E_I < 0.9$
-3	28	$1.20 < E_R < 1.23$	$0.72 < \pm E_I < 0.77$
-3	32	$1.219 < E_R < 1.230$	$0.756 < \pm E_I < 0.768$
-3	36	$1.224 < E_R < 1.228$	$0.758 < \pm E_I < 0.762$
-3	40	$1.225\,61 < E_R < 1.226\,08$	$0.759\,80 < \pm E_I < 0.760\,55$
-3		$1.225\,844$[a]	$0.760\,030$[a]
-2	20	$0.416 < E_R < 0.719$	$-0.5 < E_I < 0.5$
-2	24	$0.607 < E_R < 0.636$	$-0.03 < E_I < 0.03$
-2	28	$0.610 < E_R < 0.625$	$-0.5 \times 10^{-2} < E_I < 0.5 \times 10^{-2}$
-2	32	$0.619 < E_R < 0.625$	$-0.2 \times 10^{-2} < E_I < 0.2 \times 10^{-2}$
-2	36	$0.6203 < E_R < 0.6213$	$-0.45 \times 10^{-3} < E_I < 0.45 \times 10^{-3}$
-2	40	$0.620\,83 < E_R < 0.621\,05$	$-10^{-4} < E_I < 10^{-4}$
-2		$0.620\,9137$[a]	0[a]

[a] MRF formulation by Handy *et al* (2001a).

where $\Gamma_{p,\ell} = \sum_{\ell_v=0}^{5} \Omega_{p,\ell_v} N_{\ell_v,\ell}$. We now insert the normalization condition (i.e. solve for u_0 in terms of the first five even order moments), obtaining

$$u_p = \Gamma_{p,0} + \sum_{\ell=1}^{5} \left(\Gamma_{p,\ell} - \Gamma_{p,0}\right) u_{2\ell} \tag{37}$$

for $p \geqslant 0$. The linear programming EMM algorithm is implemented on these relations, within the context of equation (24), or the equivalent quadratic form counterpart to equation (25).

The numerical results of our analysis are given in table 1 for a selected number of α values, of interest within the asymptotic analysis by Delabaere and Trinh (2000). The reasons we do not quote more bounds, for more α values, is that the MRF analysis of Handy *et al* (HKWT, 2001a) is numerically faster, and yields results lying within the EMM bounds given here for the selected α values. This strongly suggests that the MRF analysis is correct. This is a good example of how the present 'bounding' method can be used to test other (generally much faster) estimation methods.

The MRF approach predicts that, for the lowest lying discrete states, there is a critical α value below which complex energies appear. This is given by

$$\alpha_{\text{critical}} = -2.611\,8094. \tag{38}$$

The data given in the tables (particularly table 2) is meant to test the reliability of this. It is clear that it does.

The bounds for the real and imaginary parts of the eigenenergies are very good. In the tables, $P_{\max}$ defines the maximum moment order used. That is, it is the total number of Hamburger moments used (i.e. $\{\mu_p | 0 \leqslant p \leqslant P_{\max}\}$). If the EMM procedure is applied to the $E_I = 0$ case (i.e. Handy (2001)), corresponding to symmetric $S(x)$'s, then the formalism converts to a Stieltjes moment representation which only involves the even order moments: $\{\mu_{2\rho} | 0 \leqslant \rho \leqslant P_{\max}^{(S)}\}$. Thus, a Hamburger moment order of $P_{\max}$, corresponds to a Stieltjes moment order of $P_{\max}^{(S)} = \frac{P_{\max}}{2}$. The tight bounds in Handy's original work (2001) required $P_{\max}^{(S)} = \mathrm{O}(60)$.

Our results (combined with those of HKWT (2001)) confirm the asymptotic estimates provided by Delabaere and Trinh. In particular, we can access regions in the α parameter space which were difficult within their formulation.

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

α	$P_{\max}$	$E_R^{(L)} < E_R < E_R^{(U)}$	$E_I^{(L)} < E_I < E_I^{(U)}$
−2.610	20	$0.517 < E_R < 1.920$	$-0.6 < E_I < 0.6$
−2.610	24	$0.940 < E_R < 1.800$	$-0.4 < E_I < 0.4$
−2.610	28	$1.083 < E_R < 1.586$	$-0.2 < E_I < 0.2$
−2.610	32	$1.211 < E_R < 1.361$	$-0.08 < E_I < 0.08$
−2.610	36	$1.211 < E_R < 1.360$	$-0.23 \times 10^{-1} < E_I < 0.23 \times 10^{-1}$
−2.610	40	$1.2135 < E_R < 1.2617$, $1.2617 < E_R < 1.3581$	$-0.5 \times 10^{-2} < E_I < 0.5 \times 10^{-2}$
−2.610	42	$1.2317 < E_R < 1.2367$, $1.3179 < E_R < 1.3356$	$-0.25 \times 10^{-2} < E_I < 0.25 \times 10^{-2}$
−2.610	42	1.234 216[a] and 1.332 059[a]	0[a]
−2.614	20	$0.515 < E_R < 1.925$	$-0.525 < E_I < 0.525$
−2.614	24	$0.953 < E_R < 1.808$	$-0.39 < E_I < 0.39$
−2.614	28	$1.083 < E_R < 1.589$	$-0.12 < E_I < 0.12$
−2.614	32	$1.238 < E_R < 1.326$	$0.01 < \pm E_I < 0.11$
−2.614	36	$1.256 < E_R < 1.309$	$0.030 < \pm E_I < 0.065$
−2.614	40	$1.278 < E_R < 1.286$	$0.050 < \pm E_I < 0.065$
−2.614	40	1.282 333[a]	0.053 8739[a]

[a] MRF formulation by Handy *et al* (2001a).

The numerical implementation given, of the present formalism, is meant to suggest the power of the method. Our intention is not to present an exhaustive numerical analysis over a wide range of parameter values.

3.1. Basic algebraic structure of the u-moments

Upon using equation (14) to solve for u_3 in terms of $u_{0,1}$, and incorporating this into the moment recursion equation in equation (13), we obtain

$$u_8 = \left(\frac{25\alpha E_I^2}{6} + 5\epsilon E_R\right) u_0 - \frac{25\alpha^2 E_I}{6} u_1 - \frac{5E_I^2}{2} u_2 - \frac{5\alpha^2}{3} u_4 + \frac{7E_I}{2} u_5 - \frac{8\alpha}{3} u_6 \tag{39}$$

and

$$u_{10} = \left(-\frac{31\alpha^2 E_I^2}{2} + \frac{21\epsilon^2}{2} - 12\alpha\epsilon E_R\right) u_0 + \left(\frac{31\alpha^3 E_I}{2} - 11E_I^3\right) u_1 + \left(\frac{45\alpha E_I^2}{2} + 21\epsilon E_R\right) u_2 + \left(4\alpha^3 + 12E_I^2\right) u_4 - \frac{27\alpha E_I}{2} u_5 + 5\alpha^2 u_6. \tag{40}$$

In obtaining equation (36), we must invert the relationship $\{u_8, u_{10}\} \leftrightarrow \{u_1, u_5\}$. This takes on the form

$$\begin{pmatrix} u_8 - R_8[u_0, u_2, u_4, u_6] \\ u_{10} - R_{10}[u_0, u_2, u_4, u_6] \end{pmatrix} = \begin{pmatrix} -\frac{25\alpha^2 E_I}{6}, \frac{7E_I}{2} \\ \frac{31\alpha^3 E_I}{2} - 11E_I^3, -\frac{27\alpha E_I}{2} \end{pmatrix} \begin{pmatrix} u_1 \\ u_5 \end{pmatrix} \tag{41}$$

where $R_{8,10}$ denote the remainder terms in the previous relations. The determinant of the above matrix is

$$\mathrm{Det}\,(E_I) \equiv \left\| \begin{pmatrix} -\frac{25\alpha^2 E_I}{6}, \frac{7E_I}{2} \\ \frac{31\alpha^3 E_I}{2} - 11E_I^3, -\frac{27\alpha E_I}{2} \end{pmatrix} \right\| = 2\alpha^3 E_I^2 + \frac{77}{2} E_I^4. \tag{42}$$

Accordingly,

$$\begin{pmatrix} u_1 \\ u_5 \end{pmatrix} = \frac{1}{\mathrm{Det}\,(E_I)} \begin{pmatrix} -\frac{27\alpha E_I}{2}, -\frac{7E_I}{2} \\ -(\frac{31\alpha^3 E_I}{2} - 11E_I^3), -\frac{25\alpha^2 E_I}{6} \end{pmatrix} \begin{pmatrix} u_8 - R_8[u_0, u_2, u_4, u_6] \\ u_{10} - R_{10}[u_0, u_2, u_4, u_6] \end{pmatrix}. \tag{43}$$

Thus, when $\mathrm{Det}\,(E_I) = 0$, the even order moments $\{u_0, u_2, u_4, u_6, u_8, u_{10}\}$ are constrained to satisfy two additional relations. That is, the effective dimension of the system drops from

$6 \to 5$ (before imposing a normalization constraint). The impact of this on the EMM bounds is unclear, at the present time. However, a convenient feature is that Det $(E_I) \geqslant 0$, under the conditions of lemma 4.

4. Conclusion

We have presented a non-negativity representation formalism, amenable to the EMM for generating converging bounds to the (complex) discrete eigenenergies of one-dimensional, $\mathcal{PT}$ invariant Hamiltonians. Our analysis was presented within the specific context of the $H_\alpha = P^2 + \mathrm{i}x^3 + \mathrm{i}\alpha x$ Hamiltonian, previously analysed by Delabaere and Trinh. Our formalism readily confirms (numerically) the existence of both symmetry breaking solutions and symmetry invariant solutions. The preliminary results given have focused on the properties of the low lying states near the first symmetry breaking bifurcation point, with respect to the α parameter, as predicted by the MRF eigenenergy estimation method of Tymczak *et al* (1998a, b). Our preliminary, yet highly accurate, numerical results are consistent with the asymptotic analysis methods of Delabaere and Trinh.

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5. Appendix. EMM analysis of equation (1)

In this section we focus on the structure of equation (1) and the moment equation resulting from it. This is not the most efficient approach, as indicated earlier. Instead, it is best to derive the moment equation for S by first working with the coupled S, P, J equations, deriving the corresponding coupled moment equations, and then reducing these to one moment equation for S. Nevertheless, for the sake of completeness, we outline the issues that need to be addressed if one wants to go from equation (1) directly to a moment equation.

The fourth-order equation for the $p^2 + \mathrm{i}x^3 + \alpha \mathrm{i}x$ Hamiltonian is

$$\frac{1}{\Lambda(x)} S^{(4)}(x) + \frac{\alpha + 3x^2}{\Lambda^2(x)} S^{(3)}(x) + \frac{4E_R}{\Lambda(x)} S^{(2)}(x) + + \frac{4E_R(\alpha + 3x^2)}{\Lambda^2(x)} S^{(1)}(x) - 4\Lambda(x) S(x) = 0 \tag{44}$$

where $\Lambda(x) = E_I - x(\alpha + x^2)$.

The function coefficient $\frac{1}{\Lambda(x)}$ introduces singularities on the physical domain, $\Lambda(\tau) = 0$. However, all of the solutions to equation (44) will be regular (Handy 2001). These roots are the effective 'turning points' of the differential equation. They satisfy

$$\tau^3 + \alpha\tau = E_I. \tag{45}$$

The extremal points of the function $V_I(x) \equiv x^3 + \alpha x$ satisfy $x_e^2 = -\frac{\alpha}{3}$.

If $\alpha \geqslant 0$, then there is only one real root to equation (45). If $\alpha < 0$, then there could be one or three roots, depending on E_I. That is, $x_e^{(\pm)} = \pm\sqrt{\frac{|\alpha|}{3}}$ and $V_I(x_e^{(\pm)}) = \mp\beta$, where $\beta \equiv \frac{2|\alpha|^{\frac{3}{2}}}{3\sqrt{3}}$. If $|E_I| \leqslant \beta$, or $|E_I| \leqslant 0.3849|\alpha|^{\frac{3}{2}}$, then there are three roots.

It is best to translate equation (44) to any one of the real τ roots, in order to simplify the structure of the ensuing moment equation. Therefore, we will work with the translated variable, $\xi = x - \tau$. Let us define the power moments

$$\mu_p = \int_{\mathcal{C}} \mathrm{d}\xi\, \xi^p S(\xi) \tag{46}$$

where $\mathcal{C}$ is a contour in the complex ξ plane that sits on top of the real ξ axis and deviates around the origin. Since all the solutions (physical or not) to equation (44) are regular in ξ, we see that, if $p \geqslant 0$, then for the physical solutions, we can deform the $\mathcal{C}$ contour to be identical to the real ξ axis. If $p < 0$, we cannot do this, and must retain $\mathcal{C}$. The $p \geqslant 0$ power moments are referred to as the Hamburger moments.

We note that $\Lambda(\xi) = \xi\Upsilon(\xi)$, where $\Upsilon(\xi) = 3\tau^2 - \alpha + 3\tau\xi + \xi^2$. If there are three, real, τ roots, then $\Upsilon(\xi)$ has two zeros along the real axis. If there is only one τ root, then Υ has no zeros along the real axis.

Multiplying equation (44) (translated by an amount τ) by $\xi^p(\Lambda(\xi))^2$, and integrating by parts over the contour $\mathcal{C}$, we obtain a moment equation valid for $-\infty < p < +\infty$:

$$\begin{aligned}
-(3\tau^2+\alpha)p(4-4p-p^2+p^3)\mu_{p-3} - 3\tau p(-4-p+4p^2+p^3)\mu_{p-2} \\
-p(p+2)(6+12\tau^2E_R+4\alpha E_R+7p+p^2)\mu_{p-1} \\
-12\tau E_R(4+5p+p^2)\mu_p - 4E_R(12+8p+p^2)\mu_{p+1} \\
+0\mu_{p+2} + 4(3\tau^2+\alpha)^3\mu_{p+3} + 36\tau(3\tau^2+\alpha)^2\mu_{p+4} \\
+12(36\tau^4+15\alpha\tau^2+\alpha^2)\mu_{p+5} + 36(9\tau^3+2\tau\alpha)\mu_{p+6} \\
+(144\tau^2+12\alpha)\mu_{p+7} + 36\tau\mu_{p+8} + 4\mu_{p+9} = 0.
\end{aligned} \tag{47}$$

As argued by Handy and Wang (2001), as well as Handy *et al* (2001b), in order for EMM to yield converging bounds, it is important that the proper (Hamburger) moment equation uniquely corresponds to the desired system. Let us represent equation (44) as $\mathcal{O}_\xi S(\xi) = 0$. Now consider a more general problem corresponding to $\mathcal{O}_\xi S(\xi) = \mathcal{D}(\xi)$, where the inhomogeneous term corresponds to a distribution-like expression, supported at the zeros of $\Lambda(\xi)$. When we multiply this system by $\Lambda(\xi)^2$, the corresponding inhomogeneous term can (effectively) disappear. If one is not careful, and solely restricts the moment index to non-negative values, then the resulting moment equation cannot distinguish between the desired problem (corresponding to $\mathcal{D} = 0$) and those for which $\mathcal{D} \neq 0$. In such cases, the EMM algorithm will not generate any bounds.

In order to ensure that our moment equation refers to $\mathcal{D} = 0$, we must work with the moment equation evaluated for $p \geqslant -2$, which represents the most singular function coefficient remaining after equation (44) is multiplied by $\Upsilon(\xi)$. In the work by Handy and Wang (2001), the moment equation for $p = -2, -1$ yielded additional constraints for the Hamburger moments. The same is true in the present case. Thus, the moment equation for $p = -2$ becomes

$$\begin{aligned}
4(3\tau^2+\alpha)^3\mu_1 + 36\tau(3\tau^2+\alpha)^2\mu_2 + 12(36\tau^4+15\alpha\tau^2+\alpha^2)\mu_3 \\
+36(9\tau^3+2\tau\alpha)\mu_4 + (144\tau^2+12\alpha)\mu_5 + 36\tau\mu_6 + 4\mu_7 = \Sigma(\mu_{-2}, \mu_{-4})
\end{aligned} \tag{48}$$

where

$$\Sigma(\mu_{-2}, \mu_{-4}) = -(24\tau E_R\mu_{-2} + 36\tau\mu_{-4}). \tag{49}$$

The moment equation for $p = -1$ becomes

$$\begin{aligned}
-20E_R\mu_0 + 4(3\tau^2+\alpha)^3\mu_2 + 36\tau(3\tau^2+\alpha)^2\mu_3 + 12(36\tau^4+15\alpha\tau^2+\alpha^2)\mu_4 \\
+36(9\tau^3+2\tau\alpha)\mu_5 + (144\tau^2+12\alpha)\mu_6 + 36\tau\mu_7 + 4\mu_8 \\
= \frac{(\alpha+3\tau^2)}{6\tau}\Sigma(\mu_{-2}, \mu_{-4}).
\end{aligned} \tag{50}$$

By combining the previous two relations, we can express μ_8 in terms of the Hamburger moment $\{\mu_0, \mu_1, \ldots, \mu_7\}$:

$$4\mu_8 + \left(34\tau - \frac{2\alpha}{3\tau}\right)\mu_7 + (6\alpha + 126\tau^2)\mu_6 + \left(252\tau^3 + 42\alpha\tau - \frac{2\alpha^2}{\tau}\right)\mu_5 + 90\tau^2 V_I'(\tau)\mu_4 - 2(\alpha - 6\tau^2)\frac{(V_I'(\tau))^2}{\tau}\mu_3 - 2(V_I'(\tau))^3\mu_2 - \frac{2}{3\tau}(V_I'(\tau))^4\mu_1 - 20E_R\mu_0 = 0. \tag{51}$$

This is an important additional constraint on the Hamburger moments, as noted in the work by Handy and Wang (2001). Since the only bounded and positive solutions to equation (44) are the physical solutions, EMM will work directly on the moment equation in equation (47) supplemented by the above relation (which is essential, otherwise no bounds will be generated).

The EMM numerical implementation of the above would involve (for fixed α) using τ as the variable parameter (and then computing E_I from equation (45)), in addition to E_R. Of course, this means that, for some τ values, one would be recovering the same E_I (i.e. those satisfying the condition $|E_I| < \beta$, defined previously); however, since the EMM procedure is invariant under affine maps, this is just a redundancy. In this manner, bounds on τ (or, equivalently, E_I) and E_R would be generated. Our actual numerical results confirm this, and are consistent with the bounds quoted in the tables.

We can enhance the above by including an additional constraint corresponding to equation (14). This is obtained as follows. From the Schrödinger equation, we know that $E = \frac{\int |\Psi'(x)|^2 + \mathrm{i}\int (x^3+\alpha x)S(x)}{\int S(x)}$, or (with respect to the imaginary part of the energy)

$$E_I = \frac{\int ((\xi+\tau)^3 + \alpha(\xi+\tau))S(\xi)}{\int S(\xi)} \tag{52}$$

which reduces to (i.e. from equation (45))

$$\mu_3 + 3\tau\mu_2 + (3\tau^2 + \alpha)\mu_1 = 0. \tag{53}$$

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