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Moment problem quantization within a generalized scalet-Wigner (auto-scaling) transform representation

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Abstract

For one-dimensional Schrödinger quantum systems, the correlation expression $S(x,\tau,a) \equiv \Psi^*\left(x-\frac{\tau}{2}/a\right)\Psi\left(x+\frac{\tau}{2}\right)$ satisfies a fourth-order linear differential equation with regard to x. This generalizes the result previously derived by Handy (2001 *J. Phys. A: Math. Gen.* **34** L271), and Handy and Wang (2001 *J. Phys. A: Math. Gen.* **34** 8297), with regard to $S(x,0,1)$. We are then able to incorporate this within a generalized Wigner transform representation, through the use of scalets (Handy C R and Brooks H A 2001 *J. Phys. A: Math. Gen.* **34** 3577). Energy quantization is achieved through a moment problem positivity analysis (focusing on the moments of the probability density, $|\Psi|^2$) at $a=1$, $\tau=0$. The wavefunction, Ψ, is then generated through a multiscale analysis proceeding from the unity scale, extended into the zero scale limit. The power moments, $\mu_p = \int \mathrm{d}x\, x^p \Psi(x)$, can be generated through a similar procedure. We present the general formalism and apply it to the $(\mathrm{i}x)^3$ potential.

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1. Introduction

In a series of recent works, Handy (2001a, 2001b) and Handy and Wang (2001) showed how the one-dimensional Schrödinger equation, for arbitrary (complex) potential ($V(x) = V_R(x) + \mathrm{i}V_I(x)$), could be transformed into a fourth-order, linear, ordinary differential equation for the probability density, $S(x) \equiv |\Psi(x)|^2$, of the form

$$-\frac{1}{V_I - E_I} S^{(4)}(x) - \left(\frac{1}{V_I - E_I}\right)' S^{(3)}(x) + 4\left(\frac{V_R - E_R}{V_I - E_I}\right) S^{(2)}(x) + \left[4\left(\frac{V_R - E_R}{V_I - E_I}\right)' + 2\frac{V_R'}{V_I - E_I}\right] S^{(1)}(x) + \left(4(V_I - E_I) + 2\left(\frac{V_R'}{V_I - E_I}\right)'\right) S(x) = 0. \tag{1}$$

Within this representation, the discrete states are uniquely positive and bounded, allowing the implementation of the eigenvalue moment method (EMM), as developed by Handy *et al* (1988), which quantizes through the generation of converging lower and upper bounds to the desired (complex) eigenenergy, $E = E_R + \mathrm{i}E_I$.

In general, moment-based quantization methods are capable of producing high-accuracy results, of relevance to strong coupling/singular perturbation type (linear) systems, including those with multiple singular regions (i.e. turning points, etc). The EMM does this through the generation of tightly converging eigenenergy bounds; however, the wavefunction cannot be recovered. Another very successful method, the multiscale reference function (MRF) approach, can generate impressively high-accuracy results (Tymczak *et al* 1998a, 1998b, Handy *et al* 2001). However, it may be too slowly convergent in recovering the local structure of the wavefunction. Our principal objective in this work is to show how a positivity representation, combined with EMM analysis, can be used to generalize the formalism in equation (1) so as to recover the wavefunction. Our formalism also has a strong overlap with the Wigner transform representation. We comment on this below, although we will not develop this relationship, fully, here.

The EMM approach works within a moment equation representation for equation (1), involving the power moments of the probability density,

$$U_q \equiv \int \mathrm{d}x\, x^q S(x). \tag{2}$$

In principle, we are interested in generating both the wavefunction, $\Psi(x)$, and its power moments,

$$\mu_q = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^q \Psi(x) \tag{3}$$

from knowledge of the set of moments, $\left\{U_q \equiv \int \mathrm{d}x\, x^q |\Psi(x)|^2\right\}$.

Consider the correlation type, wavefunction product:

$$S(x,\tau,\alpha) = \Psi^*\left(\alpha\left(x - \frac{\tau}{2}\right)\right)\Psi\left(x + \frac{\tau}{2}\right) \tag{4}$$

where $\alpha > 0$ corresponds to an inverse scale, $\alpha \equiv \frac{1}{a}$. So far as our ultimate objective is to analyse these structures with regard to real α values, the above definition is suitable; however, questions of analyticity with respect to α should be made with regard to $S^*(x,\tau,\alpha)$, which will generally admit a complex extension into the α-complex plane.

Two important results follow. The first is that $S(x,\tau,\alpha)$ satisfies a linear differential equation with respect to the x dependence, thereby generalizing equation (1). Because of this, the corresponding power moments,

$$U_q(\tau,\alpha) = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^q S(x,\tau,\alpha) \tag{5}$$

admit a recursive, linear, moment equation, with respect to the q-index, of order $1 + m_s$ (which is problem dependent). This takes on the form

$$U_q(\tau,\alpha) = \sum_{\ell=0}^{m_s} M_{q,\ell}(\tau,\alpha,E)U_\ell(\tau,\alpha) \qquad q \geqslant 0 \tag{6}$$

where the energy-dependent coefficients, $M_{q,\ell}(\tau,\alpha,E)$, are known. At each scale value, the first $1 + m_s$ moments, $\{U_\ell(\tau,\alpha)|0 \leqslant \ell \leqslant m_s\}$, otherwise referred to as the *missing moments*, generate all the other moments.

The second important result is that the first-order derivative of the $U_q(\tau,\alpha)$ moments, with respect to the a-variable (or inverse scale, α), can be expressed as a linear combination of the missing moments. Thus, one can generate a *scalet*-like equation (Handy and Brooks 2001), corresponding to a finite set of coupled, linear, differential equations (for the missing moments) of first order in α. The scalet equation is symbolized by

$$\partial_\alpha U_{\ell_1}(\tau,\alpha) = \sum_{\ell_2=0}^{m_s} \mathcal{M}_{\ell_1,\ell_2}(\tau,\alpha,E) U_{\ell_2}(\tau,\alpha) \qquad 0 \leqslant \ell_1 \leqslant m_s. \tag{7}$$

There will also be another scalet equation with respect to the τ direction:

$$\partial_\tau U_{\ell_1}(\tau,\alpha) = \sum_{\ell_2=0}^{m_s} \mathcal{N}_{\ell_1,\ell_2}(\tau,\alpha,E) U_{\ell_2}(\tau,\alpha) \qquad 0 \leqslant \ell_1 \leqslant m_s. \tag{8}$$

Our computational implementation will explicitly derive the form for $\mathcal{M}$ and $\mathcal{N}$, for a particular potential.

At $\tau = 0, a = 1$, the $U_q(0,1)$ moments become the power moments of the probability density, as symbolized by equation (2). We can then use EMM to determine the physical energy and all the $U_\ell(0,1)$ missing moments (after imposing an appropriate normalization condition).

Having solved the problem at $\tau = 0, a = 1$, we then use equation (8) to generate the $U_\ell(\tau,1)$ moments, over any desired τ region. Finally, using these moment configurations, equation (7) can be integrated either in the zero scale limit, generating the wavefunction, or in the infinite scale limit, generating the μ_ℓ, as detailed below.

In the zero scale limit, provided $\mu_0^* \equiv \int \mathrm{d}x\, \Psi^*(x) \neq 0$, we recover the wavefunction through the asymptotic relation (i.e. translate by $x \to x + \frac{\tau}{2}$, perform the change of variables $y \equiv \frac{x}{a}$ and expand the integral $\int \mathrm{d}y\, a\left(ay + \frac{\tau}{2}\right)^q \Psi^*(y)\Psi(ay+\tau)$ in powers of a):

$$\text{Zero scale limit}: \begin{cases} \lim_{a\to 0} \left(\dfrac{U_q(\tau,a)}{a\left(\frac{\tau}{2}\right)^q \mu_0^*} \right) = \Psi(\tau) \qquad \forall\tau \quad \text{if} \quad q=0 \quad \text{or} \quad \tau \neq 0 \quad \text{if} \quad q \neq 0 \\ \lim_{a\to 0} \left(\dfrac{1}{a^{1+q}} U_q(0,a) \right) = \mu_q^* \Psi(0) \qquad \text{if} \quad \tau = 0. \end{cases} \tag{9}$$

Since we implicitly impose a normalization at scale value $a = 1$, through the EMM procedure, the above limit expressions only generate the wavefunction up to a uniform factor (i.e. it will not necessarily be normalized to a global probability of unit value).

We can also generate the wavefunction's power moments by studying the infinite scale limit, provided $\Psi^*(0) \neq 0$. That is

$$\lim_{a\to\infty} \left(\frac{1}{\Psi^*(0)} U_q(0,a) \right) = \mu_q. \tag{10}$$

Again, because of the implicit EMM normalization at scale $a = 1$, the power moments, μ_q, are generated up to a normalization factor.

The extension of the preceding relations for the cases $\mu_0 = 0$ and $\Psi(0) = 0$ can be derived, and will be discussed elsewhere.

From the above relations, it is clear that the expression in (4) is equivalent to having the wavefunction become its own scaling function (i.e. auto-scaling), in the spirit of the analysis outlined in the work of Handy and Murenzi (1996–1999).

In the recent works by Handy and Murenzi (HM) (Handy and Murenzi 1996, 1997, 1998, 1999), they developed a *scalet* formalism for generating the wavefunction. This procedure is identically equivalent to the, multiscale, continuous wavelet theory formalism of Grossmann and Morlet (1984), although more efficient and accurate, for low-dimensional systems. Consistent with the wavelet philosophy, scalet analysis defines a procedure for efficiently generating the local properties of the wavefunction, based on integrating over all scale contributions. In this approach, one generates the local properties of a wavefunction, at a given point, through a systematic multiscale procedure which incorporates all scale contributions at the same point (within the scalet representation), or alternatively, at all other points as well (within the wavelet representation). Although such approaches are more expensive, computationally, than conventional (i.e. numerical integration) methods, it can offer greater numerical stability and accuracy. We explain this below.

Consider a one-dimensional problem with multi-singular regions (Bender and Orszag 1978). In order to generate the wavefunction, conventionally, one must successfully integrate through each of the contributing singular regimes. The scalet–wavelet analysis does not require this. Instead, the wavefunction is generated by systematically determining how the larger scale structure affects the smaller scale behaviour, recursively. Doing this, at any desired point, eventually recovers the local structure of the wavefunction, at that point, in the zero scale limit. In this approach, generation of the wavefunction, at a given point, is explicitly independent of the wavefunction's value at any other point. Clearly, although greater computation is required, this approach is potentially more accurate than conventional numerical integration schemes, for the reasons stated.

The HM analysis involves the non-local, integral, expressions $\mathcal{U}_q(\tau, a) \equiv \int \mathrm{d}x\, x^q \mathcal{S}\big(\frac{\tau - x}{a}\big)\Psi(x)$, where the scaling function, $\mathcal{S}$, is a known function (i.e. Gaussians, etc). For this reason, these are referred to as *scalets*.

Presently (*scalet-Wigner* analysis), we are taking the scaling function to be the wavefunction itself (although, clearly, it is not known *a priori*).

The HM scalets satisfy a differential scalet equation with regard to the inverse scale variable, α. The scalet equation is to be regarded as an initial value problem, where specification of the starting scale configuration, $\mathcal{U}_q(\tau, \alpha = 0)$, is then used to recover the wavefunction through relations similar to those in equation (9). The infinite scale, scalet, configurations, $\mathcal{U}_q(\tau, \alpha = 0)$, are linearly dependent on the power moments of the wavefunction, $\{\mu_q\}$. These can be obtained, in turn, by various moment quantization methods such as the multiscale reference function method, or EMM theory (for the ground state case). Excellent results were always obtained using this procedure, for arbitrary, one-dimensional, rational fraction potential systems (Handy and Murenzi 1996, 1997, 1998, 1999).

As stated, we wish to duplicate this procedure but in terms of the $U_q(\tau, \alpha)$ moments.

In the following sections, we illustrate the above formalism with respect to the important non-Hermitian potential problem defined by $V(x) = \mathrm{i}x^3$. As originally argued by Bender and Boettcher (2001), and subsequently confirmed by many other investigators such as Dorey *et al* (2001a, 2001b), including the relevant works by Handy (2001a, 2001b), Handy and Wang (2001) and Handy *et al* (2001), the discrete states have real eigenenergies ($E = E_R$).

For generating the scalet equations in the α and τ directions, we will make use of the relations (i.e. first translate by $x \rightarrow x + \frac{\tau}{2}$):

$$\partial_\tau U_q(\tau, \alpha) = \frac{q}{2} U_{q-1}(\tau, \alpha) + W_q(\tau, \alpha) \tag{11}$$

where

$$W_q(\tau, \alpha) = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^q J(x, \tau, \alpha) \tag{12}$$

is the moment of the configuration

$$J(x, \tau, \alpha) \equiv \Psi^*\left(\alpha\left(x - \frac{\tau}{2}\right)\right)\Psi'\left(x + \frac{\tau}{2}\right). \tag{13}$$

The W_q moments will be shown to be linearly dependent on the U-scalets. Using this relationship, we transform equation (11) into a U-scalet differential equation in the τ direction.

Integration in the τ direction, for $\alpha = 1$, generates the starting scalet configuration necessary for recovering the wavefunction (equation (9)) or its moments (equation (10)).

A differential relation ensues in the α direction from the relation (i.e. take $x \to x + \frac{\tau}{2}$, $\partial_\alpha \Psi^*(\alpha x) = \frac{x}{\alpha}\partial_x \Psi^*(\alpha x)$, and then integrate by parts)

$$\partial_\alpha U_q(\tau,\alpha) = -\frac{1}{\alpha}\int \mathrm{d}x\ \Psi^*(\alpha x)\partial_x \left(x\left(x+\frac{\tau}{2}\right)^q \Psi(x+\tau)\right) \tag{14}$$

or

$$-\alpha\partial_\alpha U_q(\tau,\alpha) = (q+1)U_q(\tau,\alpha) - \frac{q\tau}{2}U_{q-1}(\tau,\alpha) + W_{q+1}(\tau,\alpha) - \frac{\tau}{2}W_q(\tau,\alpha). \tag{15}$$

Substituting the linear W–U relationship alluded to the above (and to be derived in the following sections), we can convert equation (15) into equation (7).

These are the basic relations enabling the present scalet-Wigner formulation.

For completeness, we note that the Wigner transform of the wavefunction, Ψ, is given by (Wigner 1932, Cohen 1989)

$$W(x,k) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\tau\ \Psi^*\left(x-\frac{\tau}{2}\right)\Psi\left(x+\frac{\tau}{2}\right)\mathrm{e}^{-\mathrm{i}k\tau}. \tag{16}$$

It defines a two-dimensional *phase-space* extension of the one-dimensional quantum system, and has been extensively investigated and exploited, over the last seven decades in the study of both quantum systems and signal processing. A related expression is the *ambiguity function*,

$$A(\eta,\tau) = \int_{-\infty}^{+\infty} \mathrm{d}u\ \Psi^*\left(u-\frac{\tau}{2}\right)\Psi\left(u+\frac{\tau}{2}\right)\mathrm{e}^{\mathrm{i}\eta u} \tag{17}$$

which is the inverse Fourier transform of the Wigner transform:

$$A(\eta,\tau) = \int\int \mathrm{d}x\,\mathrm{d}k\ \exp(\mathrm{i}\eta x + \mathrm{i}\tau k)W(x,k). \tag{18}$$

Our formalism generalizes the above definition by introducing an explicit scale variable, a:

$$A(\eta,\tau,a) = \int_{-\infty}^{+\infty} \mathrm{d}u\ \Psi^*\left(\frac{u-\frac{\tau}{2}}{a}\right)\Psi\left(u+\frac{\tau}{2}\right)\mathrm{e}^{\mathrm{i}\eta u}. \tag{19}$$

Within the context of one-dimensional, rational fraction potential, bound state problems, it is more natural to work with power moments. For bound state configurations, the ambiguity transform (Wigner transform) will usually be analytic in η (k), therefore the above becomes the generator of the power moments:

$$(-\mathrm{i}\partial_\eta)^q A(\eta,\tau,a)|_{\eta=0} = U_q(\tau,a). \tag{20}$$

2. Deriving the S–J moment equations

In order to generate the required scalet equations defined in equations (7) and (8), we must relate the $U_q(\tau,\alpha)$ and $W_q(\tau,\alpha)$ moments defined in equations (5) and (12), respectively. This means that we must transform the Schrödinger equation into a set of differential relations for the $S(x,\tau,\alpha)$ and $J(x,\tau,\alpha)$ configurations defined in equations (4) and (13), respectively. We do this below. The present analysis is modelled after the derivation presented in the work by Handy and Wang (2001), which solely focuses on these configurations for $\tau = 0$ and $\alpha = 1$.

Consider the (rescaled) Schrödinger equation,

$$-\Psi''(x) + V(x)\Psi(x) = E\Psi(x) \tag{21}$$

and its counterpart for $\Phi(x) \equiv \Psi^*(\alpha(x-\tau))$

$$-\Phi''(x) + U(x)\Phi(x) = \mathcal{E}\Phi(x) \tag{22}$$

where we assume E is real (if not, its imaginary part can be incorporated within V), and

$$U(x) = \alpha^2 V^*(\alpha(x-\tau)) \tag{23}$$

$$\mathcal{E} = \alpha^2 E. \tag{24}$$

Let us refer to the differential equations in equations (21) and (22) as (I) and (II), respectively. If we multiply equation (I) by $\Phi(x)$, and equation (II) by $\Psi(x)$, and add/subtract the resulting expressions, we obtain

$$-\tilde{S}''(x) + 2\tilde{P}(x) + V_+(x)\tilde{S}(x) = 0 \tag{25}$$

and

$$-2\tilde{J}'(x) + \tilde{S}''(x) + V_-(x)\tilde{S}(x) = 0 \tag{26}$$

where $\tilde{S}(x) \equiv \Phi(x)\Psi(x)$, $\tilde{P}(x) \equiv \Phi'(x)\Psi'(x)$, $\tilde{J}(x) = \Phi(x)\Psi'(x)$ and $V_\pm(x) \equiv V(x) \pm U(x) - (E \pm \mathcal{E})$.

If we multiply (I) by $\Phi'(x)$, and (II) by $\Psi'(x)$, and again take the sum and difference of the resulting expressions, we obtain

$$-\tilde{P}'(x) + [V(x) - E]\tilde{S}'(x) - V_-(x)\tilde{J}(x) = 0 \tag{27}$$

and

$$-\tilde{\mathcal{W}}(x) + [V(x) - E]\tilde{S}'(x) - V_+(x)\tilde{J}(x) = 0 \tag{28}$$

where $\tilde{\mathcal{W}}(x) \equiv \Phi'(x)\Psi''(x) - \Psi'(x)\Phi''(x)$.

The last equation serves to define $\tilde{\mathcal{W}}$. The first three (equations (25)–(27)) can be reduced to one fourth-order differential equation for $\tilde{S}$, as derived below. However, in practice, it is preferable to generate all moment relations directly from equations (25)–(27), as opposed to the single fourth-order differential equation for $\tilde{S}$. This is because, depending on the potential, additional moment constraints can be overlooked, upon performing the successive differentiations required for deriving the fourth-order equation.

To obtain the fourth-order differential equation for $\tilde{S}$, we first make use of equation (25), written as $\tilde{P}'(x) = \frac{1}{2}(\tilde{S}''(x) - V_+(x)\tilde{S}(x))'$. Substituting this in equation (27), dividing the resulting expression by $V_-(x)$ and differentiating again, allows us to substitute for $\tilde{J}'$ in equation (26). Thus, we obtain

$$\partial_x\left(\frac{\frac{1}{2}(\tilde{S}''(x) - V_+(x)\tilde{S}(x))' - (V(x) - E)\tilde{S}'(x)}{V_-(x)}\right) + \frac{1}{2}(\tilde{S}''(x) + V_-(x)\tilde{S}(x)) = 0. \tag{29}$$

The *S/J* configurations are of particular interest to us, in light of the discussion in the previous section. They correspond to $S(x) \equiv S(x,\tau,\alpha) = \tilde{S}(x+\tau/2)$, and similarly, $J(x) \equiv J(x,\tau,\alpha) = \tilde{J}(x+\tau/2)$, $P(x) \equiv P(x,\tau,\alpha) = \tilde{P}(x+\tau/2)$. Making this explicit, and substituting the original expressions, we obtain (we emphasize that the S, P, J configurations cited below are not to be confused with those appearing in Handy and Wang (2001)):

$$-S''(x) + 2P(x) + \mathcal{V}_+(x)S(x) = 0 \tag{30}$$

$$-2J'(x) + S''(x) + \mathcal{V}_-(x)S(x) = 0 \tag{31}$$

$$P'(x) - \left(V\left(x + \frac{\tau}{2}\right) - E\right)S'(x) + \mathcal{V}_-(x)J(x) = 0 \tag{32}$$

where $\mathcal{V}_\pm(x) = V_\pm\big(x + \frac{\tau}{2}\big)$, or

$$\mathcal{V}_\pm(x) \equiv V\left(x + \frac{\tau}{2}\right) \pm \alpha^2 V^*\left(\alpha\left(x - \frac{\tau}{2}\right)\right) - E(1 \pm \alpha^2). \tag{33}$$

The corresponding fourth-order differential equation for S then becomes

$$\partial_x\left(\frac{\frac{1}{2}\big(S''(x) - V_+\big(x+\frac{\tau}{2}\big)S(x)\big)' - \big(V\big(x+\frac{\tau}{2}\big) - E\big)S'(x)}{V_-\big(x+\frac{\tau}{2}\big)}\right)$$
$$+\frac{1}{2}\left(S''(x) + V_-\left(x + \frac{\tau}{2}\right)S(x)\right) = 0. \tag{34}$$

One can now use these equations to generate the necessary moment equation for the U_q moments defined in section 1. It is best to demonstrate this in the context of a specific example, as discussed in the following section.

3. A pedagogic example: the $V(X) = X^2$ potential

To better appreciate the previous formalism, we examine the case of the harmonic oscillator potential problem correspondingly defined by

$$-\Psi''(x) + x^2\Psi(x) = E\Psi(x). \tag{35}$$

We limit the following analysis to the ground state case only. Although it is possible to use EMM to quantize the system, we work directly with the known solution, corresponding to $E = 1$, $\Psi_{gr}(x) = \exp\big(-\frac{x^2}{2}\big)$, and zeroth-order moment $\mu_0 = \sqrt{2\pi}$. For this case, the scalets become

$$U_q(\tau,\alpha) = \sqrt{\frac{2\pi}{1+\alpha^2}}\exp\left(-\frac{\tau^2(1+\alpha^2)}{8}\right)(-\partial_\beta)^q \exp\left(\frac{\beta^2}{2(1+\alpha^2)}\right) \tag{36}$$

where $\beta \equiv \frac{\tau}{2}(1-\alpha^2)$.

Consistent with the results in equation (9), we see that for $q = 0$, the scalet is $U_0(\tau,\alpha) = \sqrt{\frac{2\pi}{1+\alpha^2}}\exp\big(-\frac{\tau^2}{8}\frac{4\alpha^2}{1+\alpha^2}\big)$, which becomes in the zero scale limit ($a \to 0, \alpha \to \infty$),

$$\lim_{\alpha\to\infty} U_0(\tau,\alpha) = \frac{\mu_0}{\alpha}\Psi_{gr}(\tau). \tag{37}$$

For the U_1 scalet, we obtain $U_1(\tau,\alpha) = -\frac{\tau}{2}\frac{1-\alpha^2}{1+\alpha^2}U_0(\tau,\alpha)$. In the zero scale limit, for $\tau \neq 0$, we also recover the wavefunction, as indicated in equation (9).

The scalet equations are now derived. First, we note that for the harmonic oscillator problem, we have

$$\mathcal{V}_\pm(x) = \left(x + \frac{\tau}{2}\right)^2 \pm \alpha^2\left[\alpha\left(x - \frac{\tau}{2}\right)\right]^2 - E(1 \pm \alpha^2) \tag{38}$$

or

$$\mathcal{V}_\pm(x) = g_\pm x^2 + b_\pm x + c_\pm \tag{39}$$

where $\alpha^n|_\pm \equiv 1 \pm \alpha^n$, $c_\pm \equiv -E\alpha^2|_\pm + \frac{\tau^2}{4}\alpha^4|_\pm$, $b_\pm \equiv \tau\alpha^4|_\mp$ and $g_\pm \equiv \alpha^4|_\pm$.

The harmonic oscillator representation of equations (30)–(32) yields the necessary moment equations (obtained by integrating both sides with respect to x^q and performing the necessary integration by parts). First, we use equation (30) to generate the $V_q(\tau,\alpha)$ scalets in terms of the U_q:

$$V_q(\tau,\alpha) = \tfrac{1}{2}(q(q-1)U_{q-2}(\tau,\alpha) - [c_+(\tau,\alpha)U_q(\tau,\alpha)$$
$$+ b_+(\tau,\alpha)U_{q+1}(\tau,\alpha) + g_+(\tau,\alpha)U_{q+2}(\tau,\alpha)]). \tag{40}$$

From equation (31), one obtains the moment equation

$$2qW_{q-1}(\tau,\alpha) + q(q-1)U_{q-2}(\tau,\alpha) + c_-(\tau,\alpha)U_q(\tau,\alpha) + b_-(\tau,\alpha)U_{q+1}(\tau,\alpha) + g_-(\tau,\alpha)U_{q+2}(\tau,\alpha) = 0. \tag{41}$$

However, we will ignore the constraint defined by the $q = 0$ relation, since to incorporate it will complicate the necessary algebra. The legitimacy of this step lies in the fact that (through EMM, for example) we know the physical energy and starting moment values (for $\tau = 0, \alpha = 1$). The generation of the scalet configurations, for all desired (τ, α) values, can proceed regardless of whether we use the $q = 0$ relation.

Taking $q \to q + 1$ in the previous moment equation, we can solve for $W_q(\tau, \alpha)$ in terms of the U-moment/scalets as well:

$$W_q(\tau,\alpha) = \frac{-1}{2(q+1)}(q(q+1)U_{q-1}(\tau,\alpha) + c_-(\tau,\alpha)U_{q+1}(\tau,\alpha) + b_-(\tau,\alpha)U_{q+2}(\tau,\alpha) + g_-(\tau,\alpha)U_{q+3}(\tau,\alpha)). \tag{42}$$

The final moment equation follows from equation (32):

$$-qV_{q-1}(\tau,\alpha) + (q+2)U_{q+1}(\tau,\alpha) + \tau(q+1)U_q(\tau,\alpha) + \left(\frac{\tau^2}{4} - E\right)qU_{q-1}(\tau,\alpha) + c_-(\tau,\alpha)W_q(\tau,\alpha) + b_-(\tau,\alpha)W_{q+1}(\tau,\alpha) + g_-(\tau,\alpha)W_{q+2}(\tau,\alpha) = 0. \tag{43}$$

Upon substituting for V and W, a recursive, linear finite difference equation of order 5 ensues for the U-moments. This takes on the form

$$\sum_{j=-3}^{5} C_j(q;\tau,\alpha)U_{q+j}(\tau,\alpha) = 0 \tag{44}$$

where

$$C_j(q;\tau,\alpha) \equiv \begin{cases} \dfrac{(-q)(1-q)(2-q)}{2} & j=-3 \\ 0 & j=-2 \\ \dfrac{q(\tau^2\alpha^4|_+ - 4\alpha^2|_+)}{4} & j=-1 \\ \dfrac{\tau}{2}(1+2q)\alpha^4|_- & j=0 \\ 2+q+\dfrac{\alpha^4|_+q}{2} - \alpha^4|_-\left(\dfrac{3+\frac{5q}{2}+\frac{q^2}{2}}{3+q}\right) - \dfrac{1}{2(q+1)}\left(\alpha^2|_- - \dfrac{\alpha^4|_-\tau^2}{4}\right)^2 & j=1 \\ \dfrac{\alpha^2|_-\alpha^4|_+(3+2q)\tau(4-\alpha^2|_+\tau^2)}{8(q+1)(q+2)} & j=2 \\ -\dfrac{(\alpha^4|_+)^2\tau^2}{2(q+2)} - \dfrac{\alpha^2|_-\alpha^4|_-}{8}(\alpha^2|_+\tau^2-4)\left[\dfrac{1}{q+1}+\dfrac{1}{(3+q)}\right] & j=3 \\ -\dfrac{\alpha^8|_-(5+2q)\tau}{2(2+q)(3+q)} & j=4 \\ -\dfrac{(\alpha^4|_-)^2}{2(3+q)} & j=5. \end{cases} \tag{45}$$

From the above moment equation relation, we can solve for U_{q+5} in terms of the lower order moments. This then requires that the $\{U_0(\tau,\alpha),\ldots,U_4(\tau,\alpha)\}$ *missing moments* be specified before all the other moments can be generated through the linear relation

$$U_q(\tau,\alpha) = \sum_{\ell=0}^{4} M_{q,\ell}(\tau,\alpha) U_\ell(\tau,\alpha) \tag{46}$$

where the M-coefficients are readily generated, since they satisfy the previous moment equation with respect to the q-index, in addition to the initialization conditions:

$$M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2} \qquad \text{for} \quad 0 \leqslant \ell \leqslant m_s \equiv 4. \tag{47}$$

Since the W are known in terms of the missing moments/scalets, we can generate the necessary coupled scalet equations in the τ and α directions (as given in equations (11) and (15)), respectively:

$$\partial_\tau \begin{pmatrix} U_0(\tau,\alpha) \\ U_1(\tau,\alpha) \\ U_2(\tau,\alpha) \\ U_3(\tau,\alpha) \\ U_4(\tau,\alpha) \end{pmatrix} = \begin{pmatrix} \mathcal{N}_{0,0}(\tau,\alpha), \mathcal{N}_{0,1}(\tau,\alpha), \mathcal{N}_{0,2}(\tau,\alpha), \mathcal{N}_{0,3}(\tau,\alpha), \mathcal{N}_{0,4}(\tau,\alpha) \\ \mathcal{N}_{1,0}(\tau,\alpha), \mathcal{N}_{1,1}(\tau,\alpha), \mathcal{N}_{1,2}(\tau,\alpha), \mathcal{N}_{1,3}(\tau,\alpha), \mathcal{N}_{1,4}(\tau,\alpha) \\ \mathcal{N}_{2,0}(\tau,\alpha), \mathcal{N}_{2,1}(\tau,\alpha), \mathcal{N}_{2,2}(\tau,\alpha), \mathcal{N}_{2,3}(\tau,\alpha), \mathcal{N}_{2,4}(\tau,\alpha) \\ \mathcal{N}_{3,0}(\tau,\alpha), \mathcal{N}_{3,1}(\tau,\alpha), \mathcal{N}_{3,2}(\tau,\alpha), \mathcal{N}_{3,3}(\tau,\alpha), \mathcal{N}_{3,4}(\tau,\alpha) \\ \mathcal{N}_{4,0}(\tau,\alpha), \mathcal{N}_{4,1}(\tau,\alpha), \mathcal{N}_{4,2}(\tau,\alpha), \mathcal{N}_{4,3}(\tau,\alpha), \mathcal{N}_{4,4}(\tau,\alpha) \end{pmatrix} \begin{pmatrix} U_0(\tau,\alpha) \\ U_1(\tau,\alpha) \\ U_2(\tau,\alpha) \\ U_3(\tau,\alpha) \\ U_4(\tau,\alpha) \end{pmatrix} \tag{48}$$

for $\alpha^2 \neq 1$, and

$$\partial_\alpha \begin{pmatrix} U_0(\tau,\alpha) \\ U_1(\tau,\alpha) \\ U_2(\tau,\alpha) \\ U_3(\tau,\alpha) \\ U_4(\tau,\alpha) \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{0,0}(\tau,\alpha), \mathcal{M}_{0,1}(\tau,\alpha), \mathcal{M}_{0,2}(\tau,\alpha), \mathcal{M}_{0,3}(\tau,\alpha), \mathcal{M}_{0,4}(\tau,\alpha) \\ \mathcal{M}_{1,0}(\tau,\alpha), \mathcal{M}_{1,1}(\tau,\alpha), \mathcal{M}_{1,2}(\tau,\alpha), \mathcal{M}_{1,3}(\tau,\alpha), \mathcal{M}_{1,4}(\tau,\alpha) \\ \mathcal{M}_{2,0}(\tau,\alpha), \mathcal{M}_{2,1}(\tau,\alpha), \mathcal{M}_{2,2}(\tau,\alpha), \mathcal{M}_{2,3}(\tau,\alpha), \mathcal{M}_{2,4}(\tau,\alpha) \\ \mathcal{M}_{3,0}(\tau,\alpha), \mathcal{M}_{3,1}(\tau,\alpha), \mathcal{M}_{3,2}(\tau,\alpha), \mathcal{M}_{3,3}(\tau,\alpha), \mathcal{M}_{3,4}(\tau,\alpha) \\ \mathcal{M}_{4,0}(\tau,\alpha), \mathcal{M}_{4,1}(\tau,\alpha), \mathcal{M}_{4,2}(\tau,\alpha), \mathcal{M}_{4,3}(\tau,\alpha), \mathcal{M}_{4,4}(\tau,\alpha) \end{pmatrix} \begin{pmatrix} U_0(\tau,\alpha) \\ U_1(\tau,\alpha) \\ U_2(\tau,\alpha) \\ U_3(\tau,\alpha) \\ U_4(\tau,\alpha) \end{pmatrix}. \tag{49}$$

The explicit forms for these matrix coefficients, even in the present case, are very complicated. We do not detail them here.

It is important to note that for $\alpha = 1$, the form of the scalet equation simplifies considerably. Included in this is a reduction in the number of missing moments. Thus, for $\alpha = 1$, we have

$$C_j(q;\tau,1) = \begin{cases} -\frac{p(2-3p+p^2)}{2} & j=-3 \\ 0 & j=-2 \\ -p\left(2-\frac{\tau^2}{2}\right) & j=-1 \\ 0 & j=0 \\ 2(p+1) & j=1 \\ 0 & j=2 \\ -\frac{2\tau^2}{2+p} & j=3. \end{cases} \tag{50}$$

The associated τ-scalet equation is

$$\partial_\tau \begin{pmatrix} U_0(\tau,1) \\ U_1(\tau,1) \\ U_2(\tau,1) \end{pmatrix} = \begin{pmatrix} 0, 0, -\tau \\ 0, -\frac{1}{\tau}, 0 \\ \frac{1}{\tau} - \frac{\tau}{4}, 0, -\frac{2}{\tau} \end{pmatrix} \begin{pmatrix} U_0(\tau,1) \\ U_1(\tau,1) \\ U_2(\tau,1) \end{pmatrix}. \tag{51}$$

It will be noted that this equation, despite the singular matrix elements, is satisfied by the regular functions

$$\begin{pmatrix} U_0(\tau,1) \\ U_1(\tau,1) \\ U_2(\tau,1) \end{pmatrix} = \sqrt{\pi}\, \mathrm{e}^{-\frac{\tau^2}{4}} \begin{pmatrix} 1 \\ 0 \\ \frac{1}{2} \end{pmatrix} \tag{52}$$

which follows from equation (36). Combining equations (44) and (50) allows us to generate $U_3(\tau,1)$ and $U_4(\tau,1)$ as required for implementing our wavefunction recovery program.

4. Singularities in the α space

For simplicity, assume that the physical wavefunction behaves as $\Psi(x) \approx \mathrm{e}^{-P(x)}$, where $P(x)$ is some function which generates a decaying wavefunction, at infinity, along the real axis. The scalet moments, $(U_q(\tau,\alpha))^*$, should then be analytic in α, with singularities wherever $\lim_{x\to\pm\infty} \mathrm{Real}\big(P^*\big(\alpha\big(x-\frac{\tau}{2}\big)\big) + P\big(x+\frac{\tau}{2}\big)\big) < 0$. If cx^d is the highest degree term in P, then this becomes $\mathrm{Re}(c^*\alpha^{*d} + c) < 0$.

For the $V(x) = -\mathrm{i}x^3$ case to be considered in the next section, from WKB theory (Bender and Orszag 1978), we have that $P(x) = \pm\frac{2}{5}(-\mathrm{i})^{\frac{1}{2}}|x|^{\frac{5}{2}}$, depending on $x \to \pm\infty$. The singularity condition becomes $\mathrm{i}^{\frac{1}{2}}(\alpha^*)^{\frac{5}{2}} + (-\mathrm{i})^{\frac{1}{2}} = 0$, or $(\alpha^*)^{\frac{5}{2}} = \pm\mathrm{i}$. Since our coupled differential scalet equations are algebraic in structure (i.e. no explicit fractional powers are possible in the generated coefficients), these singularities in α must appear in the form $\alpha^5 = -1$, or $1 + \alpha^5 = 0$. Thus, the scalet equations to be derived involve no singular coefficients within the physical regime for the inverse scale variable (i.e. $\alpha > 0$).

For the harmonic oscillator case, $d = 2$ and $c = 1$ yield the singularity condition $1 + \alpha^{*2} = 0$. Accordingly, $\alpha^2 = -1$, and one expects that because of similar 'algebraic' reasons, as explained above, the coupled differential scalet equations will involve coefficients with singularities at $\alpha^4 = 1$. Clearly then, eventhough the physical scalet configurations are not singular at $\alpha = 1$, the scalet equation coefficients do become singular there. To deal with this complication, numerically, we must simply perform a power series expansion, in $\alpha - 1$, at $\alpha = 1$, followed by numerical (Runge–Kutta) integration.

Fortunately, the $-\mathrm{i}x^3$ potential's analysis, as discussed in the next section, can be done through numerical integration, starting at $\alpha = 1$. In this regard, it is simpler to implement, numerically, than that for conventional (real) anharmonic potentials.

5. The $V(X) = -IX^3$ potential

We examine the previous formalism within a specific context. Consider the non-Hermitian potential problem, $V(x) = -\mathrm{i}x^3$, which has received much recent attention. For this case, we will work directly with equations (30)–(32); also

$$\mathcal{V}_\pm(x) = -E(1\pm\alpha^2) - \left(\frac{\mathrm{i}\tau^3}{8} + \frac{3\mathrm{i}\tau}{2}x^2\right)(1\pm\alpha^5) - \left(\frac{3\mathrm{i}\tau^2}{4}x + \mathrm{i}x^3\right)(1\mp\alpha^5). \tag{53}$$

Define the moments

$$\begin{pmatrix} U_q(\tau,\alpha) \\ V_q(\tau,\alpha) \\ W_q(\tau,\alpha) \end{pmatrix} = \begin{pmatrix} \int_{-\infty}^{+\infty} \mathrm{d}x\, x^q S(x,\tau,\alpha) \\ \int_{-\infty}^{+\infty} \mathrm{d}x\, x^q P(x,\tau,\alpha) \\ \int_{-\infty}^{+\infty} \mathrm{d}x\, x^q J(x,\tau,\alpha) \end{pmatrix}. \tag{54}$$

Assuming that one is working with the physical, bounded, solutions, applying x^q to both sides of equations (30)–(32), and integrating by parts, yields the following coupled moment equations.

From equation (30), we obtain

$$V_q(\tau,\alpha) = \sum_{j=-2}^{3} \Omega_{1,j}(q,\tau,\alpha) U_{q+j}(\tau,\alpha) \tag{55}$$

where the Ω-coefficients are given in the appendix.

From equation (31), we obtain

$$\sum_{j=0}^{3} \Lambda_j(\tau,\alpha) U_j(\tau,\alpha) = 0 \tag{56}$$

and

$$W_q(\tau,\alpha) = \sum_{j=-1}^{4} \Omega_{2,j}(q,\tau,\alpha) U_{q+j}(\tau,\alpha) \tag{57}$$

for $q \geqslant 0$. The coefficients are given in the appendix.

Finally, from equation (32) we obtain

$$q V_{q-1}(\tau,\alpha) + \sum_{j=-1}^{2} \Omega_{3,j}(q,\tau,\alpha) U_{q+j}(\tau,\alpha) + \sum_{j=0}^{3} \Gamma_j(\alpha,\tau) W_{q+j}(\tau,\alpha) = 0. \tag{58}$$

For clarity, the E dependence of the Ω, Λ and Γ coefficients is implicitly assumed. These coefficients are given in the appendix.

We can now substitute the relations in equations (55) and (57) into equation (58), to obtain

$$U_{q+7}(\tau,\alpha) = \sum_{j=-3}^{6} \Upsilon_{q,j}(\tau,\alpha,E) U_{q+j}(\tau,\alpha) \tag{59}$$

for $q \geqslant 0$. The specific form of this equation is discussed in the appendix. We do not have to generate the Υ explicitly, in order to implement the rest of the formalism.

From the previous equation, one observes that all the U_q-scalets can be expressed as linear combinations of the first seven $\{U_\ell(\tau,\alpha) | 0 \leqslant \ell \leqslant 6\}$, through the relation (as symbolized in equation (6))

$$U_q(\tau,\alpha) = \sum_{\ell=0}^{6} M_{q,\ell}(\tau,\alpha,E) U_\ell(\tau,\alpha) \tag{60}$$

where the $M_{q,\ell}(\tau,\alpha,E)$ satisfy the moment equation in equation (59), with respect to the q-index,

$$M_{q+7,\ell}(\tau,\alpha,E) = \sum_{j=-3}^{6} \Upsilon_{q,j}(\tau,\alpha,E) M_{q+j,\ell}(\tau,\alpha,E) \qquad 0 \leqslant \ell \leqslant 6 \tag{61}$$

and also the initialization conditions

$$M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2} \qquad 0 \leqslant \ell_{1,2} \leqslant 6. \tag{62}$$

There is an additional constraint on the U from equation (56). Although we could incorporate this, it would complicate the notation. It is not necessary for recovering the wavefunction, since we can derive a closed set of differential scalet equations. This is discussed in the next section.

5.1. The scalet equations

The $W_q(\tau, \alpha)$ are linearly determined by the basic scalet configurations. This follows from combining equations (57) and (60):

$$W_q(\tau, \alpha) = \sum_{\ell=0}^{6} N_{q,\ell}(\tau, \alpha, E) U_\ell(\tau, \alpha) \tag{63}$$

where

$$N_{q,\ell}(\tau, \alpha, E) = \sum_{j=-1}^{4} \Omega_{2,j}(q, \tau, \alpha) M_{q+j,\ell}(\tau, \alpha, E). \tag{64}$$

Both equations (11) and (15) reduce to coupled, finite-dimensional, first-order differential equations in the τ and α directions (i.e. the *scalet equations*), respectively (i.e. restrict the q-index on the LHS of these equations to the basic scalet configuration indices):

$$\partial_\tau U_\ell(\tau, 1) = \sum_{\ell_v=0}^{6} \left(\frac{\ell}{2} M_{\ell-1,\ell_v}(\tau, 1, E) + N_{\ell,\ell_v}(\tau, 1, E) \right) U_{\ell_v}(\tau, 1) \tag{65}$$

and

$$\begin{aligned} -\alpha \partial_\alpha U_\ell(\tau, \alpha) = \sum_{\ell_v=0}^{6} \bigg(& (\ell+1) M_{\ell,\ell_v}(\tau, \alpha, E) - \frac{\ell\tau}{2} M_{\ell-1,\ell_v}(\tau, \alpha, E) \\ & + N_{\ell+1,\ell_v}(\tau, \alpha, E) - \frac{\tau}{2} N_{\ell,\ell_v}(\tau, \alpha, E) \bigg) U_{\ell_v}(\tau, \alpha) \end{aligned} \tag{66}$$

for $0 \leqslant \ell \leqslant 6$.

5.2. Numerical implementation

5.2.1. Solving for the initial configurations at $\tau = 0, \alpha = 1$. The $\{U_\ell(\tau = 0, \alpha = 1) | 0 \leqslant \ell \leqslant 6\}$ moments, and the corresponding bound state energy, E, are determined through the eigenvalue moment method (EMM), as discussed in the recent work by Handy (2001). We provide a brief overview here.

The physical bound state solution, $|\Psi(x)|^2 = S(x, 0, 1)$, must be integrable and nonnegative. Therefore, it must satisfy the moment problem constraints:

$$\int_{-\infty}^{+\infty} \left(\sum_{q=0}^{Q} C_q x^q \right)^2 |\Psi(x)|^2 > 0 \tag{67}$$

for arbitrary $Q \geqslant 0$, and arbitrary C (other than the zero vector). This becomes the quadratic form expression

$$\sum_{q_1,q_2=0}^{Q} C_{q_1} U_{q_1+q_2}(0, 1) C_{q_2} \geqslant 0. \tag{68}$$

Table 1. (EMM) Ground state energy and missing moments[a], $U_\ell(0,1)$, for $-ix^3$ potential.

E_{gr}	1.156 267 072
$U_0(0,1)$	0.244 411 8149
$U_1(0,1)$	0
$U_2(0,1)$	0.126 609 0790
$U_3(0,1)$	0
$U_4(0,1)$	0.187 019 7824
$U_5(0,1)$	0
$U_6(0,1)$	0.441 959 3237

[a] Adopted EMM normalization: $\sum_{\ell=0}^{6} U_\ell(0,1) = 1$.

It is implicitly assumed that $|\Psi(x)|^2$ satisfies some normalization condition. One convenient choice is

$$\sum_{\ell=0}^{6} U_\ell(0,1) = 1. \tag{69}$$

Constraining (for instance) $U_0(0,1) = 1 - \sum_{\ell=1}^{6} U_\ell(0,1)$, and substituting in equation (60) we get

$$U_q(0,1) = \hat{M}_{q,0}(E) + \sum_{\ell=1}^{6} \hat{M}_{q,\ell}(E) U_\ell(0,1) \tag{70}$$

where

$$\hat{M}_{q,0}(E) = M_{q,0}(0,1,E) \tag{71}$$

and

$$\hat{M}_{q,\ell}(E) = M_{q,\ell}(0,1,E) - M_{q,0}(0,1,E) \tag{72}$$

for $1 \leqslant \ell \leqslant 6$.

In terms of the unconstrained U, equation (68) becomes

$$\sum_{\ell=1}^{5} A_{Q;\ell}[C;E] U_\ell(0,1) < B_Q[C;E] \tag{73}$$

where

$$A_{Q;\ell}[C;E] = -\sum_{q_1,q_2=0}^{Q} C_{q_1} \hat{M}_{q_1+q_2,\ell}(E) C_{q_2} \tag{74}$$

for $1 \leqslant \ell \leqslant 5$, and

$$B_Q[C;E] = \sum_{q_1,q_2=0}^{Q} C_{q_1} \hat{M}_{q_1+q_2,0}(E) C_{q_2}. \tag{75}$$

These relations can be solved for the physical energy and $\{U_\ell(0,1)\}$ through EMM. These in turn can be used as the initial conditions in integrating equation (65), for arbitrary τ. Finally, knowledge of $\{U_\ell(\tau,1)\}$ becomes the initial conditions in integrating equation (66) either in the zero scale limit ($\alpha : 1 \to \infty$) or in the large scale limit ($\alpha : 1 \to 0$). From equations (9)–(10), these asymptotic limits generate either the wavefunction, Ψ, or its power moments (up to a factor in each case), respectively.

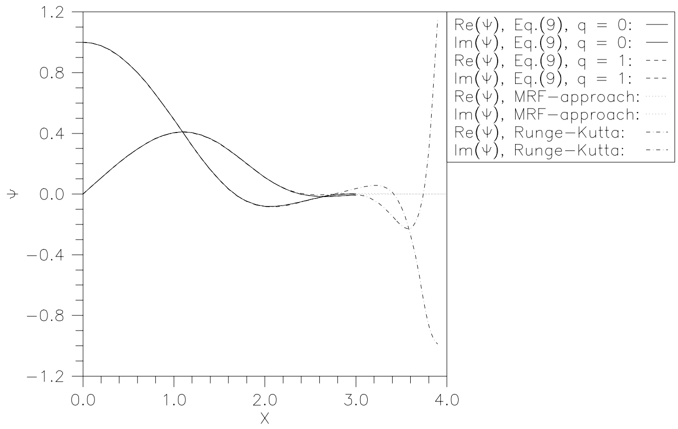

Figure 1. Generation of $\Psi(x)$ for the ground state of the $-ix^3$ potential using the scalet-Wigner (accelerated) analysis for $q = 0, 1$ as given in equation (9); the MRF analysis of Tymczak *et al* (1998); and Runge–Kutta integration.

Table 2. Missing moment ratios from scalet-Wigner and MRF analysis.

q	Scalet-Wigner[a] $\frac{\mu_q}{\mu_0}$	MRF $\frac{\mu_q}{\mu_0}$
0	(1.0, 0.0)	(1.0, 0.0)
1	(0.0, 0.659 078 862)	(0.0, 0.659 080 091)
2	(0.217 192 566, 0.0)	(0.217 192 69, 0.0)
3	(0.0, 1.156 266 23)	(0.0, 1.156 267 62)
4	(−0.762 072 626, 0.0)	(−0.762 072 968, 0.0)
5	(0.0, 2.251 137 14)	(0.0, 2.251 132 88)
6	(−5.291 441 54, 0.0)	(−5.291 435 35, 0.0)

[a] $N_c = 7$, from equation (76), and $\alpha = O(8)$.

For the $\mathcal{PT}$-invariant ground state solution, EMM gives the energy bounds $1.156\,267\,071\,853\,13 < E_{gr} < 1.156\,267\,072\,054\,77$, by working with $Q = 80$ (however, the results in table 2 correspond to $Q = 60$). Similar bounds can be generated for the missing moments $\{U_\ell(0,1)|0 \leqslant \ell \leqslant 6\}$; however, in table 1 we only quote the first ten significant digits for the energy and missing moments. Using these values, we then integrate equation (48) in the τ direction, and subsequently equation (49) in the α direction in order to recover the wavefunction and/or moments. The wavefunction is given in figure 1 (calculated through four different methods, as itemized below). The convergence behaviours of the scalet-Wigner approximants, at particular points on the x-axis, are given in figures 2–8.

5.2.2. Summary of results. We note that, in agreement with the analysis previously given pertaining to the singularity structure in the α-plane, an examination of the Υ-coefficients in equation (61), as explained in the appendix, reveals that the scalet equations will have a $(1+\alpha^5)^{-m}$ singularity (i.e. from equation (A6), and the required division by $\Omega_{2,4}$ and Γ_3, both of which are specified in equations (A1) and (A3), respectively). Thus, the closest singularities to the α-real axis are $\alpha_{\text{pole}} = e^{i\frac{\pi}{5}}$ and its complex conjugate. These should not pose any problems for the numerical integration of the scalet equation.

In figure 1, we compare the scalet-Wigner generated wavefunction (normalized to unity at the origin), as given by equation (9) for $q = 0, 1$, with those obtained by two other methods. The first is the multiscale reference function (MRF) analysis, first presented in the works

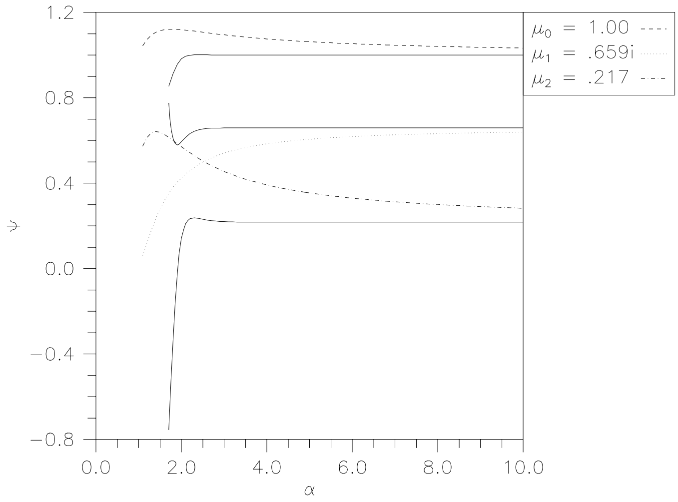

Figure 2. Behaviour of the scalet-Wigner results for the first three moments of Ψ, normalized according to $\mu_0 = 1$. The accelerated results are depicted in terms of the solid, continuous curves.

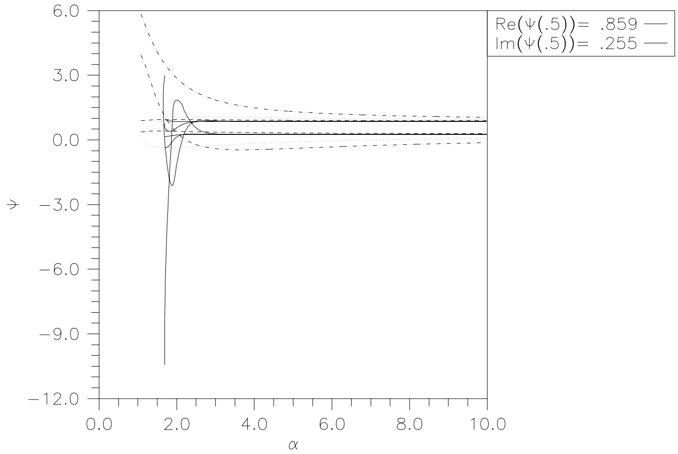

Figure 3. Scalet-Wigner results for the real and imaginary parts of $\frac{\Psi(\tau=0.5)}{\Psi(0)}$ (broken curves) and their accelerated counterparts (solid curves).

by Tymczak *et al* (1998a, 1998b), and subsequently used in various other cases, particularly in the $-ix^3 + i\alpha x$ complex potential case (Handy *et al* 2001). The numerical results of this approach were confirmed by Runge–Kutta integration, utilizing the approximate form for the wavefunction derivative, at the origin, as given by the MRF approach. All four cases agree very well (i.e. scalet-Wigner ($q = 0, 1$), MRF and Runge–Kutta). We only give the scalet-Wigner results up to $x \leqslant 3$. The MRF results are very small, for $x > 3$, and appear as dots very close to the x-axis. The Runge–Kutta integration becomes unstable, at relatively large x, as shown in figure 1.

We remind the reader that the quantization performed at scale value $a = 1$ adopts a particular normalization for $|\Psi(x)|^2$ which cannot easily be represented in terms of Ψ. Furthermore, the asymptotic relations in equation (9) do not allow us to determine $\Psi(0)$. The best we can do is generate $\frac{\Psi(\tau)}{\Psi(0)}$, and similarly for the ratios of the moments of Ψ: $\frac{\mu_q}{\mu_0}$. As such,

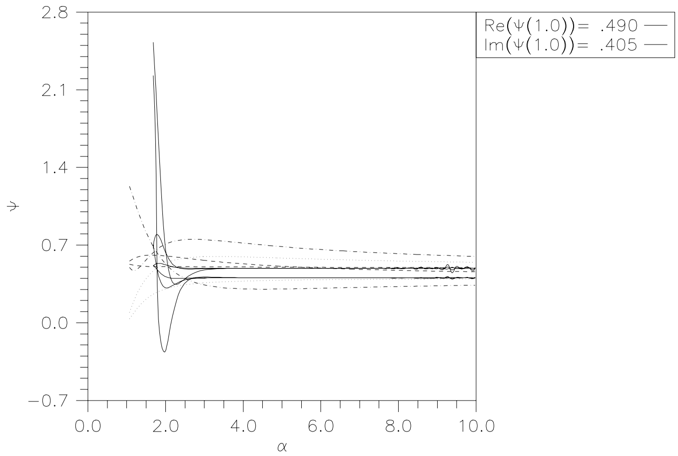

Figure 4. Scalet-Wigner results for the real and imaginary parts of $\frac{\Psi(\tau=1.0)}{\Psi(0)}$ (broken curves) and their accelerated counterparts (solid curves).

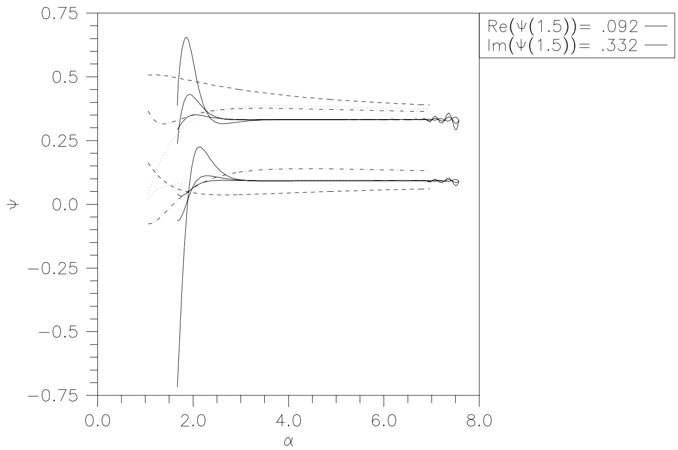

Figure 5. Scalet-Wigner results for the real and imaginary parts of $\frac{\Psi(\tau=1.5)}{\Psi(0)}$ (broken curves) and their accelerated counterparts (solid curves).

the (complex) wavefunction given in figure 1 is set to unity at the origin. The same is done in figure 2.

The convergence rate of the scalet-Wigner formalism can be slow, particularly for the $-ix^3$ problem. To improve this, we adopted a convergence acceleration technique, first used in the scalet–wavelet work of Handy and Murenzi (1996, 1997, 1998, 1999). This involves representing the large α values of the scalet-Wigner integrated results in terms of the corresponding asymptotic form expression, for small scale values, and extracting the theoretical limiting form for the wavefunction. This approach significantly speeds up the convergence rate. It is this approach which is used in all the figures. This is particularly the case in figire 2. We give the scalet-Wigner approximants, as functions of α, for the first three (normalized) moments of the wavefunction: $\frac{\mu_q}{\mu_0}, q = 0, 1, 2$. These correspond to the broken curves in figure 2. For each of these, the corresponding accelerated result is represented by a continuous, unbroken, curve. In table 2 we compare the scalet-Wigner generated moment ratios with those derived from the MRF method.

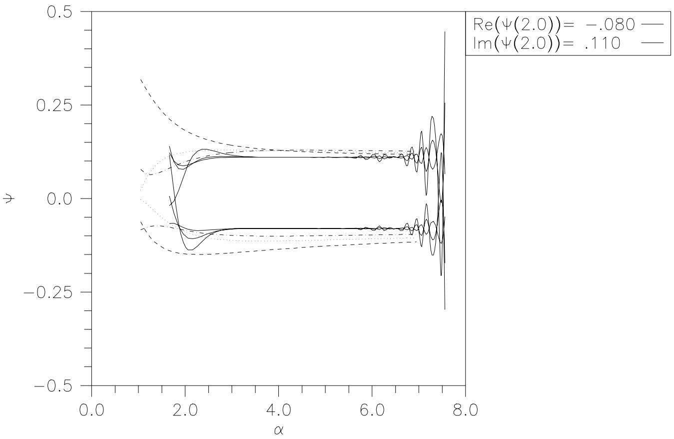

Figure 6. Scalet-Wigner results for the real and imaginary parts of $\frac{\Psi(\tau=2.0)}{\Psi(0)}$ (broken curves) and their accelerated counterparts (solid curves).

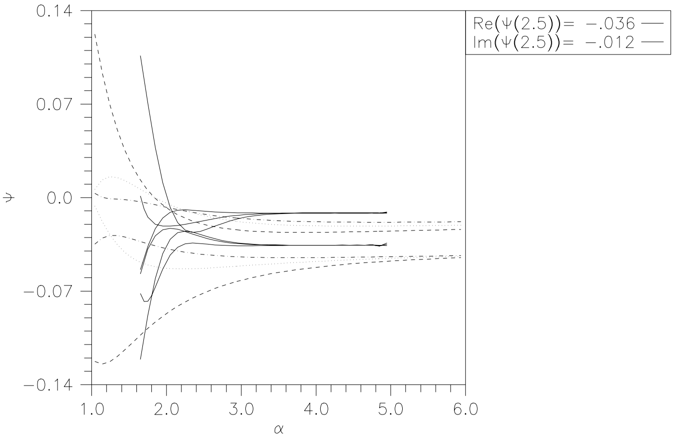

Figure 7. Scalet-Wigner results for the real and imaginary parts of $\frac{\Psi(\tau=2.5)}{\Psi(0)}$ (broken curves) and their accelerated counterparts (solid curves).

We detail the form of the accelerated sequence analysis. The integrated scalet-Wigner moment is evaluated at arbitrarily large values of the inverse scale, $\alpha_j \gg 1$, and this is equated to a truncated asymptotic expansion for small scale values $\left(\alpha_j \equiv \frac{1}{a_j}\right)$:

$$\begin{pmatrix} \alpha_j \frac{U_q(\tau,\alpha_j)}{\left(\frac{\tau}{2}\right)^q} & \text{if} \quad \tau \neq 0 \\ \alpha_j^{1+q} U_q(0,\alpha_j) & \text{if} \quad \tau = 0 \end{pmatrix} = \sum_{n=0}^{N_c} A_n^{(q)}(\tau) a_j^n. \tag{76}$$

Upon picking $N_c + 1$ different α_j values, at which the qth scalet-Wigner configuration is determined (through numerical integration of the α-scalet equation), one can solve for the $N_c + 1$ coefficients, $A_n^{(q)}(\tau)$, of which the $A_0^{(q)}(\tau)$ coefficient approximates the desired asymptotic limit, as given in equation (9). Accordingly, we obtain

$$A_0^{(q)}(\tau) = \begin{cases} \mu_0^* \Psi(\tau) & \text{if} \quad \tau \neq 0 \\ \mu_q^* \Psi(0) & \text{if} \quad \tau = 0. \end{cases} \tag{77}$$

All the accelerated results depicted in the figures correspond to $N_c = 7$. In figures 3–8 we give the scalet-Wigner results for the wavefunction ratio, $\frac{\Psi(\tau)}{\Psi(0)}$, for different τ values. For both

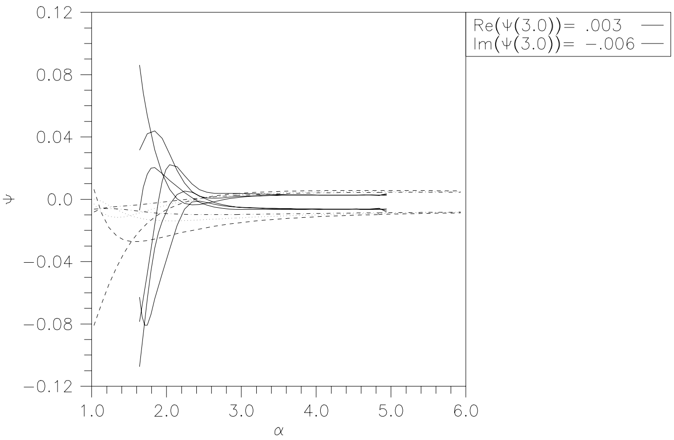

Figure 8. Scalet-Wigner results for the real and imaginary parts of $\frac{\Psi(\tau=3.0)}{\Psi(0)}$ (broken curves) and their accelerated counterparts (solid curves).

the real and imaginary parts of the wavefunctions, three distinct scalet-Wigner approximants are shown (i.e. $q = 0, 1, 2$ from equation (9)). These correspond to broken curves. For each of these, there will be a corresponding accelerated sequence. These are depicted by a solid, continuous curve. The three such curves for the real part of the wavefunction, as well as the three curves for the imaginary part, converge to their corresponding limit, quickly, as noted in the figures. These values correspond to the values given in figure 1 for the real and imaginary parts of the wavefunction. At (relatively) large α values, the accelerated curves manifest numerical instability. We show this, whereever possible.

The extension of the previous analysis to the much more difficult case of complex eigenenergies for PT-symmetry breaking systems, as first discussed by Delabaere and Trinh (2000), and subsequently studied by Handy *et al* (2001) through moment problem quantization methods, is presented elsewhere (Handy 2001c).

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Appendix

The various coefficients required in the preceding analysis are given below.

$$\Omega_{1,j}(q,\tau,\alpha) = \begin{cases} \frac{q(q-1)}{2} & j=-2 \\ 0 & j=-1 \\ \frac{1}{2}\left(E + E\alpha^2 + \frac{\mathrm{i}\tau^3}{8}(1+\alpha^5)\right) & j=0 \\ \frac{3\mathrm{i}}{8}\tau^2(1-\alpha^5) & j=1 \\ \frac{3\mathrm{i}}{4}\tau(1+\alpha^5) & j=2 \\ \frac{\mathrm{i}}{2}(1-\alpha^5) & j=3 \end{cases} \tag{A1}$$

$$\Lambda_j(\tau,\alpha) = \begin{cases} \left(E - E\alpha^2 + \frac{\mathrm{i}\tau^3}{8}(1-\alpha^5)\right) & j=0 \\ \frac{3\mathrm{i}}{4}\tau^2(1+\alpha^5) & j=1 \\ \frac{3\mathrm{i}}{2}\tau(1-\alpha^5) & j=2 \\ \mathrm{i}(1+\alpha^5) & j=3 \end{cases} \tag{A2}$$

$$\Omega_{2,j}(q,\tau,\alpha) = \begin{cases} -\frac{q}{2} & j=-1 \\ 0 & j=0 \\ \frac{1}{2(q+1)}\left(E(1-\alpha^2) + \frac{\mathrm{i}\tau^3}{8}(1-\alpha^5)\right) & j=1 \\ \frac{3\mathrm{i}\tau^2(1+\alpha^5)}{8(q+1)} & j=2 \\ \frac{3\mathrm{i}\tau(1-\alpha^5)}{4(q+1)} & j=3 \\ \frac{\mathrm{i}(1+\alpha^5)}{2(q+1)} & j=4 \end{cases} \tag{A3}$$

$$\Omega_{3,j}(q,\tau,\alpha) = \begin{cases} \left(E + \frac{\mathrm{i}\tau^3}{8}\right)q & j=-1 \\ \frac{3\mathrm{i}}{4}\tau^2(q+1) & j=0 \\ \frac{3\mathrm{i}}{2}(q+2)\tau & j=1 \\ \mathrm{i}(q+3) & j=2 \end{cases} \tag{A4}$$

and

$$\Gamma_j(\tau,\alpha) = \begin{cases} \left(E(1-\alpha^2) + \frac{\mathrm{i}\tau^3}{8}(1-\alpha^5)\right) & j=0 \\ \frac{3\mathrm{i}}{4}\tau^2(1+\alpha^5) & j=1 \\ \frac{3\mathrm{i}}{2}\tau(1-\alpha^5) & j=2 \\ \mathrm{i}(1+\alpha^5) & j=3. \end{cases} \tag{A5}$$

With regard to equation (41), we note that upon substituting equations (37) and (39) in equation (40), we obtain the expression

$$q\sum_{j=-2}^{3}\Omega_{1,j}(q-1,\tau,\alpha)U_{q-1+j}(\tau,\alpha) + \sum_{j=-1}^{2}\Omega_{3,j}(q,\tau,\alpha)U_{q+j}(\tau,\alpha) + \sum_{j_1=0}^{3}\Gamma_{j_1}(\tau,\alpha)\left(\sum_{j_2=-1}^{4}\Omega_{2,j_2}(q+j_1,\tau,\alpha)U_{q+j_1+j_2}(\tau,\alpha)\right) = 0. \tag{A6}$$

From this relation, the highest order moment is easily isolated, yielding

$$\begin{aligned} -\Gamma_3(\tau,\alpha)\Omega_{2,4}(q+3,\tau,\alpha)U_{q+7}(\tau,\alpha) &= q\sum_{j=-2}^{3}\Omega_{1,j}(q-1,\tau,\alpha)U_{q-1+j}(\tau,\alpha) \\ &+ \sum_{j=-1}^{2}\Omega_{3,j}(q,\tau,\alpha)U_{q+j}(\tau,\alpha) + \sum_{j_1=0}^{3}\Gamma_{j_1}(\tau,\alpha) \\ &\times\left(\sum_{j_2=-1}^{3}\Omega_{2,j_2}(q+j_1,\tau,\alpha)U_{q+j_1+j_2}(\tau,\alpha)\right) \\ &+ \sum_{j_1=0}^{2}\Gamma_{j_1}(\tau,\alpha)\Omega_{2,4}(q+j_1,\tau,\alpha)U_{q+j_1+4}(\tau,\alpha). \end{aligned} \tag{A7}$$

We can generate the M-coefficients in equation (43) from the related expression:

$$
\begin{aligned}
-\Gamma_3(\tau,\alpha)\Omega_{2,4}(q+3,\tau,\alpha)M_{q+7,\ell}(\tau,\alpha) &= q\sum_{j=-2}^{3}\Omega_{1,j}(q-1,\tau,\alpha)M_{q-1+j,\ell}(\tau,\alpha)\\
&\quad+\sum_{j=-1}^{2}\Omega_{3,j}(q,\tau,\alpha)M_{q+j,\ell}(\tau,\alpha)+\sum_{j_1=0}^{3}\Gamma_{j_1}(\tau,\alpha)\\
&\quad\times\left(\sum_{j_2=-1}^{3}\Omega_{2,j_2}(q+j_1,\tau,\alpha)M_{q+j_1+j_2,\ell}(\tau,\alpha)\right)\\
&\quad+\sum_{j_1=0}^{2}\Gamma_{j_1}(\tau,\alpha)\Omega_{2,4}(q+j_1,\tau,\alpha)M_{q+j_1+4,\ell}(\tau,\alpha).
\end{aligned}
\tag{A8}
$$

If one expands the above, and regroups the appropriate terms, one can define the Υ representation in equation (41). However, this approach is cumbersome, and unnecessary, in order to generate the desired M coefficients.

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