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Scalets, wavelets and (complex) turning point quantization

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Abstract

Despite the many successes of wavelet analysis in image and signal processing, the incorporation of continuous wavelet transform theory within quantum mechanics has lacked a compelling, *first principles*, motivating analytical framework, until now. For arbitrary one-dimensional rational fraction Hamiltonians, we develop a simple, unified formalism, which clearly underscores the complementary, and mutually interdependent, role played by moment quantization theory (i.e. via scalets, as defined herein) and wavelets. This analysis involves no approximation of the Hamiltonian within the (equivalent) wavelet space, and emphasizes the importance of (complex) multiple turning point contributions in the quantization process. We apply the method to three illustrative examples. These include the (double-well) quartic anharmonic oscillator potential problem, $V(x) = Z^2x^2 + gx^4$, the quartic potential, $V(x) = x^4$, and the very interesting and significant non-Hermitian potential $V(x) = -(\mathrm{i}x)^3$, recently studied by Bender and Boettcher.

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1. Introduction

Despite the many accomplishments of wavelet theory (Grossmann and Morlet 1984, Daubechies 1988), its incorporation into quantum mechanics has lacked a compelling theoretical motivation, until now. We depart from the conventional approach of emphasizing the compact support character of the dual-wavelet basis (Cho *et al* 1993, Wei and Chou 1996, Tymczak and Wang 1997) in making variational computations numerically economical. Instead, we focus on redefining the bound state quantization problem in a manner that is faithful to the essence of wavelet analysis: a space-scale parameter-dependent, multiscale formalism, for efficiently analysing and recovering the important local features of a configuration, $\Psi(x)$ (i.e. signal, image or wavefunction), with minimal distortion. This mandates that the quantization problem be reformulated so as to emphasize the significant localized

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characteristics of a given system. We can achieve this through the turning point quantization approach developed here.

Consider the bound state Schrödinger–Hamiltonian representation,

$$\epsilon \partial_x^2 \Psi(x) = (V(x) - E)\Psi(x) \tag{1}$$

where ϵ is the kinetic energy expansion parameter. It is easy to argue (Handy, Murenzi, Bouyoucef and Brooks 2000 (hereafter HMBB)), both within quantum operator theory and wavelet theory, that the most important local structures of the system are the inflection points of the solution, $\partial_x^2 \Psi(x_i) = 0$, where the kinetic energy is zero. These are of two types: nodal points, $\Psi(x_n) = 0$, where the wavefunction changes signature; and turning points,

$$V(\tau_\ell) = E \tag{2}$$

$\{\tau_\ell(E) | 0 \leqslant \ell \leqslant m_s\}$. Since the latter are known, *a priori*, as functions of the energy, E, they become the most accessible localized features of the wavefunction around which to build a wavelet-based, turning point quantization analysis. In the case of one-dimensional problems, we will be emphasizing all of the turning points, including those in the complex plane. For multidimensional problems (not discussed here), one would consider particular points on the real turning hypersurfaces (HMBB 2000).

Having identified the (complex) turning points as the important localized features of the physical quantum system, a multiscale analysis must proceed by generating the solution through a constructive process that starts at the largest possible scale ($a = \infty$), and identifies each of the important, successively smaller scale contributions ($a \to 0$).

In principle, this is possible through a moment equation (ME) representation of the Schrödinger equation. This involves transforming the Schrödinger equation into an ME relation involving the power moments of the solution: $\mu_p \equiv \int \mathrm{d}x\, x^p \Psi(x)$, for $p \geqslant 0$. The determination of the physical energy, and other global characteristics of the physical solution (i.e. expectation values, etc), can be obtained through various moment quantization (MQ) formulations (Blankenbekler *et al* 1980, Killingbeck *et al* 1985, Handy and Bessis 1985, Handy *et al* 1988a b, Fernandez and Ogilvie 1993). One of the salient features of the ME representation, as repeatedly emphasized in the works of Handy (1981), Handy and Bessis (1985), Handy *et al* (1988a, b) and HMBB (2000) is that kinetic energy ϵ-expansions are analytic. Furthermore, the zeroth-order form of this expansion depends explicitly on all the (complex) turning points of the system.

The use of the ME relation, in generating the physical wavefunction, can be difficult. This is one of the important aspects of the classic *moment problem* (Shohat and Tamarkin 1963) in pure mathematics. However, various important formulations have been developed, as itemized below (Handy 1996, Tymczak *et al* 1998a, b). A more efficient reformulation of this problem is to work with the generalized, space-scale-dependent moments, $\mu_p(a, b) = \int \mathrm{d}x\, (x-b)^p\, S(\frac{x-b}{a})\Psi(x)$, referred to as *scalets*. These are defined in terms of an appropriately chosen scaling function, S. Assuming the normalization $S(0) \equiv 1$, the infinite scale scalet configurations, $\mu_p(a = \infty, b)$, correspond to linear superpositions with respect to the power moments: $\mu_p(a = \infty, b) = \int \mathrm{d}x\, (x - b)^p \Psi(x) = \sum_{q=0}^{p} \binom{p}{q} (-b)^{p-q} \mu_q$.

Scalets are inextricably linked to wavelet analysis, as developed here. They acquire, and impart to wavelet theory, all the important properties manifested within the ME representation pertaining to the analyticity of kinetic energy expansions and (complex) turning point contributions.

There is one fundamental manifestation of the intimate relationship between the moment problem and wavelet analysis. Both critically depend on, or are impacted by, the group of affine maps: $x \to \frac{x-b}{a}$ (in one dimension). Specifically, the affine group is used in wavelet

theory to generate the dual-wavelet basis (described in equations (4) and (5)); whereas the ME representation is naturally invariant under the affine group. The former is clarified below and in the next section.

With respect to the latter, the power moments, μ_p, can be regarded as the 'projection of Ψ' onto the monomial-basis functions, x^p. Given the affine map invariance of polynomial spaces, any transformation of the Schrödinger equation into an ME representation should simplify the underlying wavelet analysis. This has been confirmed through the moment-wavelet formalism of Handy and Murenzi (hereafter HM) (1997, 1998a, b, 1999).

Related to this is the fact that the referenced (MQ) works by Handy and Bessis (1985), and Handy *et al* (1988a, b), can be characterized as defining an affine map invariant, variational quantization procedure, based on knowledge of the signature structure of the physical wavefunction (i.e. knowing the location of all the nodal points of the wavefunction). This approach uses polynomial sampling functions to test for 'localized' deviations from the underlying positivity constraints (of the moment problem), in a multiscale manner. This procedure yielded excellent results for singular perturbation/strong coupling-type problems.

Other examples of the multiscale robustness of MQ methods include the multiscale reference function (MRF) variational representation of Handy (1996), and the MRF quantization methods of Tymczak *et al* (1998a, b). Both of these approaches are based on an MRF representation (i.e. equation (3)) which exploits the analytic properties of certain Fourier space basis representations, within a multi-wavelet, basis-like, expansion. The MRF representation is also intimately related, if not identical, to the distributed approximating functionals (DAFs) method of Hoffman, Kouri, and co-workers (1993).

For the important, and large, class of one-dimensional, bound-state, rational fraction potentials, the number of (complex) turning points is exactly the same as the dimension of the linear, moment equation representation for the Schrödinger equation (i.e. $1+m_s$). This permits the implementation of an exact (closed) turning point quantization (TPQ) analysis.

There are two approaches for doing this. The first was developed by HMBB (2000), and makes use of the MRF basis expansion for the wavefunction,

$$\Psi_{MRF}(x) = \sum_{n=0}^{\infty} a_n[\mu_0, \ldots, \mu_{m_s}; E](-\partial_x)^n R(x) \tag{3}$$

where the *reference function*, $R(x)$, is arbitrary, and the coefficients are linear in the $1 + m_s$ independent variables of the ME representation. Imposing the TPQ conditions, $\partial^2_{\tau_\ell} \Psi_{MRF}(\tau_\ell(E)) = 0$, then leads to a determinantal equation for the energy. This approach yields excellent physical estimates, but also many spurious solutions. In order to discriminate between the physical and spurious solutions, in a scale consistent manner, HMBB employed some specialized, wavelet-based, methods (we review, and expand upon, their formalism in the appendix).

1.1. Result no 1

The reason that many spurious ('noise') solutions are generated within the TPQ-MRF representation is that the underlying basis functions used, $(-\partial_x)^n R(x)$, are not necessarily well suited to the localized nature of the TPQ conditions (despite the robustness, and algebraic simplicity, of the MRF representation when used in the *non-localized* context of Tymczak *et al*'s (1998a, b) quantization formalism). Any approximation errors in the MRF representation are exacerbated upon evaluating the highly localized, kinetic energy operator. What is required is a basis representation that results in less 'noise' generation, upon evaluating the second-order

derivative expression. This is possible through a wavelet (DCWT) representation, as developed in this work (refer to sections 2–4), which takes the form

$$\Psi_{DCWT}(x) = \frac{1}{\nu} \sum_{-\infty<l,\ j<+\infty} w_{l,j}[\mu_0, \ldots, \mu_{m_s}; E]\ \frac{1}{\sqrt{2^l}} \mathcal{D}\left(\frac{x - j2^l}{2^l}\right) \tag{4}$$

within the dyadic wavelet basis representation (Daubechies 1991, HM 1999). The dual basis functions, $\mathcal{D}$, are multiplied by (wavelet-transform-generated) coefficients, $w_{l,j}$, that are also linear with respect to the ME-independent variables, μ_ℓs. They are given by the wavelet transform relation

$$w_{l,j} = \frac{1}{\sqrt{2^l}} \int \mathrm{d}x\, \mathcal{W}\left(\frac{x - j2^l}{2^l}\right) \Psi(x) \tag{5}$$

where $\mathcal{W}$ is referred to as the *mother wavelet*.

We show in this work that the TPQ conditions applied to the DCWT representation,

$$\partial_\tau^2 \Psi_{DCWT}(\tau_\ell(E)) = 0 \tag{6}$$

$0 \leqslant \ell \leqslant m_s$, also produces a determinantal equation for the energy which yields significantly fewer (or no) spurious solutions. This defines the second (and preferred) TPQ approach.

An important part of the proposed TPQ-DCWT method is that the $w_{l,j}$ coefficients are linearly dependent on the μ_ℓ variables. This comes from studying the properties of the *scalet equation*,

$$\partial_\alpha \overrightarrow{\mu}(\alpha, b) = \mathcal{M}(\alpha, b; E, \epsilon) \overrightarrow{\mu}(\alpha, b) \tag{7}$$

where $\overrightarrow{\mu}(\alpha, b) = (\mu_0(\alpha, b), \ldots, \mu_{m_s}(\alpha, b))$. The scalet equation corresponds to transforming the Schrödinger equation into a *scaling* transform representation, defined in terms of the generalized, space-scale-dependent, moments,

$$\mu_\ell(a, b) \equiv \int \mathrm{d}x\, x^\ell S\left(\frac{x}{a}\right) \Psi(x + b) \tag{8}$$

$\alpha \equiv \frac{1}{a}$, for a suitable scaling function, S (i.e. $\int \mathrm{d}x\, S(x) \neq 0$). The $\mu_\ell(a, b)$s are referred to as *scalets*. The scalets can be regarded as the generators of the DCWT expansion coefficients (i.e. the $w_{l,j}$s). Depending on the scale regime of interest, $a \approx \infty$, or $a \approx 0$, we will use the notation '$\mu_p(\alpha, b)$', or '$\mu_p(a, b)$', respectively.

The implementation of the TPQ-DCWT analysis is done by first defining the general scalet solution

$$\overrightarrow{\mu}(\alpha, b) = \sum_{\ell=0}^{m_s} \mu_\ell \overrightarrow{\mathcal{B}^{(\ell)}}(\alpha, b; E, \epsilon) \tag{9}$$

where each *basic* scalet solution $\overrightarrow{\mathcal{B}^{(\ell)}}(\alpha, b; E, \epsilon)$ satisfies equation (7), subject to certain initial, infinite scale ($\alpha = 0$), conditions. Using this general solution, one then generates the $w_{l,j}$-wavelet coefficients. (We restrict our analysis to mother wavelets whose wavelet transforms can be expressed as linear superpositions over the scalets.) In this manner, the Ψ_{DCWT} representation in equation (4) is obtained.

1.2. Result no 2

If the scaling function, S, decreases more slowly than the physical wavefunction, $\lim_{|x|\to\infty} \Psi(x)/S(x) = 0$, then the matrix function in the scalet equation will be analytic in α. This means that all scalet solutions will be analytic in α (and absolutely convergent as well). The ϵ dependence of $\mathcal{M}$ will be in terms of powers of $\epsilon\alpha^{\rho}$ (i.e. ρ = integer). Thus, any ϵ-expansion, within the scalet representation, will involve a resummation with respect to the underlying α-expansion. This is expected to produce an analytic ϵ power series as well. Accordingly, ϵ-perturbation is analytic within the scalet representation (refer to section 5).

We develop the ϵ-perturbative expansion for the scalets, and show that the associated configurations manifest a localized structure within the extended space-scale parameter domain (α, b). The importance of this is that these localized, basis-like, scalet configurations are manifestly well adapted to the underlying physics of the problem in question. One of the challenges of wavelet analysis is that the selection of an optimal dual-wavelet basis (i.e. $\mathcal{D}$ and $\mathcal{W}$) is not evident at the outset. In this regard, the kinetic energy scalet expansion representation may be a better alternative to the DCWT representation.

The ϵ-perturbation formalism is an exact reformulation of the (approximate) high-temperature lattice expansion methods proposed by Bender and Sharp (1981) and Handy (1981).

1.3. Result no 3

For the physical energy, E, and power moments, $\{\mu_\ell | 0 \leqslant \ell \leqslant m_s\}$, in equation (7) or equation (9), the scalets will converge to the physical wavefunction, in the zero-scale limit (HM 1997, 1998a, b, 1999),

$$\lim_{a\to 0} \frac{\mu_\ell(a,b)}{a^{1+\ell}\nu_\ell} = \Psi(b) \tag{10}$$

provided $\nu_\ell \equiv \int \mathrm{d}x\, x^\ell S(x) \neq 0$.

This is always true for $\ell = 0$, by definition of the scaling function. For this case, the zero-scale asymptotic expansion is given by $\frac{\mu_0(a,b)}{a\nu_0} = \Psi(b) + a^2 \frac{\nu_2}{2\nu_0}\partial_b^2\Psi(b) + \mathrm{O}(a^3)$, assuming $\nu_1 = 0$. Thus, one can calculate $\partial_b^2\Psi(b)$ by taking the zero-scale limit of $\partial_b^2\big(\frac{\mu_0(a,b)}{a\nu_0}\big)$, or identifying the second-order term of the asymptotic expansion. The latter is preferable, since it avoids any numerical second-order differencing of $\frac{\mu_0(a,b)}{a\nu_0}$, with respect to the translation variable, b. We will denote this process by $\frac{\nu_0}{\nu_2}\partial_a^2\big(\frac{\mu_0(a,b)}{a\nu_0}\big)$, although no actual differentiation is done. That is, in practice, we generate numerically the a-scale dependence of the $\mathcal{B}^{(\ell)}$s, and identify the second-order asymptotic expansion term.

One would think that it should be possible to bypass the TPQ-DCWT analysis and directly implement a TPQ-scalet analysis by constraining the general scalet solution according to $\partial_a^2\big(\frac{1}{a\nu_0}\mu_0(a, \tau_\ell(E); E, \epsilon, \mu_0, \ldots, \mu_{m_s})\big) = 0$, or equivalently

$$\partial_a^2\left(\frac{1}{a\nu_0}\sum_{\ell_1=0}^{m_s} \mu_{\ell_1}\mathcal{B}_0^{(\ell_1)}(a, \tau_{\ell_2}(E); E, \epsilon)\right) = 0 \tag{11}$$

$0 \leqslant \ell_1 \leqslant m_s$, for some sufficiently small-scale value, $a \approx 0$. This would lead to a $1 + m_s$ determinantal equation for the energy, $\mathrm{Det}(\Delta(E)) = 0$, where $\Delta_{\ell_1,\ell_2}(E) = \partial_a^2\big(\frac{1}{a\nu_0}\mathcal{B}_0^{(\ell_1)}(a, \tau_{\ell_2}(E); E, \epsilon)\big)$.

We show in section 6 that such a pure TPQ-scalet analysis cannot work because these conditions will be satisfied, for any E (physical or unphysical), by some set of μ_ℓs. Thus, the

above TPQ-scalet conditions cannot distinguish between the physical and unphysical energy values.

The precise reason for the above is that for any E, there will always be a set of μ_ℓs for which the corresponding scalet solution converges to the Schrödinger equation. That is, the zero-scale asymptotic expansion of the general scalet solution, for any E, and appropriate $\{\mu_\ell | 0 \leqslant \ell \leqslant m_s\}$ values,

$$\mu_0(a,b) = a\nu_0\left(\Psi_0(b) + \frac{a^2\nu_2}{2\nu_0}\Psi_2(b) + \mathrm{O}(a^3)\right) \tag{12}$$

(where it is assumed that $\Psi_2(b) = \partial_b^2\Psi_0(b)$) generates configurations that satisfy the corresponding Schrödinger equation: $-\epsilon\Psi_2(b) + V(b)\Psi_0(b) = E\Psi_0(b)$.

However, any solution to the Schrödinger equation, physical or not, has zero kinetic energy at all the (complex) turning points. Thus, a purely TPQ-scalet ansatz cannot distinguish between the physical and unphysical solutions.

We prove the above in two ways. The first, and more general argument (refer to section 6.1), shows that the compactly supported scalets, $\mu_\ell^{-\delta_1,\delta_2}(a,b) \equiv \int_{-\delta_1}^{\delta_2} \mathrm{d}x\, x^\ell\, S(x/a)\Psi(x+b)$, which exist for any physical (bounded) or unphysical (unbounded) Schrödinger equation solution, Ψ, define an ME representation which is asymptotic to the ME relation for the $\mu_\ell(a,b)$s. Furthermore, the $\mu_\ell^{-\delta_1,\delta_2}(a,b)$s also satisfy equation (10). This explains why the scalet equation can generate (physical or unphysical) configurations that satisfy the Schrödinger equation.

The second argument (refer to sections 6.2 and 6.3) is to study the leading, zero-scale asymptotic behaviour of the scalet equation for the three problems studied here: the double-well quartic anharmonic oscillator, the quartic oscillator, and the non-Hermitian potential problem $V(x) = -(\mathrm{i}x)^3$, recently investigated by Bender and Boettcher (1998). In all three cases, we show that for any E, almost all of the scalet modes decay rapidly, with one surviving mode converging to the Schrödinger equation, in the manner suggested by equation (12).

It is important to stress that we have not studied the translation variable dependence, b, of the basic scalet modes, $\overrightarrow{\mathcal{B}^{(\ell)}}(\alpha, b; E, \epsilon)$. Since the scalet equation matrix is analytic in b, we expect these modes to be analytic in b as well, for finite α. These modes (essentially) converge to solutions of the Schrödinger equation, in the zero-scale limit, $\lim_{\alpha\to\infty}\left(\frac{\alpha}{\nu_0}\mathcal{B}_0^{(\ell)}(\alpha, b; E, \epsilon)\right) \to \Psi_E(b)$. For unphysical energy values, if $\Psi_E(b)$ is continuously differentiable, up to second order, then it must be unbounded in (one or both of) the asymptotic limit(s), $b \to \pm\infty$. As noted, these unbounded, Schrödinger equation solutions satisfy the zero kinetic energy conditions at all the (complex) turning points.

By way of contrast, the (appropriately truncated) $\Psi_{DCWT}(x)$ representation, in which the scalets generate the wavelet coefficients, represents both physical (bounded) and unphysical (unbounded) solutions in terms of the bounded, dual basis functions, $\mathcal{D}\left(\frac{x-j2^l}{2^l}\right)$. The imposition of the TPQ (zero kinetic energy) conditions at the turning points, on such bounded representations, creates an inconsistency that can only be satisfied by the physical solutions. That is, a bounded approximation to an unbounded (unphysical) solution, cannot be expected to satisfy all the TPQ conditions. Thus, combining the DCWT representation with the TPQ conditions can discriminate between the physical and unphysical solutions.

However, it is also possible (and more likely) that the basic scalet modes, in the zero-scale limit, generate piecewise differentiable, spline-like, solutions, $\Psi_E(b)$, with discontinuous (first-order) derivatives at the turning points. In this case, these asymptotically generated, Schrödinger equation solutions, could be bounded (in the $b \to \pm\infty$ limit), for unphysical Es.

Consider the two configurations $f_-(b) \equiv (c_0 + c_1^{(-)}b + c_0b^2)\mathrm{e}^{-b^2}$, for $b < 0$, and $f_+(b) \equiv (c_0 + c_1^{(+)}b + c_0b^2)\mathrm{e}^{-b^2}$, for $b > 0$. The first-order derivatives at the origin are: $f'_-(0) = c_1^{(-)}$ and

$f'_+(0) = c_1^{(+)}$. However, the second-order derivatives are $f''_\pm(0) = 0$. The scaling transform for this function, in the zero-scale limit, becomes $\underline{Sf}(a, b = 0) = c_0 + a(c_1^{(+)} - c_1^{(-)})\nu_1^{(+)} + \mathrm{O}(a^3)$, where $\nu_1^{(+)} = \int_0^{+\infty} \mathrm{d}y\, yS(y)$ (recall $\nu_1 \equiv 0$). Thus, this corresponds to a simple scenario in which the zero kinetic energy condition can be met at the turning point (i.e. $b = 0$), for a bounded, spline-like configuration, with discontinuous first-order derivatives at the turning point ($f'_-(0) \neq f'_+(0)$).

This behaviour is suggested by the kinetic energy, ϵ-perturbation structure of the scalet modes, as discussed in section 5. That is, to any finite order in ϵ, and $\alpha \neq 0$, the generated expansion for the scalets will be bounded, as $|b| \to \infty$. The generated expansion, to any finite order in ϵ, is analytic in b. Thus, as in the truncated DCWT analysis, we expect the application of the TPQ conditions, on the ϵ-perturbative, kinetic energy scalet expansion, will pick out the physical solution (provided it is implemented at the appropriate scale). The details of this are not discussed here.

1.4. Result no 4. On the complex extension of DCWT

Since we will be analysing $\Psi(x)$, at the complex turning points, it is important to assess the suitability of the DCWT representation within the complex x-plane. The argument presented below is also relevant in determining the conditions under which equation (10) holds, for complex b. That is, although the $\mu_\ell(\alpha, b)$ scalets can be analytically continued onto the complex b-plane, they do not necessarily converge to $\Psi(b)$, in the small-scale limit.

The DCWT representation corresponds to a particular scaling transform of the wavefunction, $\underline{S_2\Psi}(a, x) = \frac{1}{\nu}\int \frac{\mathrm{d}\xi}{a} S_2(\frac{\xi - x}{a})\Psi(\xi)$, where the scaling function, S_2, is determined by the dual and mother wavelet functions (as reviewed in the following section). At appropriate points (as defined below), the zero-scale limit recovers the wavefunction, $\lim_{a\to 0} \underline{S_2\Psi}(a, x) = \Psi(x)$.

At finite scales, $a = 2^L$, for the dyadic case, we have (refer to equation (4))

$$\underline{S_2\Psi}(2^L, x) = \frac{1}{\nu}\sum_{l=L}^{+\infty}\sum_{j=-\infty}^{+\infty} w_{l,j}\,\frac{1}{\sqrt{2^l}}\mathcal{D}\left(\frac{x - j2^l}{2^l}\right). \tag{13}$$

Assuming that S_2 is well behaved (i.e. bounded along the real x-axis, analytic everywhere, and $\nu \equiv \int \mathrm{d}x\, S_2(x) \neq 0$), the derivations given by HM (1998a, b, 1999) show that so long as $\Psi(x)$ is entire (and bounded along the real axis), then the DCWT representation is appropriate within the complex x-plane. This is because $\underline{S_2\Psi}(a, x)$ will be analytic in $\alpha = \frac{1}{a}$ and x.

The same is true for all turning points lying within the widest, infinite strip, parallel to the real axis, $\mathcal{S}_\mathcal{A}$, within which the wavefunction is analytic.

The more general case, allowing for pole or branch cut singularities at the boundary of $\mathcal{S}_\mathcal{A}$, is more complicated. A brief analysis is presented in appendix A showing under what conditions one can expect the DCWT representation to converge to $\Psi(x)$, for $x \notin \mathcal{S}_\mathcal{A}$.

In this work, we deal only with potential problems for which the Schrödinger equation solutions are entire functions.

2. Overview

In this section we make explicit the relevance of dual-wavelet analysis for singular perturbation problems. This comprehensive discussion will serve to emphasize the basic wavelet philosophy that they define a multiscale process for analysing and reconstructing the local structures of a configuration. Wavelets connect the large-scale structure to the small-scale (transient)

behaviour of the system, in the neighbourhood of a given point. This large–small scale interaction is most efficient at the turning points. We review the basic wavelet relations in the following subsection.

The wavelet representation's effectiveness (i.e. convergence properties, etc) is dictated by the underlying scaling transform representation. This motivates defining scaling transform representations for the Schrödinger equation. We can do so, in terms of a closed (and thereby exact) formulation, by working within the class of problems corresponding to bound state, rational fraction, potentials. The multiscale dynamics of the system (i.e. how large- and small-scale features interact) is revealed through the *scalet equation*. Its dimension is equal to the total number of (complex) turning points. Further justification for first focusing on the scalet equation is that, for a large class of mother wavelet functions, the associated wavelet transform (which defines the coefficients of the signal (Ψ)-wavelet expansion, Ψ_{DCWT} in equation (4)), can be defined as a superposition over the scalets. We discuss all of the above, including the derivation of the scalet equation, in subsection 2.2. Additional properties of the scaling transform representation are discussed in appendix B.

An important feature of the scalet equation is that kinetic energy (ϵ-perturbation) expansions are analytic (regular). We motivate this through a discussion of the associated moment equation representation for the Schrödinger equation. We give the zeroth-order form for both the ME solution, and the scalet equation solution. In both of these, the zeroth-order contribution of all the (complex) turning points is immediate. All of this is presented in subsection 2.3.

Finally, in subsection 2.4 we emphasize the initial-value nature of the scalet equation, and define various basic scalet solutions.

2.1. Singular perturbation theory and wavelet analysis

One of the most challenging types of problems in physics are those involving strong coupling interactions. Usually, these require singular perturbation analysis (Bender and Orszag 1978), because the physical solutions manifest important small-scale transient, behaviours, and, consequently, the interplay between large- and small-scale 'dynamics' becomes important. Various multiscale methods have been developed to tackle most of these kinds of problems, with varying success.

Over the previous 16 years, since the seminal work of Grossmann and Morlet (1984), wavelet analysis has emerged as a general multiscale approach suitable for addressing many of these singular-perturbation–strong-coupling problems. The primary reason for this is that it involves an explicit space- (b)–scale- (a) dependent basis expansion, where the basis functions are the affine map transforms of a chosen *dual* function, $\mathcal{D}(\frac{x-b}{a})$. For a given configuration, Ψ, its wavelet decomposition involves the superposition over all $\mathcal{D}(\frac{x-b}{a})$ basis functions, for arbitrary scale ($a > 0$) and translation ($|b| < \infty$) values. For the continuous wavelet transform (CWT) case, the corresponding signal(Ψ)–wavelet inversion formula is given by (HM 1998a, b)

$$\Psi(x) = \frac{1}{\nu}\int_0^{+\infty} \frac{\mathrm{d}a}{a^{5/2}} \int_{-\infty}^{+\infty} \mathrm{d}b\, \mathcal{D}\left(\frac{x-b}{a}\right) \underline{W\Psi}(a,b) \tag{14}$$

where $\nu \neq 0$ (defined below), and the basis expansion coefficients, $\underline{W\Psi}(a,b)$, correspond to the wavelet transform:

$$\underline{W\Psi}(a,b) = \frac{1}{\sqrt{a}} \int_{-\infty}^{+\infty} \mathrm{d}\xi\ \mathcal{W}\left(\frac{\xi-b}{a}\right) \Psi(\xi) \tag{15}$$

where the *mother wavelet*, $\mathcal{W}$, must satisfy certain basic conditions. These follow from the basic requirement that both $\mathcal{D}$ and $\mathcal{W}$ generate a *scaling function*, S, which is bounded,

with a non-zero integral, $\nu \equiv \int \mathrm{d}x\, S(x) \neq 0$, and otherwise well behaved. In the Fourier representation, the relation between all three functions becomes (HM 1998a, b):

$$-k\partial_k \hat{S}(k) = \sqrt{2\pi}\hat{\mathcal{D}}(k)\,\hat{\mathcal{W}}(k). \tag{16}$$

From this, all of the basic properties for $\mathcal{W}$ can be derived. The most important of these is that $\hat{\mathcal{W}}(0) = 0$. Although it is not necessary for the dual function to be a mother wavelet, it can be taken as such. One popular choice is the *Mexican hat* mother wavelet $\mathcal{W}_{mh}(x) = -\mathcal{N}_{mh}\partial_x^2 \mathrm{e}^{-x^2/2}$, where $\mathcal{N}_{mh} = \frac{2}{\sqrt{3\sqrt{\pi}}}$.

The scaling function is very important. For any dual-wavelet pair that generate the same scaling function, the convergence properties of the signal–wavelet inversion formula, with respect to the scale variable integration, are unchanged. In order to clarify this, define the *scaling transform*

$$\underline{S\Psi}(a, x) \equiv \frac{1}{\nu_0}\int_{-\infty}^{+\infty} \frac{db}{a}\, S\left(\frac{x-b}{a}\right)\Psi(b). \tag{17}$$

Clearly, one can recover the wavefunction through the zero-scale pointwise convergent (at a given translation point, x), asymptotic limit relation

$$\lim_{a\to 0} \underline{S\Psi}(a, x) = \Psi(x). \tag{18}$$

This defines a particular representation for the dirac distribution, $\lim_{a\to 0} \frac{1}{a\nu_0} S((x-b)/a) = \delta(x-b)$.

This pointwise convergent character is also inherent to equation (14), since one can derive it directly from equation (18) (HM 1998a, b):

$$\underline{S\Psi}(a, x) = \frac{1}{\nu}\int_a^{+\infty} \frac{\mathrm{d}a_v}{{a_v}^{5/2}} \int_{-\infty}^{+\infty} \mathrm{d}b\, \mathcal{D}\left(\frac{x-b}{a_v}\right) \underline{W\Psi}(a_v, b). \tag{19}$$

Thus, the signal–wavelet inversion formula (i.e. equation (14)) is implicitly pointwise convergent, in the above sense, and represents a multiscale resummation process proceeding from the largest scale ($a = \infty$) to the smallest ($a = 0$). That is, equation (14) is not meant to suggest that it is a global, uniformly convergent, basis expansion representation. Instead, it is to be used to recover the local properties of the configuration Ψ, near the point x, through a multiscale process that samples over smaller and smaller scale contributions.

The non-uniformity of the (zero-scale) convergence characteristics of equation (19) is further evidenced by the fact that $\underline{S\Psi}(a, x)$ converges fastest at the inflection points of the configuration, $\partial_x^2\Psi(x_i) = 0$, provided the scaling function satisfies $\nu_1 = \int \mathrm{d}x\, xS(x) = 0$. This immediately follows from a small-scale asymptotic expansion of the scaling transform (i.e. perform the change of variables $y = \frac{x-b}{a}$):

$$\underline{S\Psi}(a, x) = \Psi(x) + \frac{a^2\nu_2}{2\nu_0}\partial_x^2\Psi(x) + \mathrm{O}(a^3). \tag{20}$$

If $x \neq x_i$, then $\underline{S\Psi}(a, x) = \Psi(x) + \mathrm{O}(a^2)$. If $x = x_i$, the convergence is at least $\mathrm{O}(a^3)$.

Instead of the complicated two-dimensional integration, CWT representation, one can work with an exact discretization of it, to be referred to as DCWT. This is made possible by the subset of affine maps corresponding to the A-adic scale and translation values: $a = a_0\rho^l$, and $b = j \times fa_0\rho^l$, for $-\infty < l, j < +\infty$, and $\rho > 1$. From a moment quantization perspective (without explicitly introducing 'frames'), HM derived the corresponding (DCWT) signal–wavelet inversion formula

$$\Psi(x) = \frac{1}{\tilde{\nu}}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty} \mathcal{D}\left(\frac{x - fa_0 j\rho^l - \delta_l[x]}{fa_0\rho^l}\right)\frac{1}{\sqrt{\rho^l}}\,\underline{W\Psi}(\rho^l,\, fa_0 j\rho^l + \delta_l[x]) \tag{21}$$

where x is arbitrary (continuous), and $\delta_l[x]$ is the residual amount, at scale ρ^l, satisfying the equation $x = n_l[x]\rho^l + \delta_l[x]$, for an optimal integer value, $n_l[x]$. Note that $\lim_{l\to-\infty}\delta_l[x] = 0$, and $\partial_x\delta[x] = 1$, except at $x = j\rho^l$, where the residual is discontinuous.

The DCWT (A-adic) inversion formula is valid, so long as the dual-wavelet pair generate a scaling function, S_2, that satisfies (in terms of the Fourier transform)

$$\hat{S}_2(k) - \hat{S}_2(\rho k) = \left(\sum_{j=-\infty}^{+\infty} \mathcal{D}(j)\,\mathrm{e}^{\mathrm{i}fjk}\right)\hat{\mathcal{W}}\left(\frac{k}{a_0}\right) \tag{22}$$

where $\tilde{\nu} \equiv \int \mathrm{d}x\, S_2(x) \neq 0$.

For the dyadic case, $\rho = 2$ ($a_0 = f = 1$), working with the Mexican hat mother wavelet, and dual (i.e. $\mathcal{D}_{mh}(x) = \mathcal{W}_{mh}(x)$), one obtains the DCWT inversion relation (HM 1998a, b)

$$\Psi(x) = \frac{1}{3.427}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty}\mathcal{W}_{mh}\left(\frac{x - j2^l - \delta_l[x]}{2^l}\right)\frac{1}{\sqrt{2^l}}\,\underline{W_{mh}\Psi}(2^l,\, j2^l + \delta_l[x]). \tag{23}$$

This compares favourably with Daubechies' (1991) frame-based analysis

$$\Psi(x) \approx \frac{1}{3.410}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty}\mathcal{W}_{mh}\left(\frac{x - j2^l}{2^l}\right)\frac{1}{\sqrt{2^l}}\,\underline{W_{mh}\Psi}(2^l,\, j2^l). \tag{24}$$

In our numerical implementation of the TPQ-DCWT method, instead of (second-order) differentiating the DCWT inversion formula, with respect to x (so as to calculate the kinetic energy at the turning points), it will be more convenient to work with the DCWT inversion relation for the second-order derivative configuration, $\partial_x^2\Psi(x)$. In this case, we simply have

$$\partial_x^2\Psi(x) = \frac{1}{3.427}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty}\mathcal{W}_{mh}\left(\frac{x - j2^l - \delta_l[x]}{2^l}\right)\frac{1}{\sqrt{2^l}}\,\underline{W_{mh}\Psi^{(2)}}(2^l,\, j2^l + \delta_l[x]) \tag{25}$$

where

$$\underline{W_{mh}\Psi^{(2)}}(a, b) = \frac{1}{\sqrt{a}}\int \mathrm{d}\xi\, \mathcal{W}_{mh}\left(\frac{\xi - b}{a}\right)\partial_\xi^2\Psi(\xi). \tag{26}$$

As argued in the introduction, for the one-dimensional Schrödinger equation representation (i.e. equation (1)), there are two types of inflection points: nodal points, x_n, and turning points, $\tau_\ell(E)$. Since the latter are known, *a priori*, as functions of the energy, E, they become the more convenient local objects around which to implement a TPQ analysis. Since some of these turning points will be complex, the residual term, $\delta_l[\tau]$, will absorb the imaginary component of the complex turning point, τ.

There are additional, important relations, for the scaling transform. These are reviewed in appendix B.

2.2. The scalet equation representation

The scalets can be used to either generate the wavefunction directly, through pointwise converging approximations (i.e. equation (10)), or generate the wavelet transforms, which in turn define the expansion coefficients in the Ψ_{DCWT} representation (i.e. equation (4)). As discussed in the previous section, the Ψ_{DCWT} representation implicitly generates another scaling function, S_2 (i.e. equation (22)), different from that used to define the scalets, S (and not necessarily identical to that in equation (16)). The convergence properties of the S_2-based scaling transform, with respect to recovering Ψ, may be better (i.e. faster) than

those associated with the scaling transform for S (which are, in fact, the scalets themselves). Beyond these practical advantages, the use of the scalets to generate Ψ_{DCWT} also gives us a basis representation for approximating the properties of the wavefunction in the vicinity of any chosen point. This is not possible in terms of the 'pointwise convergent' application of the scalets (equation (10)), which only gives us numerical estimates for Ψ. However, within the kinetic energy, ϵ-expansion representation discussed in section 5, we can generate localized scalet-basis configurations, with which to represent the local structure of the wavefunction. This approach is under investigation.

The scalet equation (i.e. equation (7)) is derived by first generating the scalet moment equation, which corresponds to the Schrödinger equation's representation in terms of the $\mu_p(a, b)$s, for $p \geqslant 0$. This scalet moment equation is linearly dependent on the first $1 + m_s$ scalets, $\{\mu_\ell(a, b)|0 \leqslant \ell \leqslant m_s\}$, and can be transformed into a differential relation that relates scalets at one scale to scalets at another scale. One of the important features of the scalet representation is that kinetic energy expansions are analytic. This is already manifested at the moment equation level, which also involves the turning points. We outline the theoretical structure of all of these issues in the following subsections.

2.2.1. Scalets as pointwise generators of Ψ. Given the importance of the scaling transform within wavelet analysis, it is then reasonable to emphasize the transformation of the Schrödinger equation into a scaling transform representation. Consider any bound state, rational fraction, potential problem,

$$V(x) = \frac{\sum_{i=0}^{T} N_i x^i}{\sum_{j=0}^{B} D_j x^j} \tag{27}$$

where $1 + m_s \equiv \max\{T, B\}$. As emphasized in the introduction, this number represents the total number of all turning points, including those in the complex plane. Let us choose a scaling function of the form $S(x) = \mathrm{e}^{-Q(x)}$, where $Q(x)$ is an appropriate polynomial. We can then transform the associated Schrödinger equation into a set of coupled, linear, first-order differential equations with respect to the scalet configurations (i.e. equation (7), HM 1997, 1998a, b, 1999, HMBB 2000):

$$\partial_\alpha \begin{pmatrix} \mu_0(\alpha, b) \\ \cdot \\ \cdot \\ \mu_{m_s}(\alpha, b) \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{0,0}(\alpha, b; E, \epsilon), \ldots, \mathcal{M}_{0,m_s}(\alpha, b; E, \epsilon) \\ \cdots \\ \cdots \\ \mathcal{M}_{m_s,0}(\alpha, b; E, \epsilon), \ldots, \mathcal{M}_{m_s,m_s}(\alpha, b; E, \epsilon) \end{pmatrix} \begin{pmatrix} \mu_0(\alpha, b) \\ \cdot \\ \cdot \\ \mu_{m_s}(\alpha, b) \end{pmatrix} \tag{28}$$

where $\alpha \equiv \frac{1}{a}$, and $0 \leqslant \ell \leqslant m_s$. As previously noted, we will interchange the notation '$\mu_\ell(\alpha, b)$' and '$\mu_\ell(a, b)$', depending on the scale regime of interest (i.e. $a = \infty$, or $a = 0$, respectively).

The scalet expressions, $\mu_\ell(\alpha, b)$, are so designated, because they are, essentially, proportional to particular scaling transforms of some derivative of the wavefunction. Thus, $\mu_\ell(a, b) = \int \mathrm{d}x\, x^\ell S(x/a)\Psi(x + b) = a^{1+\ell} \int \frac{\mathrm{d}x}{a} \left(\frac{x-b}{a}\right)^\ell S(\frac{x-b}{a})\Psi(x)$. If $\nu_\ell = \int \mathrm{d}x\, x^\ell S(x) \neq 0$, then $\mu_\ell(a, b)$ is proportional to the scaling transform of Ψ with respect to the scaling function $x^\ell S(x)$. If $\nu_\ell = 0$, then from the zero-scale asymptotic expansion

$$\mu_\ell(a, b) = a^{1+\ell} \sum_{q=0}^{\infty} \frac{a^q \nu_{\ell+q}}{q!} \partial_b^q \Psi(b) \tag{29}$$

one obtains

$$\lim_{a\to 0} \frac{q_\ell^*!\mu_\ell(a,b)}{a^{1+\ell+q_\ell^*}\nu_{\ell+q_\ell^*}} = \partial_b^{q_\ell^*}\Psi(b) \tag{30}$$

where q_ℓ^* corresponds to the smallest non-negative integer for which $\nu_{\ell+q_\ell^*} \neq 0$. Thus, in the zero-scale limit, the $\mu_\ell(a,b)$ configuration is proportional to the S-scaling transform of the $\partial_x^{q_\ell^*}\Psi(x)$ configuration.

The scalet equation is to be regarded as an initial-value problem. Specification of the infinite scale, scalet configurations, $\mu_\ell(\alpha = 0, b)$, and energy parameter, E, allow one to generate the corresponding scalet solution within the entire space-scale domain, $\{(\alpha,b)|0 \leqslant \alpha < \infty, -\infty < b < +\infty\}$. The $\mu_\ell(0,b)$ depend, linearly, on the infinite scale, zero translation ($b = 0$) scalets, which are simply the ordinary power moments, $\mu_\ell \equiv \int \mathrm{d}x\, x^\ell \Psi(x)$. This is further discussed in subsection 2.4.

In the works of HM (1997, 1998a, b, 1999), they exploited the initial-value nature of the scalet equation in order to obtain pointwise converging approximations to the physical wavefunction. They used moment quantization methods (described below) to solve for the physical μ_ℓs, and the energy. They then integrated the scalet equation, and made use of the zero-scale asymptotic relations (i.e. equation (30)), to approximate the wavefunction. Excellent results were obtained, for a variety of rational fraction potentials.

When one performs this type of scalet equation analysis, one is directly testing the effectiveness of the underlying scaling function, $S(x) = \mathrm{e}^{-Q(x)}$, in approximating the physical solution.

It is important to emphasize that the scalet equation involves the translation variable, b, as a parameter. Thus, for any fixed b, one is generating the scalet solution as a function of α. One can reformulate the scalet equation as a partial differential equation in α and b. However, we prefer the simplicity of the current formulation. In keeping with this, we do not explicitly study the b-dependent behaviour of the scalet solutions. We have assumed (as is the case for the physical solution), that the general scalet solution, for finite α, is analytic in b (i.e. the scalet matrix elements will always be polynomials in b). We do focus on the behaviour of the (basic) scalet solutions in the asymptotic $\alpha \to \infty$, or zero-scale limit.

2.2.2. Scalets as generators of the wavelet transform. One can also use the scalet equation in order to generate the wavelet transform coefficients for a mother wavelet of the form $\mathcal{W}(x) = P(x)\,\mathrm{e}^{-Q(x)}$, where $P(x)$ is an appropriate polynomial. In this case, once the desired dual function, $\mathcal{D}(x)$, is prescribed, the corresponding scaling function, S_2, satisfying equation (22), will be very different from $S = \mathrm{e}^{-Q(x)}$ (which now becomes the 'generator' for the chosen mother wavelet).

For mother wavelets of the above type, the wavelet transform becomes a superposition over the scalets:

$$\underline{W\Psi}(a,b) = \sum_{\ell_v=0}^{m_s} C_{\ell_v}(a,b)\mu_{\ell_v}(a,b) \tag{31}$$

involving known coefficient functions, $C_{\ell_v}(a,b)$. For the Mexican hat wavelet transform, one has

$$\underline{W_{mh}\Psi}(\alpha,b) = \mathcal{N}_{mh}\sqrt{\alpha}\big(\mu_0(\alpha,b) - \alpha^2\mu_2(\alpha,b)\big) \tag{32}$$

where $\mu_\ell(\alpha,b) = \int \mathrm{d}x\; x^\ell\, \mathrm{e}^{-(\alpha x)^2/2}\Psi(x+b)$. For the second-order derivative, $\partial_x^2\Psi(x)$, the corresponding wavelet transform is

$$\underline{W_{mh}\Psi^{(2)}}(\alpha,b) = -\mathcal{N}_{mh}\alpha^{5/2}\big(3\mu_0(\alpha,b) - 6\alpha^2\mu_2(\alpha,b) + \alpha^4\mu_4(\alpha,b)\big). \tag{33}$$

2.2.3. The scalets' moment equation. The Schrödinger equation, for rational fraction potentials, can be easily transformed into a scalet equation. One must first obtain a moment equation for all the scalets, $\mu_p(\alpha, b)$, $p \geqslant 0$ (not just the first $1+m_s$). We outline the essentials by first focusing on the infinite-scale, zero-translation, scalets (i.e. the μ_ps, or power moments).

Knowledge of the physical power moments defines an implicit multiscale analysis; although it is not as efficient as the scalets in probing small-scale structures. For bounded, physical, configurations, the Fourier transform will generally exist and be analytic,

$$\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx} \Psi(x) \tag{34}$$

defining the k-space power series

$$\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \sum_{p=0}^{\infty} (-\mathrm{i}k)^p \frac{\mu_p}{p!}. \tag{35}$$

This is effectively an expansion in inverse powers of a basic length scale, $k \approx \mathrm{O}(\frac{1}{\text{length}})$. As the order of the Fourier expansion increases, one is probing over smaller and smaller length scales. However, this expansion is not too efficient for very small scales, since large moment orders are required, together with high-precision numerical capabilities (in dealing with the associated large degrees, x^p). Nevertheless, working with the power moments leads to the more efficient scalet representation.

For the class of problems identified, we can transform the Schrödinger equation into a finite-difference, recursive relation for the μ_ps. It takes on the form (Handy and Bessis 1985, Handy *et al* 1988a, b)

$$\mu_p = \sum_{\ell=0}^{m_s} M_{p,\ell}(E, \epsilon) \mu_\ell \tag{36}$$

where the readily determinable coefficients, $M_{p,\ell}(E, \epsilon)$ will be rational fractions in E, and polynomially dependent on ϵ. They satisfy the 'initial' conditions $M_{\ell_1,\ell_2}(E, \epsilon) = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_1, \ell_2 \leqslant m_s$. The independent moments, $\{\mu_\ell | 0 \leqslant \ell \leqslant m_s\}$ are referred to as the *missing moments*. The missing moments are explicitly ϵ independent; whereas the other, dependent, moments are explicitly ϵ dependent.

For concreteness, consider the quartic potential problem $-\epsilon \partial_x^2 \Psi(x) + x^4 \Psi(x) = E\Psi(x)$. For the physical solution, we can integrate both sides of this equation by x^p, obtaining the ME equation

$$\mu_{p+4} = E\mu_p + \epsilon p(p-1)\mu_{p-2} \tag{37}$$

for $p \geqslant 0$. The missing moments are $\{\mu_0, \mu_1, \mu_2, \mu_3\}$. Only the dependent (non-missing) moments acquire an ϵ dependence (i.e. actually, all the moments of order six and higher acquire an explicit ϵ dependence).

In general, for any rational fraction potential, the form of the above relations persists. For the general, rational fraction, bound state potential problem

$$-\epsilon \partial_x^2 \Psi(x) + \frac{\sum_{i=0}^{T} N_i x^i}{\sum_{j=0}^{B} D_j x^j} \Psi(x) = E\Psi(x) \tag{38}$$

upon multiplying both sides by the denominator polynomial, and integrating with respect to x^p, one obtains the ME relation

$$-\epsilon \sum_{j=0}^{B} D_j (p+j)(p+j-1)\mu_{p+j-2} + \sum_{i=0}^{T} N_i \mu_{p+i} = E \sum_{j=0}^{B} D_j \mu_{p+j} \tag{39}$$

where $p \geqslant 0$. The highest-order moment is given by $p + \max\{T, B\}$, or $1 + p + m_s$, where $1+m_s = \max\{T, B\}$. This is also the degree of the polynomial relation derived from the turning point condition $V(\tau_\ell) = E$. Upon isolating the highest moment-order term in equation (39), one obtains the corresponding, recursive, ME relation, as symbolized by equation (36).

For future reference, in connection with $\mathcal{M}(\alpha, b; E, \epsilon)$s ϵ dependence (i.e. equation (28)), it is important to understand which of the moments are explicitly ϵ dependent. To this extent, we have

Lemma 1. *The maximum moment order m_*, for which μ_{m_*} is ϵ independent is $m_* = m_s + 2, m_s + 1, m_s$, for $B = 0, 1, \geqslant 2$, respectively.*

Proof. From equation (39), the moments acquire a polynomial dependence in ϵ. The first $1 + m_s$ moments (the missing moments) are ϵ independent. For the case $B = 0$ (polynomial potential, hence $T = 1 + m_s$) the moments μ_{m_s+1} and μ_{m_s+2} (i.e. $p = 0, 1$ in equation (39)), are also ϵ independent. If $B = 1$, only μ_{m_s+1} is ϵ independent. If $B \geqslant 2$ then μ_{m_s+1} takes on an ϵ dependence. □

Lemma 2. *The moments μ_{m_*+1} through $\mu_{3+m_*+m_s-B}$ will be of first order in ϵ.*

Proof. In general, from equation (39), we see that only the kinetic-energy-related terms will affect the degree to which ϵ contributes to a particular moment. So long as $p+B-2 \leqslant m_*$, none of the kinetic energy moments (i.e. the ϵ terms in equation (39)) will be dependent on ϵ, and the generated moments, μ_{p+m_s+1}, will acquire, at most, an ϵ dependence. Thus, $p \leqslant 2 + m_* - B$, and the generated moments (i.e. μ_{p+m_s+1}) are $\mu_{\leqslant 3+m_*+m_s-B}$. For the problems considered here, where $B = 0$, the moments $\mu_{m_s+3}, \ldots, \mu_{2m_s+5}$ will be of degree one in ϵ. □

One can quantize the energy within the ME representation in equation (39). This is referred to as moment quantization. Various procedures have been proposed by Blankenbecler *et al* (1980), Killingbeck *et al* (1985), Handy and Bessis (1985), Handy *et al* (1988), Fernandez and Ogilvie (1993), Handy (1996), Tymczak *et al* (1998a, b) and HMBB (2000). However, the methods of Handy and Bessis, and Handy *et al* define an affine map invariant variational procedure that yields converging lower and upper bounds to the energy, once the signature properties of the wavefunction are given. This was used to solve the difficult, singular perturbation, quadratic Zeeman effect for strong magnetic fields. This further suggests the relevance of MQ methods to wavelet analysis, and singular perturbation theory. However, with the exception of the MRF representation methods developed by Handy (1996), Tymczak *et al* (1998a, b) and HMBB (2000), none of the other formulations enabled the generation of the wavefunction.

A similar formalism, as given above, applies for the scalets, $\mu_p(\alpha, b)$, $p \geqslant 0$. To derive their ME relation, one translates the Schrödinger equation by an amount b: $[-\epsilon\partial_x^2 + V(x + b)]\Psi(x+b) = E\Psi(x+b)$. Since the scalets involve the scaling function $e^{-Q(x)}$, we define the configuration $\Phi_{a,b}(x) \equiv e^{-Q(x/a)}\Psi(x + b)$, and substitute $\Phi_{a,b}$ for $\Psi(x + b)$. The resulting differential equation for Φ is

$$-\epsilon\left(\partial_x^2 + 2\alpha Q'(\alpha x)\partial_x + \alpha^2[(Q'(\alpha x))^2 + Q''(\alpha x)]\right)\Phi_{a,b}(x) + V(x + b)\Phi_{a,b}(x) = E\Phi_{a,b}(x). \tag{40}$$

Upon repeating the same steps as followed in deriving the ME relation for the μ_ps, one obtains the moment equation for the moments $\int dx\, x^p \Phi_{a,b}(x) = \mu_p(a, b)$, which becomes the moment equation for the scalets:

$$\mu_p(\alpha, b) = \sum_{\ell=0}^{m_s} M_{p,\ell}(\alpha, b; E, \epsilon)\mu_\ell(\alpha, b) \tag{41}$$

$p \geqslant 0$, and $M_{\ell_1,\ell_2}(\alpha, b; E, \epsilon) = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_1, \ell_2 \leqslant m_s$. Note that for notational simplicity, we are not making explicit the E, ϵ dependence of the generated scalets.

So long as

$$\lim_{|x|\to\infty} \frac{Q'(x)}{\sqrt{V(x)}} = 0 \tag{42}$$

(or equivalently, $\mathrm{e}^{-Q(x)}$ does not decrease more rapidly than the physical wavefunction) the order of the finite-difference equation in equation (41), $1 + m_s$, remains the same as that for the μ_p moments (HM 1997). We emphasize that this is not a necessary restriction, but is one for which the eventual form of the scalet equation will become analytic in α and ϵ. If one departs from this, then singular terms are introduced into the scalet equation. Such problems have been dealt with by HM (1997) in their extension of the present formalism to the Bohr atom case.

Let $Q(x) = \sum_{j=0}^{J_Q} \Xi_j\, x^j$. Then, if Deg[$Q$] denotes the degree of Q, we have Deg[Q] = J_Q. The above asymptotic condition forces

$$\mathrm{Deg}\left[\frac{(Q')^2}{V}\right] = 2(J_Q - 1) - (T - B) \leqslant -1 \tag{43}$$

or $J_Q - 1 \leqslant \frac{T-B-1}{2}$. In generating the scalet ME relation (equation (41)), one must consider the product of $V(x + b)$'s denominator polynomial and the kinetic energy terms in equation (40). The respective degrees will be (upon multiplying by x^p and integrating by parts): $p + B - 2$, $p + B + J_Q - 2$, $p + B + 2(J_Q - 1)$, and $p + B + J_Q - 2$. The second and third expressions satisfy: $p + B + J_Q - 2 \leqslant p + \frac{T+B-3}{2}$, and $p + B + 2(J_Q - 1) \leqslant p + T - 1$. Hence all of the original, first three expressions, are strictly less than $p + \max\{T, B\} = p + m_s + 1$. This confirms the previous assertion that the order of the scalet finite-difference ME relation, $1+m_s$, is not changed from that for the μ_ps.

Let us rewrite the shifted potential as $V(x + b) = \sum_{i=0}^{T} N_i(b)x^i / \sum_{j=0}^{B} D_j(b)x^j$. The kinetic energy terms to consider are

$$x^p\left(\sum_{j=0}^{B} D_j(b)x^j\right) \times \begin{cases} \partial_x^2 \Phi_{\alpha,b}(x) \\ 2\alpha\left(\sum_{j_2=0}^{J_Q} \Xi_{j_2}\, j_2 (\alpha x)^{j_2-1}\right)\partial_x \Phi_{\alpha,b}(x) \\ \alpha^2\left(\sum_{j_2,j_3=0}^{J_Q} \Xi_{j_2}\Xi_{j_3}\, j_2 j_3 (\alpha x)^{j_2+j_3-2}\right)\Phi_{\alpha,b}(x) \\ \alpha^2\left(\sum_{j_2=0}^{J_Q} \Xi_{j_2}\, j_2(j_2-1)(\alpha x)^{j_2-2}\right)\Phi_{\alpha,b}(x). \end{cases} \tag{44}$$

The recursive scalet moment equation corresponds to

$$\begin{aligned} -\epsilon\Bigg(&\sum_{j=0}^{B} D_j(b)\,(p+j)(p+j-1)\mu_{p+j-2}(\alpha,b) \\ &-2\alpha\sum_{j_1=0}^{B}\sum_{j_2=0}^{J_Q} D_{j_1}(b)\Xi_{j_2} j_2 (p + j_1 + j_2 - 1)\alpha^{j_2-1}\mu_{p+j_1+j_2-2}(\alpha,b) \\ &+\alpha^2\sum_{j_1=0}^{B}\sum_{j_2,j_3=0}^{J_Q} D_{j_1}(b)\Xi_{j_2}\Xi_{j_3}\, j_2 j_3 (\alpha)^{j_2+j_3-2}\mu_{p+j_1+j_2+j_3-2}(\alpha,b) \end{aligned}$$

$$+\alpha^2 \sum_{j_1=0}^{B} \sum_{j_2=0}^{J_Q} D_{j_1}(b)\,\Xi_{j_2}\, j_2(j_2-1)(\alpha)^{j_2-2}\mu_{p+j_1+j_2-2}(\alpha,b)\Bigg)$$

$$+\sum_{i=0}^{T} N_i(b)\ \mu_{p+i}(\alpha,b) = E\sum_{j=0}^{B} D_j(b)\ \mu_{p+j}(\alpha,b) \tag{45}$$

where $p \geqslant 0$. Note that one of the last two series expressions contain the highest-order scalet moment, $\mu_{p+\mathrm{Max}\{T,B\}}(\alpha,b) = \mu_{p+m_s+1}(\alpha,b)$. When $p = 0$, the corresponding scalet $\mu_{m_s+1}(\alpha,b)$ is of first degree in ϵ (so long as $\alpha \neq 0$).

In general, the $\mu_\ell(\alpha,b)$, for $0 \leqslant \ell \leqslant m_s$ will not have an explicit ϵ dependence. The recursively generated scalets (i.e. $\mu_{p+m_s+1}(\alpha,b)$, $p \geqslant 0$), which are of first order in ϵ, must satisfy:

$$m_s \geqslant \begin{cases} p+B-2 \\ p+B+J_Q-2 \\ p+B+2(J_Q-1) \end{cases} \tag{46}$$

since then, the contributing kinetic energy terms will only involve scalets of (explicit) zeroth-order form in ϵ. Thus $0 \leqslant p \leqslant \mathrm{Min}\{m_s - B + 2, m_s - B - J_Q + 2, m_s - B - 2(J_Q - 1)\}$. The smallest of these is the last one: $p \leqslant m_s - B + 2 - 2J_Q$. Accordingly, we have:

Lemma 3. *The scalets, $\mu_{m_s+1}(a,b)$ through $\mu_{2m_s+1-(B+2(J_Q-1))}(a,b)$, will be of first degree in ϵ. (Proof given above.)*

2.2.4. Deriving the scalet equation. We note that the scaling function will be of the form $S(x) = \mathrm{e}^{-Q(x)}$, where $Q(x) = \sum_{j=0}^{J_Q} \Xi_j x^j$ is a suitable polynomial. Accordingly, the derivative $\partial_\alpha S(\alpha x)$ takes on the form: $\partial_\alpha \mathrm{e}^{-Q(\alpha x)} = (-\sum_{j=0}^{J_Q} j\,\Xi_j \alpha^{j-1} x^j)\mathrm{e}^{-Q(\alpha x)}$. It follows from the definition of $\mu_p(a,b)$ that

$$\partial_\alpha \mu_p(\alpha,b) = -\sum_{j=0}^{J_Q} j\,\Xi_j \alpha^{j-1}\mu_{p+j}(\alpha,b). \tag{47}$$

However, for $0 \leqslant p \leqslant m_s$, the $\mu_{p+j}(\alpha,b)$ scalets depend on the first $1+m_s$ scalets. Thus, one obtains a closed relation, which becomes the scalet equation:

$$\partial_\alpha \mu_p(\alpha,b) = -\sum_{j=0}^{J_Q} j\,\Xi_j \alpha^{j-1}\Bigg(\sum_{\ell=0}^{m_s} M_{p+j,\ell}(\alpha,b;E,\epsilon)\mu_\ell(\alpha,b)\Bigg) \tag{48}$$

or ($p \to \ell_1$)

$$\partial_\alpha \mu_{\ell_1}(\alpha,b) = \sum_{\ell_2=0}^{m_s} \mathcal{M}_{\ell_1,\ell_2}(\alpha,b;E,\epsilon)\mu_{\ell_2}(\alpha,b) \tag{49}$$

where $\mathcal{M}_{\ell_1,\ell_2}(\alpha,b;E,\epsilon) \equiv -\sum_{j=0}^{J_Q} j\,\Xi_j \alpha^{j-1} M_{\ell_1+j,\ell_2}(\alpha,b;E,\epsilon)$. The details are worked out for the explicit examples considered.

At moderately large scale values, one can use MQ methods on the scalets, in order to quantize the energy. This was done for the Bohr atom, scalet analysis, of HM (1997). This approach also requires the introduction of a 'scalet equation'-type relation in the b-direction.

2.3. Analyticity of kinetic energy perturbation in the scalet representation

As noted previously, one of the important features of the scalet equation representation is that kinetic energy ϵ-expansions become analytic. This property is acquired from the underlying moment equation relations. We summarize the relevant relation below.

2.4. Analyticity of the moment equation with respect to ϵ

The moment equation representation for the power moments, and the scalets, is explicitly analytic (regular) in ϵ, the kinetic energy expansion parameter. One immediate indication of the analyticity in ϵ is that the order of the finite-difference moment equation does not change when $\epsilon = 0^+$ and $\epsilon = 0$.

For simplicity, let us examine the zeroth-order, in ϵ, form of the ME relation for the quartic oscillator. From equation (37) we obtain the fourth-order finite-difference equation

$$\mu^{(0)}_{p+4} = E\mu^{(0)}_p \tag{50}$$

which has the solution $\mu^{(0)}_p = \sum_{\ell=0}^{3} \mathcal{A}_\ell\,(\tau_\ell)^p$, where the $\mathcal{A}_\ell$s are arbitrary, and the τ_ℓs are all of the turning points of the problem, $\tau^4_\ell = E$. For real E values, two of the turning points are real, the other two pure imaginary. Symbolically, the configuration associated with these moments, has the form $\Psi^{(0)}(x) = \sum_{\ell=0}^{3} \mathcal{A}_\ell \delta(x - \tau_\ell)$.

The above is true in general. The zeroth-order structure for the general ME relation is (from equation (39))

$$\sum_{i=0}^{T} N_i \mu^{(0)}_{p+i} = E \sum_{j=0}^{B} D_j \mu^{(0)}_{p+j}. \tag{51}$$

The general solution for this is

$$\mu^{(0)}_p = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell\,(\tau_\ell)^p \tag{52}$$

where $\sum_{i=0}^{T} N_i \tau_\ell^{p+i} = E \sum_{j=0}^{B} D_j \tau_\ell^{p+j}$, or (upon factoring out τ_ℓ^p), $V(\tau_\ell) = E$.

The symbolic, zeroth-order configuration corresponding to the $\mu^{(0)}_p$ moments is

$$\Psi^{(0)}(x) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell \delta(x - \tau_\ell(E)) \tag{53}$$

where the $\mathcal{A}_\ell$s are arbitrary. This expression, which becomes precise in the μ_p representation, emphasizes the importance of all the turning points as the primary local structures around which to develop a wavelet analysis.

2.4.1. Analyticity of the scalet matrix function with respect to α and ϵ. So long as equation (42) is satisfied, the scalet equation matrix function, $\mathcal{M}(\alpha, b; E, \epsilon)$, will be analytic in α, and ϵ, as is evident from equations (48) and (49).

It follows that the scalet equation solutions, $\mu_\ell(\alpha, b)$, are analytic in α. In fact, they will be entire functions, with a power-series expansion of the form, $\mu_\ell(\alpha, b) = \sum_{j=0}^{\infty} \Lambda_{\ell;j}[\epsilon, b]\,\alpha^j$, where the $\Lambda_{\ell;j}[\epsilon, b]$ coefficients are polynomials in ϵ and b. These expansion are absolutely convergent. We expect that any reordering, so as to define the ϵ-expansion, $\mu_\ell(\alpha, b) = \sum_{j=0}^{\infty} \mu^{(j)}_\ell(\alpha, b)\epsilon^j$, will also be analytic in ϵ.

Given the symbolic form of the corresponding zeroth-order configuration in equation (53), we can use it to obtain the form for $\mu_p^{(0)}(\alpha, b) = \int \mathrm{d}x\, x^p\, \mathrm{e}^{-Q(\alpha x)}\Psi^{(0)}(x+b)$:

$$\mu_p^{(0)}(\alpha, b) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell(\tau_\ell(E) - b)^p \mathrm{e}^{-Q(\alpha[\tau_\ell(E)-b])}. \tag{54}$$

In section 5.2 we prove this within the scalet representation.

In generating the ϵ expansion for the scalet equation solutions, it is important to know $\mathcal{M}(\alpha, b; E, \epsilon)$'s ϵ dependence. For polynomial potentials ($B = 0$), and Gaussian scaling functions, $Q(x) = x^2/2$, the scalet matrix function will be at most of first degree in ϵ. This can be proved, as follows.

The largest moment-order term appearing in the scalet equation's derivation (i.e. $p = m_s$ in equation (47)) is $\mu_{m_s+J_Q}(\alpha, b)$. For the Gaussian scaling function, $J_Q = 2$. For polynomial potentials, $B = 0$. From lemma 3, the scalets $\mu_{m_s+1}(\alpha, b)$ through $\mu_{2m_s-1}(\alpha, b)$ will be of first degree in ϵ. If we are to have $m_s + (J_Q = 2) \leqslant 2m_s - 1$, then $m_s \geqslant 3$. Thus we have:

Lemma 4. *$\mathcal{M}(\alpha, b; E, \epsilon) = \mathcal{M}^{(0)}(\alpha, b; E) + \epsilon\mathcal{M}^{(1)}(\alpha, b; E)$, for polynomial potentials ($B = 0$), Gaussian scaling functions ($Q(x) = x^2/2$), and $m_s \geqslant 3$. (Proof given above.)*

By way of contrast, the non-Hermitian potential $V(x) = -(\mathrm{i}x)^3$, discussed in the last section, has $m_s = 2$. Its scalet matrix is of degree ϵ^2.

2.5. The scalet equation: an initial-value problem

As previously noted, the scalet equation is to be regarded as an initial-value problem, in which the infinite scale ($\alpha = 0$) configurations have to be specified. For physical, bounded, Ψ-configurations, assuming that $S(0) \equiv 1$, we have (if b is real; if not, then through its analytic continuation, $x \to x - b$)

$$\mu_{\ell_v}(\alpha = 0, b) = \int \mathrm{d}x\, x^{\ell_v}\Psi(x+b) = \int \mathrm{d}x\, (x-b)^{\ell_v}\Psi(x) \tag{55}$$

or

$$\mu_{\ell_v}(\alpha = 0, b) = \sum_{j=0}^{\ell_v} \binom{\ell_v}{j} (-b)^{\ell_v - j}\mu_j \tag{56}$$

where $\mu_j \equiv \mu_j(\alpha = 0, b = 0)$.

Although the scalet equation generates solutions that do not necessarily correspond to bounded Ψ configurations, we will restrict the set of scalet solutions to those that satisfy the above relations, at $\alpha = 0$. Under this assumption, the general scalet solution takes on the form

$$\overrightarrow{\mu}(\alpha, b) = \sum_{\ell=0}^{m_s} \mu_\ell \overrightarrow{\mathcal{B}^{(\ell)}}(\alpha, b; E, \epsilon) \tag{57}$$

where the basic scalet solutions, $\overrightarrow{\mathcal{B}^{(\ell)}}(\alpha, b)$, satisfy the scalet equation

$$\partial_\alpha \overrightarrow{\mathcal{B}^{(\ell)}} = \mathcal{M}(\alpha, b; E, \epsilon)\overrightarrow{\mathcal{B}^{(\ell)}} \tag{58}$$

subject to the conditions (i.e. take $\mu_j \equiv \delta_{j,\ell}$ in equation (56))

$$\mathcal{B}_{\ell_v}^{(\ell)}(\alpha = 0, b) = \sum_{j=0}^{\ell_v} \binom{\ell_v}{j} (-b)^{\ell_v - j}\delta_{j,\ell} \tag{59}$$

or

$$\mathcal{B}^{(\ell)}_{\ell_v}(\alpha=0,b)=\begin{cases}0 & \text{if} \quad \ell_v<\ell\\ \begin{pmatrix}\ell_v\\ \ell\end{pmatrix}(-b)^{\ell_v-\ell} & \text{if} \quad \ell_v\geqslant\ell.\end{cases} \tag{60}$$

Knowledge of the basic scalet solutions, $\overrightarrow{\mathcal{B}}^{(\ell)}$, allows us to express the wavelet transform in terms of a linear relation involving the μ_ℓs (refer to equation (31))

$$\underline{W\Psi}(a,b)=\sum_{\ell=0}^{m_s}\mu_\ell\ \Omega_\ell(a,b;E,\epsilon) \tag{61}$$

where $\Omega_\ell(a,b;E,\epsilon)=\sum_{\ell_v=0}^{m_s}C_{\ell_v}(a,b)\mathcal{B}^{(\ell)}_{\ell_v}(a,b;E,\epsilon)$. This representation facilitates the implementation of TPQ-DCWT, as indicated in the introduction.

An alternate set of initial conditions for the basic scalet solutions is to use the missing moment relation $\mu_j=\sum_{\ell_v=0}^{m_s}\mathcal{A}_{\ell_v}(\tau_{\ell_v}(E))^j$, $0\leqslant j\leqslant m_s$, which is invertible (i.e. $\mu_j\leftrightarrow\mathcal{A}_{\ell_v}$). This follows from equation (52) and the fact that the missing moments are explicitly ϵ-independent (and hence automatically of zeroth order, $\mu^{(0)}_\ell\equiv\mu_\ell$, for $0\leqslant\ell\leqslant m_s$).

One can impose that the basic scalet equation solutions satisfy (at $\alpha=0$) the conditions $\mathcal{A}_{\ell_v}=\delta_{\ell_v,\ell}$, or $\mu_j=(\tau_\ell(E))^j$, for $0\leqslant j\leqslant m_s$. That is, we can define another set of basic scalet equation solutions

$$\overrightarrow{\mu}(\alpha,b)=\sum_{\ell=0}^{m_s}\mathcal{A}_\ell\overrightarrow{\Upsilon^{(\ell)}}(\alpha,b;E,\epsilon) \tag{62}$$

whose initial ($\alpha=0$) configuration is defined as (i.e. from equation (56))

$$\Upsilon^{(\ell)}_{\ell_v}(\alpha=0,b)=\sum_{j=0}^{\ell_v}\begin{pmatrix}\ell_v\\ j\end{pmatrix}(-b)^{\ell_v-j}(\tau_\ell(E))^j \tag{63}$$

which becomes

$$\Upsilon^{(\ell)}_{\ell_v}(\alpha=0,b)=(\tau_\ell(E)-b)^{\ell_v}. \tag{64}$$

3. TPQ-scalet/wavelet analysis

We bring together the necessary components of the previous formalism which are essential to the proposed TPQ-scalet/wavelet formalism. Its numerical implementation is discussed in the next section.

In the previous discussion, we outlined the structure of the general scalet equation solution and its linear dependence on the $1+m_s$ missing moment variables, $\{\mu_\ell|0\leqslant\ell\leqslant m_s\}$. We will work with wavelet transforms that can be written as linear combinations of the scalets. These in turn, define the coefficients of the DCWT signal(Ψ)–wavelet expansion.

We will use the truncated dyadic Mexican hat DCWT representation in equation (23):

$$\Psi_{L,J}(x)=\frac{1}{3.427}\sum_{l=L_{min}}^{L_{max}}\sum_{j=-J}^{+J}\mathcal{W}_{mh}\left(\frac{x-j2^l-\delta_l[x]}{2^l}\right)$$
$$\times\frac{1}{\sqrt{2^l}}\underline{W_{mh}\Psi}(2^l,j2^l+\delta_l[x];E,\epsilon,\mu_0,\ldots,\mu_{m_s}) \tag{65}$$

where the Mexican hat wavelet transform coefficients are given in terms of the general (Gaussian) scalet solution (i.e. $\mu_p(a,\xi) = \int \mathrm{d}x\, x^p \mathrm{e}^{-\frac{x^2}{2a^2}} \Psi(x+\xi)$)

$$\underline{W_{mh}\Psi}(a,\xi) = \mathcal{N}_{mh} a^{-1/2}\left(\mu_0(a,\xi) - \frac{1}{a^2}\mu_2(a,\xi)\right). \tag{66}$$

These, in turn, are generated through the basic scalet solutions:

$$\mu_{\ell_v}(a,\xi;E,\epsilon,\mu_0,\ldots,\mu_{m_s}) = \sum_{\ell=0}^{m_s} \mu_\ell \mathcal{B}^{(\ell)}_{\ell_v}(a,\xi;E,\epsilon). \tag{67}$$

Therefore, in terms of the power moment variables, the Mexican hat wavelet transform becomes

$$\underline{W_{mh}\Psi}(a,\xi;E,\epsilon,\mu_0,\ldots,\mu_{m_s}) = \sum_{\ell=0}^{m_s} \mu_\ell\, w_{mh;\ell}(a,\xi;E,\epsilon) \tag{68}$$

where

$$w_{mh;\ell}(a,\xi;E,\epsilon) = \mathcal{N}_{mh} a^{-1/2}\left(\mathcal{B}^{(\ell)}_0(a,\xi;E,\epsilon) - \frac{1}{a^2}\mathcal{B}^{(\ell)}_2(a,\xi;E,\epsilon)\right). \tag{69}$$

We then impose the TPQ conditions

$$\partial^2_\tau \Psi_{L,J}(\tau_\ell(E)) = 0 \tag{70}$$

for $0 \leqslant \ell \leqslant m_s$. This results in a $(1+m_s)$-dimensional, determinantal equation

$$\mathrm{Det}\left(\Delta(E,L,J)\right) = 0 \tag{71}$$

where

$$\Delta_{\ell_1,\ell_2}(E,L,J) = \frac{1}{3.427}\partial^2_{\tau_{\ell_1}}\left(\sum_{l=L_{min}}^{L_{max}}\sum_{j=-J}^{+J} \mathcal{W}_{mh}\left(\frac{\tau_{\ell_1}(E) - j2^l - \delta_l[\tau_{\ell_1}(E)]}{2^l}\right)\right.$$
$$\left.\times \frac{1}{\sqrt{2^l}} w_{mh;\ell_2}(2^l, j2^l + \delta_l[\tau_{\ell_1}(E)];E,\epsilon)\right). \tag{72}$$

The $\partial^2_{\tau_{\ell_1}}$ differentiation is done numerically. Good results are obtained, as discussed in the following section. Alternatively, one can avoid such differentiation by working instead with the DCWT representation for the second derivative of the wavefunction, $\Psi^{(2)}(x) \equiv \partial^2_x \Psi(x)$.

As noted in the previous section, the Mexican hat wavelet transform for $\Psi^{(2)}(x)$ is given by

$$\underline{W_{mh}\Psi^{(2)}}(a,\xi) = -\mathcal{N}_{mh} a^{-5/2}\left(3\mu_0(a,\xi) - \frac{6}{a^2}\mu_2(a,\xi) + \frac{1}{a^4}\mu_4(a,\xi)\right). \tag{73}$$

For the problems considered here, the fourth-order scalet is dependent on the lower-order scalets, $\mu_4(a,\xi) = \sum_{\ell=0}^{m_s} M_{4,\ell}(a,\xi;E,\epsilon)\mu_\ell(a,\xi)$. In this case, we have

$$\underline{W_{mh}\Psi^{(2)}}(a,\xi;\mu_0,\ldots,\mu_{m_s}) = \sum_{\ell=0}^{m_s} \mu_\ell\, w^{(2)}_{mh;\ell}(a,\xi;E,\epsilon) \tag{74}$$

where

$$w^{(2)}_{mh;\ell}(a,\xi;E,\epsilon) = -\mathcal{N}_{mh} a^{-5/2}\left(3\mathcal{B}^{(\ell)}_0(a,\xi;E,\epsilon) - \frac{6}{a^2}\mathcal{B}^{(\ell)}_2(a,\xi;E,\epsilon)\right.$$
$$\left.+\frac{1}{a^4}\sum_{\ell_v=0}^{m_s} M_{4,\ell_v}(a,\xi;E,\epsilon)\mathcal{B}^{(\ell)}_{\ell_v}(a,\xi;E,\epsilon)\right). \tag{75}$$

We then have

$$\Psi^{(2)}_{L,J}(x) = \frac{1}{3.427}\sum_{l=L_{min}}^{L_{max}}\sum_{j=-J}^{+J}\mathcal{W}_{mh}\left(\frac{x - j2^l - \delta_l[x]}{2^l}\right) \times\frac{1}{\sqrt{2^l}}\underline{W_{mh}\Psi^{(2)}}(2^l,\, j2^l + \delta_l[x];\, E, \epsilon, \mu_0, \ldots, \mu_{m_s}). \tag{76}$$

The TPQ conditions become

$$\Psi^{(2)}_{L,J}(\tau_\ell(E)) = 0 \tag{77}$$

which similarly reduce to a $(1+m_s)$-dimensional determinantal equation. This procedure also works very well, as discussed in the following section.

4. Numerical implementation of TPQ-DCWT

In this section, we consider several important polynomial potentials in order to demonstrate the capabilities, and limitations, of the proposed TPQ-DCWT method. The first two problems will be the double-well quartic anharmonic oscillator potential, $V(x) = Z^2x^2 + gx^4$, for $Z^2 < 0$, and the quartic potential, $Z^2 = 0$. In the first case, for $Z^2 = -5$, all the turning points (within the energy interval considered, for the ground and first excited states) are real. For the quartic potential, two of the turning points are real, the other two, pure imaginary.

For both of these potentials, the implementation of TPQ-DCWT resulted in good physical estimates, with no (or very few) spurious solutions generated, in comparison to the TPQ-MRF analysis by HMBB (which was limited to the double well case).

The third example corresponds to the non-Hermitian potential $V(x) = -(\mathrm{i}x)^3$, recently considered by Bender and Boettcher (1998). For this case, a severe, exponentially growing scalet mode, appears to affect the numerical implementation of the TPQ-DCWT method. We can control the explosiveness of this mode by working in terms of complex scales; however, this is still insufficient to yield any TPQ-DCWT estimates for the ground state. By comparison, the TPQ-MRF method works exceptionally well for this problem (Handy (2000), despite the generation of spurious states that can be filtered out by the method adopted by HMBB, and reviewed in appendix C). In light of these numerical limitations, we defer consideration of this problem to section 5.4, where the asymptotic properties of the scalet equation solutions are discussed.

4.1. TPQ-DCWT analysis for the $Z^2x^2 + gx^4$ potential

We derive the moment equation for the μ_ps and the $\mu_p(\alpha, b)$s, followed by specifying the form of the scalet equation for the generic quartic anharmonic oscillator problem (i.e. double well, and quartic).

4.1.1. The moment equation: $Z^2x^2 + gx^4$. Consider the quartic anharmonic double-well oscillator,

$$-\epsilon\partial^2\Psi(x) + (Z^2x^2 + gx^4)\Psi(x) = E\Psi(x) \tag{78}$$

where $Z^2 < 0$. In the limit $Z^2 \to -\infty$, the ground and first excited state become degenerate. The μ_p- moment equation is

$$g\mu_{p+4} = -Z^2\mu_{p+2} + E\mu_p + p(p-1)\epsilon\mu_{p-2}. \tag{79}$$

It is a fourth-order finite-difference equation in which the energy, E, appears as a parameter. The missing moments correspond to $\{\mu_\ell | 0 \leqslant \ell \leqslant m_s = 3\}$. Specification of these determines all the other moments through the linear relation:

$$\mu(p) = \sum_{\ell=0}^{m_s} M_{p,\ell}(E,\epsilon)\mu(\ell) \tag{80}$$

where $M_{\ell_1,\ell_2}(E,\epsilon) = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_1, \ell_2 \leqslant m_s$. The $M_{p,\ell}(E,\epsilon)$ coefficients satisfy the moment equation with respect to the p index, for fixed ℓ, and are easily generated upon imposing the given initial conditions.

As previously noted, the moments' equation representation is regular with respect to the kinetic energy perturbation parameter, ϵ. Such expansions are relevant for strong coupling problems.

The zeroth order, $\epsilon = 0$, structure of the moment equation is

$$g\mu_{p+4}^{(0)} = -Z^2\mu_{p+2}^{(0)} + E\mu_p^{(0)} \tag{81}$$

and has the general solution $\mu_p^{(0)} = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell(\tau_\ell(E))^p$, where the $\mathcal{A}_\ell$s are arbitrary. The turning point, energy-dependent, functions are defined by $V(\tau_\ell(E)) = E$, where $V(x) = Z^2x^2 + gx^4$:

$$\tau_\ell^2 = -\frac{Z^2}{2} \pm \sqrt{E - V_{min}} \tag{82}$$

where $V_{min} = -Z^4/4$. We adopt the turning point function indexing:

$$\tau_\ell(E) = \begin{cases} -\sqrt{-\frac{1}{2}Z^2 + \sqrt{E - V_{min}}} & \ell = 0 \\ -\sqrt{-\frac{1}{2}Z^2 - \sqrt{E - V_{min}}} & \ell = 1 \\ +\sqrt{-\frac{1}{2}Z^2 - \sqrt{E - V_{min}}} & \ell = 2 \\ +\sqrt{-\frac{1}{2}Z^2 + \sqrt{E - V_{min}}} & \ell = 3. \end{cases} \tag{83}$$

Note that $\tau_0(E) = -\tau_3(E)$ and $\tau_1(E) = -\tau_2(E)$. Physical bound states must satisfy $E > V_{min}$, therefore both $\tau_{0,3}(E)$ will be real functions, so long as $Z^2 < 0$ (we will be investigating the case $Z^2 = -5$). The other two turning point functions can be complex.

4.1.2. The scalet moment equation: $Z^2x^2 + gx^4$. We now derive the moment equation for the scalets, $\mu_p(\alpha, b) = \int_{-\infty}^{+\infty} \mathrm{d}x\, x^p \mathrm{e}^{-Q(\alpha x)}\Psi(x+b)$, corresponding to an appropriate polynomial function $Q(x)$. We require that $Q(0) = 1$ and $Q(\pm\infty) = +\infty$.

Translating the Schrödinger equation by an amount b, we obtain

$$-\epsilon\partial_x^2\Psi(x+b) + (Z^2(x+b)^2 + g(x+b)^4)\Psi(x+b) = E\Psi(x+b). \tag{84}$$

Defining $\Phi(x) \equiv \mathrm{e}^{-Q(\alpha x)}\Psi(x+b)$, and making the appropriate substitutions we obtain

$$-\epsilon\big(\partial_x^2 + 2\alpha Q'(\alpha x)\partial_x + \alpha^2[Q''(\alpha x) + (Q'(\alpha x))^2]\big)\Phi(x)$$
$$+g\big(Z^2(x+b)^2 + (x+b)^4\big)\Phi(x) = E\Phi(x). \tag{85}$$

From JWKB analysis, we know that the asymptotic form for the physical states is $\Psi(x) \to \mathrm{e}^{-\frac{\sqrt{g}}{3}|x|^3}$. Therefore, taking $Q(x) = x^2/2$, satisfies the condition in equation (42)

leading to scalets which are analytic in α, as well as ϵ. The corresponding moment equation for the scalets is

$$\begin{aligned}\mu_{p+4}(\alpha,b) = &-4b\mu_{p+3}(\alpha,b) - g^{-1}[6gb^2 + Z^2 - \epsilon\alpha^4]\mu_{p+2}(\alpha,b)\\ &-g^{-1}[4gb^3 + 2Z^2b]\mu_{p+1}(\alpha,b)\\ &+g^{-1}[E - gb^4 - Z^2b^2 - \epsilon\alpha^2(2p+1)]\mu_p(\alpha,b)\\ &+\frac{\epsilon}{g}p(p-1)\mu_{p-2}(\alpha,b)\end{aligned} \tag{86}$$

where $p \geqslant 0$. We can transform this linear, fourth-order finite-difference equation into the representation

$$\mu_p(\alpha,b) = \sum_{\ell=0}^{m_s=3} M_{p,\ell}(\alpha,b;E,\epsilon)\mu_\ell(\alpha,b) \tag{87}$$

$p \geqslant 0$, and $M_{\ell_1,\ell_2} = \delta_{\ell_1,\ell_2}$, involving readily derivable M function coefficients which are regular in all the dependent variables. The $M_{p,\ell}$ satisfy the ME relation in equation (86), with respect to the p-index, and are recursively generated upon imposing the aforementioned initialization conditions.

4.1.3. The scalet equation: $Z^2x^2 + gx^4$. The scalet equation is obtained from the relations (which follow upon choosing $Q(x) = x^2/2$)

$$\partial_\alpha\mu_p(\alpha,b) = -\alpha\mu_{p+2}(\alpha,b) \tag{88}$$

or

$$\partial_\alpha\mu_p(\alpha,b) = -\alpha\sum_{\ell=0}^{m_s=3}\hat{\mathcal{M}}_{p,\ell}(\alpha,b;E,\epsilon)\mu_\ell(\alpha,b) \tag{89}$$

where

$$\hat{\mathcal{M}}_{p,\ell}(\alpha,b;E,\epsilon) = M_{p+2,\ell}(\alpha,b;E,\epsilon) \tag{90}$$

($\mathcal{M} \equiv -\alpha\hat{\mathcal{M}}$).

Since all the scalets ($p \geqslant 3$) are linearly dependent on the $\{\mu_\ell(\alpha,b)|0 \leqslant \ell \leqslant 3\}$, we can limit the above differentiation with respect to these, generating the scalet equation:

$$\partial_\alpha\begin{pmatrix}\mu_0(\alpha,b)\\ \mu_1(\alpha,b)\\ \mu_2(\alpha,b)\\ \mu_3(\alpha,b)\end{pmatrix} = -\alpha\begin{pmatrix}0,0,1\quad 0\\ 0,0,0,1\\ \hat{\mathcal{M}}_{2,0},\hat{\mathcal{M}}_{2,1},\hat{\mathcal{M}}_{2,2},\hat{\mathcal{M}}_{2,3}\\ \hat{\mathcal{M}}_{3,0},\hat{\mathcal{M}}_{3,1},\hat{\mathcal{M}}_{3,2},\hat{\mathcal{M}}_{3,3}\end{pmatrix}\begin{pmatrix}\mu_0(\alpha,b)\\ \mu_1(\alpha,b)\\ \mu_2(\alpha,b)\\ \mu_3(\alpha,b)\end{pmatrix} \tag{91}$$

where the $\hat{\mathcal{M}}$ matrix is

$$\begin{pmatrix}0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\\ -\frac{1}{g}\begin{pmatrix}\epsilon\alpha^2+\\ V(b)-E\end{pmatrix} & -\frac{V'(b)}{g} & -\frac{1}{g}\begin{pmatrix}m+6gb^2\\ -\epsilon\alpha^4\end{pmatrix} & -4b\\ 4\frac{b}{g}\begin{pmatrix}\epsilon\alpha^2+\\ V(b)-E\end{pmatrix} & -\frac{1}{g}\begin{pmatrix}3\epsilon\alpha^2-7b^2m\\ -15gb^4-E\end{pmatrix} & -\frac{1}{g}\begin{pmatrix}4\epsilon b\alpha^4\\ -2bm-20gb^3\end{pmatrix} & -\frac{1}{g}\begin{pmatrix}m-10gb^2\\ -\epsilon\alpha^4\end{pmatrix}\end{pmatrix}. \tag{92}$$

Table 1. Ground and first excited state results for $V(x) = -5x^2 + x^4$.

J_{max}	$E_{gr}(L_{min}, L_{max})$	$E_1(L_{min}, L_{max})$
5	−3.404 60 (−2, 0)	−3.250 92 (−2, 0)
5	−3.414 01 (−2, 2)	−3.260 66 (−2, 2)
7	−3.412 38 (−2, 2)	−3.258 35 (−2, 2)
11	−3.40 952 (−2, 2)	−3.249 28 (−2, 2)
	−3.410 142 761[a]	−3.250 675 362[a]

[a] Tymczak *et al* (1998a).

Table 2. Ground state results for $V(x) = x^4$.

J_{max}	$E_{gr}(L_{min}, L_{max})$
5	1.061 76(−2, 4)
11	1.061 76 (−2, 4)
	1.060 3621[a]

[a] Handy and Bessis (1985).

4.2. TPQ-DCWT results for the double-well potential, $Z^2 = -5$, $g = 1$

We numerically generated the basic scalet solutions, $\overrightarrow{\mathcal{B}}^{(\ell)}(\alpha, b; E, \epsilon)$ (i.e. refer to equation (60)), according to a fourth-order Runge–Kutta procedure, and computed the (Mexican hat) wavelet transform through equation (69). This defines the $\Psi_{DCWT} \equiv \Psi_{L,J}$, representation in equation (65), on which the numerically differentiated TPQ conditions are applied (equation (70)). Specifically, we set $\partial_\tau^2 \Psi_{L,J}(\tau) \rightarrow \big(\Psi_{L,J}(\tau + \delta\tau) + \Psi_{L,J}(\tau - \delta\tau) - 2\Psi_{L,J}(\tau)\big)/\delta\tau^2$, where $\delta\tau = 10^{-3}$. Good results were obtained, as indicated in table 1. No spurious energies were detected, as compared with the results of HMBB.

Instead of numerically differentiating, we can adopt the DCWT representation for $\partial_x^2 \Psi(x)$, as noted in equation (76), where the required wavelet transform coefficients are computed from equation (73). The corresponding TPQ condition, in equation (77), duplicates the results in table 1 (although in this case a few spurious solutions were generated).

4.2.1. TPQ-DCWT results for the quartic potential, $Z^2 = 0$, $g = 1$. The same analysis can be extended to the quartic potential problem case ($Z^2 \rightarrow 0$)

$$-\epsilon \partial_x^2 \Psi(x) + x^4 \Psi(x) = E\Psi(x). \tag{93}$$

The turning points are now real and imaginary:

$$\tau_\ell(E) = \begin{cases} \pm E^{1/4} & \text{for} \quad \ell = 1, 2 \\ \pm \mathrm{i} E^{1/4} & \text{for} \quad \ell = 0, 3. \end{cases} \tag{94}$$

We find that the implementation of the TPQ-DCWT condition yields good results. The limited results cited in table 2 ensue from the TPQ-DCWT analysis as applied to the $\partial_x^2 \Psi(x)$ formalism in equations (73)–(77).

5. Kinetic energy perturbation in the scalet representation

As we have repeatedly emphasized, the scalet equation matrix (for appropriate scaling functions, $S(x) = \mathrm{e}^{-Q(x)}$), will be analytic in the inverse scale variable, α, as well as in

the kinetic energy coupling strength, ϵ. The structure of the α power-series expansion does not suggest any interesting zeroth-order features of immediate significance to the physical system under study. However, the ϵ power series does have a very suggestive, and plausibly relevant structure, impacting bound states. We have seen in the previous discussions that the zeroth-order, in ϵ, structure of the power moment ME relation, suggests the symbolic wavefunction configuration, $\Psi^{(0)}(x) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell \delta(x - \tau_\ell(E))$, for arbitrary E. Clearly, this is to be interpreted as a superposition over bounded (i.e. Dirac distribution) configurations. The immediate issues are: can we make this precise, and can we construct the physical, bound state, solutions around such (suggestive) localized structures. The answer to both of these is yes, as developed in this section. We outline the necessary theoretical form of this, although its numerical implementation is still under study.

The scalet ϵ expansion is defined by $\overrightarrow{\mu}(\alpha, b; E, \epsilon) = \sum_{j=0}^{\infty} \epsilon^j \overrightarrow{\mu}^{(j)}(\alpha, b; E)$. We have symbolically derived the zeroth order (in ϵ) form of the scalet configuration in equation (54). We prove this explicitly within the scalet representation, for the $V(x) = Z^2x^2 + gx^4$ case, in the following subsection. The general case follows similarly (subsection (B)). We also specify in subsection 5., the recursive structure of the ϵ-expansion, scalet configurations, and indicate the nature of their localized form, both in α and b, around the respective turning points. The implementation of TPQ, within such kinetic energy expansion representations, is still under investigation. Nevertheless, the theoretical attraction of such, localized, scalet basis-like configurations, is that they are well adapted to the given problem. This is not usually the case in wavelet analysis, where the selection of an optimal dual-wavelet pair is not immediately discernible for a given problem.

5.1. The zeroth-order scalet equation solution: $Z^2x^2 + gx^4$

We show how to prove the zeroth-order form of the scalet equation solution, directly from the scalet equation. We do this for the generic quartic anharmonic oscillator problem.

From equation (86) the zeroth-order moment equation becomes

$$\mu_{p+4}^{(0)}(\alpha, b) = \sum_{\ell=0}^{m_s=3} \frac{1}{\ell!} \partial_b^\ell \mathcal{K}(b)\, \mu_{p+\ell}^{(0)}(\alpha, b) \tag{95}$$

for $p \geqslant 0$, where $\mathcal{K}(b) \equiv g^{-1}(E - V(b))$. From this, and equation (90), it follows that

$$\hat{\mathcal{M}}_{2,\ell}(\alpha, b; E, 0) = M_{4,\ell}(\alpha, b; E, 0) = \frac{1}{\ell!} \partial_b^\ell \mathcal{K}(b) \tag{96}$$

and

$$\hat{\mathcal{M}}_{3,\ell}(\alpha, b, E, 0) = \begin{cases} \dfrac{1}{m_s!} \mathcal{K}(b)\, \partial_b^{m_s} \mathcal{K}(b) & \text{for} \quad \ell = 0 \\ \dfrac{1}{(\ell-1)!} \partial_b^{\ell-1} \mathcal{K} + \dfrac{1}{\ell! m_s!} \partial_b^\ell \mathcal{K}(b)\, \partial_b^{m_s} \mathcal{K}(b) & \text{for} \quad 1 \leqslant \ell \leqslant 3. \end{cases} \tag{97}$$

We want to determine the eigenstates of the zeroth-order scalet equation. From the fourth-degree nature of the potential,

$$\sum_{\ell=0}^{4} \frac{1}{\ell!} \partial_b^\ell \mathcal{K}(b)\, \Delta^\ell = \mathcal{K}(b + \Delta). \tag{98}$$

If we take $\Delta = (\tau_{\ell_2}(E) - b)$, then

$$\sum_{\ell_1=0}^{4} \frac{1}{\ell_1!} \partial_b^{\ell_1} \mathcal{K}(b)\, (\tau_{\ell_2}(E) - b)^{\ell_1} = 0 \tag{99}$$

by definition of the turning point, and thus

$$\sum_{\ell_1=0}^{3} \mathcal{M}_{2,\ell_1}(\alpha, b, E, 0)\,(\tau_{\ell_2}(E) - b)^{\ell_1} = (\tau_{\ell_2}(E) - b)^4. \tag{100}$$

If we multiply both sides by $(\tau_{\ell_2}(E) - b)$ we obtain the desired relation

$$\sum_{\ell_1=0}^{3} \mathcal{M}_{3,\ell_1}(\alpha, b, E, 0)\,(\tau_{\ell_2}(E) - b)^{\ell_1} = (\tau_{\ell_2}(E) - b)^5. \tag{101}$$

From the preceding relations, one can easily verify that the eigenstates of the $\epsilon = 0$ scalet equation are

$$\begin{pmatrix} \mathcal{E}_0^{(\ell)}(\alpha, b) \\ \mathcal{E}_1^{(\ell)}(\alpha, b) \\ \mathcal{E}_2^{(\ell)}(\alpha, b) \\ \mathcal{E}_3^{(\ell)}(\alpha, b) \end{pmatrix} = \begin{pmatrix} (\tau_\ell(E) - b)^0 \\ (\tau_\ell(E) - b)^1 \\ (\tau_\ell(E) - b)^2 \\ (\tau_\ell(E) - b)^3 \end{pmatrix} \mathrm{e}^{-\frac{\alpha^2}{2}(\tau_\ell(E)-b)^2} \tag{102}$$

which satisfy $\partial_\gamma \overrightarrow{\mathcal{E}}^{(\ell)}(\gamma, b) = -\hat{\mathcal{M}}(b, E, \epsilon = 0)^M \overrightarrow{\mathcal{E}}^{(\ell)}(\gamma, b)$, or

$$\hat{\mathcal{M}}(b, E, \epsilon = 0)\,\overrightarrow{\mathcal{E}}^{(\ell)}(\gamma, b) = (\tau_\ell(E) - b)^2 \overrightarrow{\mathcal{E}}^{(\ell)}(\gamma, b) \tag{103}$$

where $\gamma \equiv \alpha^2/2$. Therefore, the general solution is

$$\begin{pmatrix} \mu_0^{(0)}(\alpha, b) \\ \mu_1^{(0)}(\alpha, b) \\ \mu_2^{(0)}(\alpha, b) \\ \mu_3^{(0)}(\alpha, b) \end{pmatrix} = \sum_{\ell=0}^{m_s=3} \mathcal{A}_\ell \begin{pmatrix} (\tau_\ell(E) - b)^0 \\ (\tau_\ell(E) - b)^1 \\ (\tau_\ell(E) - b)^2 \\ (\tau_\ell(E) - b)^3 \end{pmatrix} \mathrm{e}^{-\frac{\alpha^2}{2}(\tau_\ell(E)-b)^2} \tag{104}$$

which is consistent with the symbolic configuration space solution $\Psi^{(0)}(x) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell \delta(x - \tau_\ell(E))$, yielding the scaled and translated moments $\mu_\ell^{(0)}(\alpha, b) = \int \mathrm{d}x\, x^\ell \mathrm{e}^{-\frac{\alpha^2}{2}x^2} \Psi^{(0)}(x + b) = \sum_{\ell_2=0}^{m_s} \mathcal{A}_{\ell_2}(\tau_{\ell_2}(E) - b)^\ell \mathrm{e}^{-\frac{\alpha^2}{2}(\tau_{\ell_2}(E)-b)^2}$.

It will be noted that the asymptotic b dependence of the zeroth-order scalet solutions is different for $\alpha = 0$ and $\alpha \neq 0$. In the zero-scale limit, these zero-order solutions, as functions of $\mathrm{Re}(b)$, become proportional to Dirac measures sitting at $\mathrm{Re}(b) = \mathrm{Re}(\tau_\ell)$.

5.2. A more general proof for $\mu_p^{(0)}(\alpha, b) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell(\tau_\ell(E) - b)^p \mathrm{e}^{-Q(\alpha(\tau_\ell(E)-b))}$

A more general argument can be structured as follows. From equation (45), we see that the zeroth-order scalets must satisfy (as in equation (52))

$$\mu_p^{(0)}(\alpha, b) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell(\alpha, b)(\tau_\ell(b; E))^p \tag{105}$$

for $p \geqslant 0$. The 'shifted' turning points must satisfy $V(\tau_\ell(b; E) + b) = E$, or $\tau_\ell(b; E) = \tau_\ell(E) - b$.

The $\mathcal{A}_\ell(\alpha, b)$ coefficients are restricted by the defining relation $\partial_\alpha \mu_p(\alpha, b; E, \epsilon) = -\alpha \mu_{p+2}(\alpha, b; E, \epsilon)$, for the case $Q(x) = -x^2/2$. The generalization of this, for arbitrary Qs, is immediate. We then obtain

$$\sum_{\ell=0}^{m_s} \partial_\alpha \mathcal{A}_\ell(\alpha, b)(\tau_\ell(b; E))^p = -\alpha \sum_{\ell=0}^{m_s} \mathcal{A}_\ell(\alpha, b)(\tau_\ell(b; E))^{p+2} \tag{106}$$

for $p \geqslant 0$. Therefore,

$$\partial_\alpha \mathcal{A}_\ell(\alpha, b) = -\alpha(\tau_\ell(b; E))^2 \mathcal{A}_\ell(\alpha, b) \tag{107}$$

for $0 \leqslant \ell \leqslant m_s$. That is,

$$\mathcal{A}_\ell(\alpha, b) = \mathcal{A}_\ell(b) \mathrm{e}^{-\frac{\alpha^2}{2}(\tau_\ell(E)-b)^2} \tag{108}$$

hence

$$\mu_p^{(0)}(\alpha, b) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell(b)(\tau_\ell(E) - b)^p \mathrm{e}^{-\frac{\alpha^2}{2}(\tau_\ell(E)-b)^2} \tag{109}$$

for $p \geqslant 0$. Finally, from the infinite-scale initial condition in equation (64), we obtain $\mathcal{A}_\ell(b) = \mathcal{A}_\ell$.

5.3. Generating the scalet, kinetic energy, perturbative expansion

The scalet equation, for appropriate choices of scaling function, will have an analytic ϵ expansion $\overrightarrow{\mu}(\alpha, b; E, \epsilon) = \sum_{j=0}^{\infty} \epsilon^j \overrightarrow{\mu}^{(j)}(\alpha, b; E)$. From lemma 4, the scalet equation matrix will be of first order in ϵ (for polynomial potentials, $B = 0$, Gaussian scaling functions, and $m_s \geqslant 3$), facilitating the perturbative generation of the $\overrightarrow{\mu}^{(j)}(\alpha, b; E)$ configurations. Thus, from the perturbative expansion of the scalet equation, we have $\partial_\alpha \overrightarrow{\mu}^{(j+1)}(\alpha, b; E) = \mathcal{M}^{(0)}(\alpha, b; E)\overrightarrow{\mu}^{(j+1)}(\alpha, b; E) + \mathcal{M}^{(1)}(\alpha, b; E)\overrightarrow{\mu}^{(j)}(\alpha, b; E)$, or

$$\big(\partial_\alpha - \mathcal{M}^{(0)}(\alpha, b; E)\big)\overrightarrow{\mu}^{(j+1)}(\alpha, b; E) = \mathcal{M}^{(1)}(\alpha, b; E)\overrightarrow{\mu}^{(j)}(\alpha, b; E) \tag{110}$$

for $j \geqslant 0$. At $\alpha = 0$, to all orders we impose the initial conditions:

$$\overrightarrow{\mu}(\alpha = 0, b; E, \epsilon) = \sum_{\ell=0}^{m_s} c_\ell \, \overrightarrow{\mathcal{S}^{(\ell)}}(0, b) \tag{111}$$

where (from equation (57) and equation (62))

$$\overrightarrow{\mathcal{S}^{(\ell)}}(0, b) = \begin{cases} \overrightarrow{\mathcal{B}^{(\ell)}}(0, b) & c_\ell \equiv \mu_\ell \\ \overrightarrow{\Upsilon^{(\ell)}}(0, b) & \text{a } c_\ell \equiv \mathcal{A}_\ell. \end{cases} \tag{112}$$

However, these are automatically of zeroth order in ϵ, hence

$$\overrightarrow{\mu}^{(j)}(0, b; E) = \overrightarrow{0} \tag{113}$$

for all $j \geqslant 1$. The zeroth-order form of the scalet configuration, $\overrightarrow{\mu}^{(0)}(\alpha, b; E)$, was defined in the previous subsections.

From the (assumed) boundedness properties of the scaling function, $S(z) = \mathrm{e}^{-Q(z)}$, along the asymptotic $\mathrm{Re}(z) \to \pm\infty$ direction, we have that

$$\lim_{|\,\mathrm{Re}(b)| \to \infty} \overrightarrow{\mu}^{(0)}(\alpha, b; E) = 0 \tag{114}$$

exponentially fast. Similarly, for some sufficiently large $\mathrm{Re}(b)$, in the zero-scale asymptotic limit we have

$$\lim_{a \to 0} \overrightarrow{\mu}^{(0)}(\alpha, b; E) = 0 \tag{115}$$

also exponentially fast.

These properties are preserved by $\overrightarrow{\mu}^{(j+1)}(\alpha, b; E)$, for $j \geqslant 0$. The inductive argument is immediate. If the right-hand side of equation (110) goes to zero, then $\overrightarrow{\mu}^{(j+1)}(\alpha, b; E)$ are dominated by the zeroth-order modes of the scalet equation, which automatically satisfy the above.

The exact structure of the $\overrightarrow{\mu}^{(j+1)}(\alpha, b; E)$s is complicated and depends on the choice of the polynomial, Q, and the nature of the turning points. However, the $\overrightarrow{\mu}^{(0)}(\alpha, b)$ configuration, as a function of $\mathrm{Re}(b)$, corresponds to localized structures situated at the $\mathrm{Re}(\tau_\ell(E))$ values. At an arbitrary $b \approx \tau_\ell(E)$, one can have either exponentially growing or decaying behaviour, as $a \to 0$.

One of the objectives of using such kinetic energy expansions is to implement a TPQ analysis in terms of them. At each of the turning points, $\tau_\ell(E)$, the TPQ condition becomes viable only at some moderately small scale, a_ℓ. If these scales are not too small, it may be possible to work within a low-order ϵ-expansion, and generate good approximate values for the quantized states. These issues are inherent to the scaling transform extremal scale analysis reviewed in appendix B. As noted at the outset, the numerical implementation of this TPQ analysis is under investigation.

6. Zero-scale asymptotic behaviour of the scalet solutions

In the introduction, we made reference to the fact that most of the scalet equation modes, converge to the Schrödinger equation, in the zero-scale limit, regardless of the chosen energy value. We prove this here in two ways. The first is to argue that compactly supported scalets (as defined below) are asymptotic to the scalets, in the zero-scale limit. However, such compactly supported scalets are definable for any bounded or unbounded solution of the Schrödinger equation. Thus, it should be expected that most of the scalet solutions should converge to the Schrödinger equation. The second approach is to work out the leading asymptotic form of the scalet solutions, in the zero-scale limit. We do this for the generic quartic anharmonic oscillator, as well as the non-Hermitian potential discussed earlier. In all of these cases, we confirm the existence of a large number of scalet modes that converge to the Schrödinger equation; thereby preventing a direct TPQ-scalet analysis, as argued in the introduction (although such a procedure may work within the kinetic energy expansion representation discussed in the previous section).

6.1. Convergence of scalet and Schrödinger solutions

An important argument in proving that (most of) the scalet solutions should converge to the Schrödinger equation is to study the behaviour of the compactly supported scalets

$$\mu_p^{(\delta_1,\delta_2)}(a, b) \equiv \int_{-\delta_1}^{\delta_2} \mathrm{d}x\, x^p \mathrm{e}^{-Q(x/a)} \Psi(x + b). \tag{116}$$

These exist, regardless of Ψ's behaviour at infinity ($|x| \to \infty$), because they are defined on a compact domain.

The $\mu_p^{(\delta_1,\delta_2)}(a, b)$s satisfy a moment equation that is identical, in structure, to that for the scalets, except for the appearance of boundary terms. Thus, as in section 2.2.3, let $\Psi(x)$ be an arbitrary solution (bounded or not) to the Schrödinger equation, for an arbitrary energy value, E. We can translate the Schrödinger equation by an amount b, and work with $\Phi_{a,b}(x) \equiv \mathrm{e}^{-Q(x/a)}\Psi(x+b)$. We then apply $\int_{-\delta_1}^{\delta_2} \mathrm{d}x\, x^p$, to both sides of the differential equation for $\Phi_{a,b}(x)$, after first multiplying by the denominator of the potential, $V(x + b) \equiv \frac{P_N(x+b)}{P_D(x+b)}$.

The ensuing integration by parts generates the boundary terms

$$\alpha x^p P_D(x+b) Q'(\alpha x) \mathrm{e}^{-Q(x/a)} \Psi(x+b)\big|_{-\delta_1}^{\delta_2} \tag{117}$$

and

$$x^p P_D(x+b) \partial_x \big(\mathrm{e}^{-Q(x/a)} \Psi(x+b)\big)\big|_{-\delta_1}^{\delta_2} - \partial_x \big(x^p P_D(x+b)\big) \mathrm{e}^{-Q(x/a)} \Psi(x+b)\big|_{-\delta_1}^{\delta_2}. \tag{118}$$

Since both $\delta_{1,2}$ are fixed, as $a \to 0$ the exponential factor dominates, and the boundary terms go to zero. Thus the moment equation satisfied by $\mu_p^{-\delta_1,\delta_2}(a,b)$, is asymptotic to that satisfied by the $\mu_p(a,b)$s, in the zero-scale limit. That is, $\mu_p^{(-\delta_1,\delta_2)}(a,b) = \sum_{\ell=0}^{m_s} M_{p,\ell}(a,b;E,\epsilon)\mu_\ell^{(-\delta_1,\delta_2)}(a,b)$, in the zero-scale limit. We also note that $\partial_\alpha \mu_p^{-\delta_1,\delta_2}(\alpha,b) = \mu_p^{-\delta_1,\delta_2}(\alpha,b)$, exactly. Thus, the compact scalets satisfy a scalet-like differential equation which is asymptotic to the original scalet equation (with the disappearance of the boundary terms).

In the zero-scale asymptotic limit, the compact moments yield a pointwise recovery for the underlying configuration. This follows from the standard argument:

$$\mu_p^{(\delta_1,\delta_2)}(a,b) = a^{1+p} \int_{-\delta_1/a}^{\delta_2/a} \mathrm{d}y\, y^p \mathrm{e}^{-Q(y)} \Psi(ay+b) \tag{119}$$

or

$$\lim_{a\to 0} \mu_p^{(\delta_1,\delta_2)}(a,b) \to a^{1+p} \sum_{n=0}^{\infty} \frac{\nu_{n+p} a^n}{n!} \partial_b^n \Psi(b). \tag{120}$$

Thus, in the zero-scale limit we have

$$\lim_{a\to 0} \left(\frac{n_p^*! \mu_p^{(\delta_1,\delta_2)}(a,b)}{a^{1+p+n_p^*} \nu_{p+n_p^*}} \right) = \partial_b^{n_p^*} \Psi(b) \tag{121}$$

where n_p^* was defined previously (equation (30)).

The preceding analysis strongly suggests that in the zero-scale limit, a subset of the scalet solutions must become solutions of the Schrödinger equation. This is indeed verified numerically. A leading-order JWKB analysis for the scalet equation also confirms this, as is presented below.

6.2. Intermediate-scale behaviour of scalet equation: $Z^2x^2 + gx^4$

Before delving into the asymptotic, zero-scale limit, analysis of the scalet equation solutions, we outline an intermediate analysis for the quartic anharmonic oscillator class of problems. This will help us obtain a better understanding of the behaviour of the scalet equation solutions.

It is possible to obtain some qualitative properties of the scalet equation for moderate scale values. In order to do this, one should work with the generalized scaling transform expressions

$$U_\ell(\alpha,b) \equiv \frac{\alpha^{1+\ell+n_\ell^*} n_\ell^*!}{\nu_{\ell+n_\ell^*}} \mu_\ell(\alpha,b) \tag{122}$$

(refer to equation (30)).

We can convert the scalet equation into the U-representation. First, we note that $\nu_{2\rho} = (-\partial_s)^\rho \sqrt{\frac{\pi}{s}}$, for $s = \frac{1}{2}$. Accordingly, $\nu_0 = \nu_2 = \sqrt{2\pi}$ and $\nu_4 = 3\sqrt{2\pi}$. Thus we have:

$$\begin{pmatrix} U_0(a,b) \\ U_1(a,b) \\ U_2(a,b) \\ U_3(a,b) \end{pmatrix} = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} \dfrac{\mu_0(a,b)}{a} \\ \dfrac{\mu_1(a,b)}{a^3} \\ \dfrac{\mu_2(a,b)}{a^3} \\ \dfrac{\mu_3(a,b)}{3a^5} \end{pmatrix}. \tag{123}$$

That is, $n^*_\ell = \{0,1,0,1\}$ (hence $n^*_\ell! \equiv 1$), for $\ell = \{0,1,2,3\}$. We also have $\mu_\ell(a,b) = a^{n^*_\ell+\ell+1}\nu_{\ell+n^*_\ell}U_\ell(a,b)$.

Inserting this in the scalet equation (i.e. $\partial_\alpha = -a^2\partial_a$)

$$-a^2\partial_a(a^{n^*_\ell+\ell+1}\nu_{\ell+n^*_\ell}U_\ell(a,b)) = \sum_{\ell_v=0}^{m_s} \mathcal{M}_{\ell,\ell_v}(a,b)a^{n^*_{\ell_v}+\ell_v+1}\nu_{\ell_v+n^*_{\ell_v}}U_{\ell_v}(a,b) \tag{124}$$

or

$$-a^2\partial_a \overrightarrow{U}(a,b) = \mathcal{U}(E,\epsilon;a,b)\overrightarrow{U}(a,b) \tag{125}$$

where

$$\mathcal{U}_{\ell_1,\ell_2}(E,\epsilon;a,b) = \left(\left[\mathcal{M}_{\ell_1,\ell_2}(a,b)\frac{a^{n^*_{\ell_2}+\ell_2}}{a^{n^*_{\ell_1}+\ell_1}}\frac{\nu_{\ell_2+n^*_{\ell_2}}}{\nu_{\ell_1}+n^*_{\ell_1}} + a\delta_{\ell_1,\ell_2}(n^*_{\ell_1}+\ell_1+1)\right]\right) \tag{126}$$

and the $\mathcal{U}$ matrix is given by (the ensuing analysis is easier in terms of α)

$$\begin{pmatrix} \frac{1}{\alpha} & 0 & -\frac{1}{\alpha} & 0 \\ 0 & \frac{3}{\alpha} & 0 & -\frac{3}{\alpha} \\ \frac{\alpha^3}{g}\begin{pmatrix}\epsilon\alpha^2+\\ V(b)-E\end{pmatrix} & \frac{\alpha}{g}V'(b) & \frac{\alpha}{g}\begin{pmatrix}m+6gb^2\\ +\frac{3g}{\alpha^2}-\epsilon\alpha^4\end{pmatrix} & \frac{12b}{\alpha} \\ -\frac{4b\alpha^5}{3g}\begin{pmatrix}\epsilon\alpha^2+\\ V(b)-E\end{pmatrix} & \frac{\alpha^3}{3g}\begin{pmatrix}3\epsilon\alpha^2-E\\ -7b^2m-15gb^4\end{pmatrix} & \frac{\alpha^3}{3g}\begin{pmatrix}4\epsilon b\alpha^4\\ -2bm-20gb^3\end{pmatrix} & \frac{\alpha}{g}\begin{pmatrix}m-\epsilon\alpha^4\\ +\frac{5g}{\alpha^2}-10gb^2\end{pmatrix} \end{pmatrix}. \tag{127}$$

Empirically, for the double-well quartic anharmonic oscillator problem ($Z^2 = -5$, $g = 1$) one observes that as α becomes large, the basic scalet solutions (chosen either according to equation (57) or equation (62)), regardless of the energy, generate $U_\ell(\alpha,b)$s that converge, pointwise (at fixed b, $\alpha \to \infty$) to a solution of the Schrödinger equation, as indicated in equation (30).

There are two phases to this convergence. The first is an abrupt (exponential) attraction between U_0 and U_2, and U_1 and U_3. Once they become sufficiently close to each other, for the respective pairs, the differences $U_0 - U_2$ and $U_1 - U_3$ will go to zero, in an algebraic manner, consistent with the asymptotic expansion in equation (29).

In order to determine the first phase of the asymptotic behaviour for the U_ℓs we identify the dominant terms of various matrix elements given above. These are

$$\lim_{\alpha\to\infty}\mathcal{U}\to\begin{pmatrix} \frac{1}{\alpha} & 0 & -\frac{1}{\alpha} & 0 \\ 0 & \frac{3}{\alpha} & 0 & -\frac{3}{\alpha} \\ \frac{\epsilon\alpha^5}{g} & \frac{\alpha}{g}V'(b) & -\frac{\epsilon\alpha^5}{g} & \frac{12b}{\alpha} \\ -\frac{4b\epsilon\alpha^7}{3g} & \frac{\epsilon\alpha^5}{g} & \frac{4\epsilon b\alpha^7}{3g} & -\frac{\epsilon\alpha^5}{g} \end{pmatrix}. \tag{128}$$

Upon subtracting the third row from the first, and the fourth row from the second, and identifying the dominant terms, we obtain the asymptotic relations

$$\partial_\alpha\begin{pmatrix} U_0-U_2 \\ U_1-U_3 \end{pmatrix} = -\begin{pmatrix} \frac{\epsilon\alpha^5}{g} & 0 \\ -\frac{4b\epsilon\alpha^7}{3g} & \frac{\epsilon\alpha^5}{g} \end{pmatrix}\begin{pmatrix} U_0-U_2 \\ U_1-U_3 \end{pmatrix}. \tag{129}$$

Accordingly, we then have

$$\lim_{\alpha\to 0}(U_0(\alpha,b)-U_2(\alpha,b)) = \mathcal{C}\mathrm{e}^{-\frac{\epsilon}{6g}\alpha^6} \tag{130}$$

and likewise for $(U_1(\alpha,b)-U_3(\alpha,b))$.

We can define the critical scale marking the onset of the mutually attractive behaviour of the U_ℓs:

$$a_c = \left(\frac{\epsilon}{6g}\right)^{1/6}. \tag{131}$$

For $g=\epsilon=1$, $a_c\approx 0.74$ ($a=0.64$ for $\mathrm{e}^{-\alpha^6/6}=10^{-1}$).

As α increases beyond the critical value $\frac{1}{a_c}$, the various terms of the U_ℓ equation dominate in accordance with the asymptotic expansion given in equation (29).

6.3. JWKB asymptotic analysis of the scalet equation: $Z^2x^2+gx^4$

We can implement a lowest-order JWKB analysis on the generic quartic anharmonic oscillator scalet equations in order to confirm the dominant nature of the Schrödinger equation solutions, in the zero-scale limit. We do so by first reducing the scalet equations to a fourth-order ordinary differential equation. This is best done in terms of the $\mathcal{M}(\alpha,b;E,\epsilon)=\alpha\hat{\mathcal{M}}(\alpha^2,b;E,\epsilon)$, representation, which converts the scalet equation into a differential expression in the variable $\gamma\equiv\frac{1}{2}\alpha^2$, which we adopt below.

In order to facilitate the algebra, we rewrite equation (91) as

$$-\partial_\gamma\begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 0,0,1,0 \\ 0,0,0,1 \\ A,B,C,D \\ F,G,H,I \end{pmatrix}\begin{pmatrix} w \\ x \\ y \\ z \end{pmatrix} \tag{132}$$

where $(w,x,y,z)=(\mu_0(\gamma,b),\mu_1(\gamma,b),\mu_2(\gamma,b),\mu_3(\gamma,b))$, $(A,B,C,D)=(\hat{\mathcal{M}}_{2,0},\ldots)$ and $(F,G,H,I)=(\hat{\mathcal{M}}_{3,0},\ldots)$.

From the first two relations we have $y = -w'$ and $z = -x'$, thus we can reduce the above to

$$\begin{pmatrix} w'' \\ x'' \end{pmatrix} = \begin{pmatrix} A, B, C, D \\ F, G, H, I \end{pmatrix} \begin{pmatrix} w \\ x \\ -w' \\ -x' \end{pmatrix}. \tag{133}$$

The first equation (i.e. $w'' \ldots$) involves both x and x'. We want to find a relation relating these two quantities to various derivatives of w; thereby generating one differential equation for w. We do so by differentiating the first equation, twice, each time substituting the second for x''. Thus,

$$w''' = (A', B', C', D') \cdot (w, x, -w', -x') + (A, B, C, D) \cdot (w', x', -w'', -x''). \tag{134}$$

We substitute for x'', obtaining

$$\begin{aligned} w''' = {} & (A', B', C', D') \cdot (w, x, -w', -x') + (A, B, C, 0) \cdot (w', x', -w'', 0) \\ & -D\big((F, G, H, I) \cdot (w, x, -w', -x')\big) \end{aligned} \tag{135}$$

or

$$\begin{aligned} w''' = {} & (A' - DF, B' - DG, C' - DH, D' - DI) \cdot (w, x, -w', -x') \\ & +(A, B, C, 0) \cdot (w', x', -w'', 0). \end{aligned} \tag{136}$$

Repeating the same procedure, we now obtain

$$\begin{aligned} w'''' = {} & (A' - DF, B' - DG, C' - DH, D' - DI) \cdot (w', x', -w'', -x'') \\ & +(A, B, C, 0) \cdot (w'', x'', -w''', 0) \\ & +(A'' - (DF)', B'' - (DG)', C'' - (DH)', D'' - (DI)') \cdot (w, x, -w', -x') \\ & +(A', B', C', 0) \cdot (w', x', -w'', 0). \end{aligned} \tag{137}$$

Again, we substitute for the x'' contribution, $(B - D' + DI)x''$:

$$\begin{aligned} w'''' = {} & (A' - DF, B' - DG, C' - DH, 0) \cdot (w', x', -w'', 0) \\ & +(A, 0, C, 0) \cdot (w'', 0, -w''', 0) + (A'' - (DF)', B'' - (DG)', C'' \\ & -(DH)', D'' - (DI)') \cdot (w, x, -w', -x') + (A', B', C', 0) \cdot (w', x', -w'', 0) \\ & +(B - D' + DI)\big((F, G, H, I) \cdot (w, x, -w', -x')\big). \end{aligned} \tag{138}$$

Combining all the x, x' terms:

$$\begin{aligned} & w'''' + Cw''' + [2C' - DH - A]w'' + [DF - 2A' + C'' - (DH)' + (B - D' + DI)H]w' \\ & \quad +[(DF)' - A'' - (B - D' + DI)F]w = [B'' - (DG)' + (B - D' + DI)G]x \\ & \quad +[2B' - DG - D'' + (DI)' - I(B - D' + DI)]x'. \end{aligned} \tag{139}$$

We denote the left-hand side by $\sum_{j=0}^{4} \Lambda_{1j} w^{(j)}$.

Similarly, from equation (136), we have

$$w''' + Cw'' + [C' - DH - A]w' + [DF - A']w = [B' - DG]x + [DI - D' + B]x'. \tag{140}$$

We denote the left-hand side by $\sum_{j=0}^{3} \Lambda_{2,j} w^{(j)}$.

We can now solve for x and x':

$$\begin{pmatrix} x \\ x' \end{pmatrix} = \frac{1}{\mathrm{Det}} \begin{pmatrix} \Omega_{22}, -\Omega_{12} \\ -\Omega_{21}, \Omega_{11} \end{pmatrix} \begin{pmatrix} \sum_{j=0}^{4} \Lambda_{1,j} w^{(j)} \\ \sum_{j=0}^{3} \Lambda_{2j} w^{(j)} \end{pmatrix} \tag{141}$$

$$\Omega_{i,j} = \begin{cases} B'' - (DG)' + (B - D' + DI)G & \text{for } i = 1 \quad j = 1 \\ 2B' - DG - D'' + (DI)' - I(B - D' + DI) & \text{for } i = 1 \quad j = 2 \\ B' - DG & \text{for } i = 2 \quad j = 1 \\ DI - D' + B & \text{for } i = 2 \quad j = 2 \end{cases} \tag{142}$$

and

$$\Delta = \Omega_{11}\Omega_{22} - \Omega_{12}\Omega_{21}. \tag{143}$$

Substituting in the first of the two relations in equation (133), we obtain the desired fourth-order differential equation

$$w'' = (A, B, C, D) \cdot (w, x[w'''', w''', w'', w', w], -w', -x'[w'''', w''', w'', w', w]) \tag{144}$$

or

$$\Delta \times (w'' - A\ w + C\ w') = B\left(\sum_{j=0}^{4} [\Omega_{22}\Lambda_{1,j} - \Omega_{12}\Lambda_{2,j}]w^{(j)} \right) + D\left(\sum_{j=0}^{4} [\Omega_{21}\Lambda_{1,j} - \Omega_{11}\Lambda_{2,j}]w^{(j)} \right), \tag{145}$$

becoming (i.e. $\Lambda_{2,4} \equiv 0$)

$$\Delta \times (w'' - A\ w + C\ w') = \sum_{j=0}^{4} \left([(B\Omega_{22} + D\Omega_{21}]\Lambda_{1,j} - [B\Omega_{12} + D\Omega_{11}]\Lambda_{2,j}] \right) w^{(j)}. \tag{146}$$

The dominant coefficients for this differential equation are (i.e. using Mathematica)

$$\left(\left[\frac{3072\epsilon^4 b^2}{g^4} \right] \gamma^6 + \cdots \right) w(\gamma) + \left(\left[\frac{6144\epsilon^4 b^2}{g^4} \right] \gamma^7 + \cdots \right) w'(\gamma) + \left(\left[\frac{3072\epsilon^3 b^2}{g^3} \right] \gamma^5 + \cdots \right) w''(\gamma) + \left(\left[128\,\epsilon^2 \frac{Z^2 b^2}{g^3} + 256 \frac{\epsilon^2 b^4}{g^2} \right] \gamma^4 + \cdots \right) w'''(\gamma) + \left(\left[32\epsilon \frac{Z^2 b^2}{g^2} + 64\epsilon \frac{b^4}{g} \right] \gamma^2 + \cdots \right) w''''(\gamma) = 0. \tag{147}$$

We can now substitute the usual JWKB formalism $w = \mathrm{e}^W$, obtaining a fourth degree, in $W'(\gamma)$, equation ($w^{(j)} \to (W')^j \mathrm{e}^W$):

$$1 + 2\gamma W'(\gamma) + \frac{g}{\epsilon}\gamma^{-1}(W'(\gamma))^2 + \left(\frac{gZ^2}{24\epsilon^2} + \frac{b^2 g^2}{12\epsilon^2} \right) \gamma^{-2}(W'(\gamma))^3 + \frac{g}{4\epsilon} \left(\frac{gZ^2}{24\epsilon^2} + \frac{b^2 g^2}{12\epsilon^2} \right) \gamma^{-4}(W'(\gamma))^4 = 0. \tag{148}$$

Upon setting $r \equiv W'/\gamma$, the above transforms into the quartic polynomial expression $1 + c_1\gamma^2 r + c_2\gamma r^2 + c_3\gamma r^3 + c_4 r^4 = 0$. The JWKB self-consistent asymptotic solutions

follow from the three dominant term relations: (1) $1 + c_1\gamma^2 r = 0$; (2) $c_3\gamma r^3 + c_4 r^4 = 0$; and (3) $c_1\gamma^2 r + c_3\gamma r^3 = 0$. These result in the JWKB (lowest-order) asymptotic solutions:

$$W'(\gamma) = \begin{cases} -\dfrac{1}{2\gamma} \\ -\dfrac{4\epsilon}{g}\gamma^2 \\ \pm \mathrm{i}\dfrac{2\epsilon}{bg}\sqrt{\dfrac{6}{\left(1 + Z^2/2b^2g\right)}}\gamma^{3/2} \end{cases} \tag{149}$$

or ($\mu_0(\gamma, b) \equiv w(\gamma, b) = \exp(\int \mathrm{d}\gamma\, W'(\gamma))$)

$$\mu_0(\gamma, b) = \begin{cases} \dfrac{f_1(b)}{\sqrt{\gamma}} \\ f_2(b)\exp\left(-\dfrac{4\epsilon}{3g}\gamma^3\right) \\ f_\pm(b)\exp\left(\pm \mathrm{i}\dfrac{4\epsilon}{5bg}\sqrt{\dfrac{6}{\left(1 + Z^2/2b^2g\right)}}\gamma^{5/2}\right) \end{cases} \tag{150}$$

where the fs correspond to b-dependent factors. Note that the $W' \approx -\frac{1}{2\gamma}$ solution is made possible by the fact that there are inverse γ-dependent coefficients in equation (148). That is, we have a consistent asymptotic expansion, since even though $W'' \approx 2(W')^2$, $W''' \approx 8(W')^3$, etc, the inverse γ dependence of the cited coefficients allows us to ignore the nonlinear terms in equation (148), with respect to generating the first asymptotic solution, as given above.

If $c_3 = \frac{b^2g^2}{12\epsilon^2}(1 + \frac{Z^2}{2b^2g}) > 0$, and b real, rapidly oscillating solutions are introduced, to lowest order. However, a first-order correction (to the lowest-order JWKB estimate) reveals that there is a small exponential decay. Thus, taking $r \equiv r(\delta)$, where $\delta = 1$ is to be treated as a perturbation parameter, we can solve the equation

$$c_1\gamma^2 r(\delta) + c_3\gamma(r(\delta))^3 + \delta(1 + c_2\gamma r^2 + c_4 r^4) = 0 \tag{151}$$

for $r(\delta) = r_0 + \delta r_1 + \mathrm{O}(\delta^2)$. We obtain the correction

$$W'(\gamma) = \pm \mathrm{i}\frac{2\epsilon}{bg}\sqrt{\frac{6}{\left(1 + Z^2/2b^2g\right)}}\gamma^{3/2} - \frac{g}{4\epsilon c_3}\gamma + \frac{1}{4\gamma}. \tag{152}$$

For $c_3 > 0$, the second term introduces an exponential decay for the corresponding $\mu_0(\gamma, b)$ expression.

From the preceding lowest-order JWKB analysis we can see that except for some exponentially unbounded modes, all of the other scalet modes, except one, decay exponentially to zero, in the small-scale limit. The non-exponentially decaying mode is that which imitates the asymptotic behaviour of the physical solution (i.e. $\mathrm{O}(\frac{1}{\sqrt{\gamma}})$); although it is present for any E. This behaviour confirms our assertion (in the introduction) that for any E, there exist scalet solutions that converge pointwise (at fixed b) to solutions of the Schrödinger equation.

That is, for any E, we can find μ_ℓ values (i.e. the infinite-scale zero-translation scalets), such that the corresponding scalet solution does not involve the exponentially growing mode. For such solutions, the TPQ conditions are automatically satisfied, in the zero-scale limit. This is why, a pure TPQ-scalet analysis cannot work (and we must use the scalets as the generators for the wavelet transform coefficients in the Ψ_{DCWT} representation).

6.4. JWKB asymptotic analysis of the scalet equation: $V(x) = -(\mathrm{i}x)^3$

We now consider the problem

$$-\epsilon\partial_x^2\Psi(x) - (\mathrm{i}x)^3\Psi(x) = E\Psi(x) \tag{153}$$

recently studied by Bender and Boettcher (1998). They established that this non-Hermitian potential admits bound states along the real axis. The asymptotic behaviour of the wavefunction along the real axis is determined by the JWKB expression $\lim_{|x|\to\infty}\Psi(x) = \mathrm{e}^{\pm\frac{2\sqrt{\mathrm{i}}}{5}x^{5/2}}$, which dies off faster than the Gaussian. Accordingly, we can still work with $\mu_p(\alpha, b) = \int \mathrm{d}x\, x^p \mathrm{e}^{-\frac{(\alpha x)^2}{2}}\Psi(x+b)$, which will be analytic in α and b.

The $\mu_p(\gamma, b)$-moment equation is readily obtainable as before ($\gamma = \alpha^2/2$):

$$\begin{aligned}\mu_{p+3}(\gamma, b) = {} & [-3b + 4\mathrm{i}\epsilon\gamma^2]\,\mu_{p+2}(\gamma, b) - 3b^2\mu_{p+1}(\gamma, b) \\ & +[-b^3 + \mathrm{i}E - 2\mathrm{i}\epsilon\gamma(2p+1)]\,\mu_p(\gamma, b) + \mathrm{i}\epsilon p(p-1)\,\mu_{p-2}(\alpha, b).\end{aligned} \tag{154}$$

There are three missing moments $\{\mu_\ell(\gamma, b)|0 \leqslant \ell \leqslant 2\}$; thus, $m_s = 2$. The corresponding scalet equation becomes (i.e. $-\partial_\gamma\mu_p(\gamma, b) = -\mu_{p+2}(\gamma, b)$)

$$-\partial_\gamma\begin{pmatrix}\mu_0(\gamma, b)\\ \mu_1(\gamma, b)\\ \mu_2(\gamma, b)\end{pmatrix} = \begin{pmatrix}0, 0, 1\\ A, B, C\\ D, F, G\end{pmatrix}\begin{pmatrix}\mu_0(\gamma, b)\\ \mu_1(\gamma, b)\\ \mu_2(\gamma, b)\end{pmatrix} \tag{155}$$

where $A = -b^3 + \mathrm{i}E - 2\mathrm{i}\epsilon\gamma$, $B = -3b^2$, $C = -3b + 4\mathrm{i}\epsilon\gamma^2$, $D = (-b^3 + \mathrm{i}E - 2\mathrm{i}\gamma\epsilon)(-3b + 4\mathrm{i}\epsilon\gamma^2)$, $F = -3b^2(-3b + 4\mathrm{i}\epsilon\gamma^2) + (-b^3 + \mathrm{i}E - 6\mathrm{i}\epsilon\gamma)$, $G = (-3b + 4\mathrm{i}\epsilon\gamma^2)^2 - 3b^2$.

Note that the corresponding scalet equation matrix is now ϵ^2 dependent (refer to the conditions of lemma 4).

We can reduce these equations to one third-order differential equation for $\mu_0(\gamma, b)$. First, we take

$$\mu_1 = -\frac{1}{F}[\partial_\gamma\mu_2 + D\mu_0 + G\mu_2] \tag{156}$$

followed by substituting for μ_1 in the second scalet equation:

$$-\partial_\gamma\left(-\frac{1}{F}[\partial_\gamma\mu_2 + D\mu_0 + G\mu_2]\right) = A\mu_0 - \frac{B}{F}[\partial_\gamma\mu_2 + D\mu_0 + G\mu_2] + C\mu_2. \tag{157}$$

Finally, we substitute the first scalet equation, $\mu_2 = -\partial_\gamma\mu_0$:

$$\partial_\gamma\left(\frac{1}{F}[-\partial_\gamma^2\mu_0 + D\mu_0 - G\partial_\gamma\mu_0]\right) = A\mu_0 - \frac{B}{F}[-\partial_\gamma^2\mu_0 + D\mu_0 - G\partial_\gamma\mu_0] - C\partial_\gamma\mu_0 \tag{158}$$

or

$$\begin{aligned}-\mu_0''' + \left(\frac{F'}{F} - G - B\right)\mu_0'' + \left(G\frac{F'}{F} + D - G' - BG + CF\right)\mu_0' \\ +\left(-D\frac{F'}{F} + D' - FA + BD\right)\mu_0 = 0.\end{aligned} \tag{159}$$

In terms of the dominant γ terms in the coefficients:

$$\mu_0''' - 16\epsilon^2\gamma^4\mu_0'' - 64\epsilon^2\gamma^3\mu_0' - 20\epsilon^2\gamma^2\mu_0 = 0 \tag{160}$$

or (via JWKB approximation, $\mu_0 = \mathrm{e}^W$)

$$(W')^3 - 16\epsilon^2\gamma^4(W')^2 - 64\epsilon^2\gamma^3W' - 20\epsilon^2\gamma^2 = 0. \tag{161}$$

This equation cannot be used to generate the anticipated $W' \approx -\frac{1}{2\gamma}$ solution, since one would have to include all higher-order derivatives of W'. That is, since $\mu_0'' = (W'' + (W')^2)\mathrm{e}^W$, etc, and $W'' = 2(W')^2$ for $W' = -\frac{1}{2\gamma}$, etc, one would have to include the higher-order derivatives in equation (161).

From equation (160), anticipating that $\mu_0 \to f\gamma^\rho$ is a solution, we have

$$\rho(\rho-1)(\rho-2)\gamma^{\rho-3} - 16\epsilon^2\rho(\rho-1)\gamma^{\rho+2} - 64\epsilon^2\rho\gamma^{\rho+2} - 20\epsilon^2\gamma^{\rho+2} = 0. \tag{162}$$

Since $\frac{\gamma^{\rho+2}}{\gamma^{\rho-3}} \to +\infty$, we see that balancing the last three terms gives us two possible solutions (i.e. $16\rho(\rho-1) + 64\rho + 20 = 0$)

$$\rho = \begin{cases} -\frac{1}{2}, \ \mu_0(\gamma, b) \to f\gamma^{-1/2} \\ -\frac{5}{2}, \ \mu_0(\gamma, b) \to f\gamma^{-5/2}. \end{cases} \tag{163}$$

The third (asymptotic) solution can be obtained by balancing the first two terms in equation (161), yielding

$$W' = 16\epsilon^2\gamma^4 \tag{164}$$

or

$$\mu_0(\gamma, b) \to f\mathrm{e}^{\frac{16\epsilon^2}{5}\gamma^5}. \tag{165}$$

The presence of this mode will seriously impact any direct numerical integration of the scalet equations, for γ real. However, we can regulate the contribution of this mode by taking γ along a complex direction,

$$\gamma = |\gamma|\,\mathrm{e}^{\mathrm{i}\theta} \tag{166}$$

so long as

$$\cos(5\theta) < 0. \tag{167}$$

We recall that the Ψ_{DCWT} wavelet expansion is equivalent to the scaling transform $\frac{1}{\nu}\int \frac{\mathrm{d}b}{a} S_2(\frac{x-b}{a})\Psi(x)$, for a scaling function satisfying equation (22). If we are to work with complex scales, $a = |a|\mathrm{e}^{-\mathrm{i}\frac{\theta}{2}}$ (i.e. $\gamma = \frac{1}{2|a|^2\mathrm{e}^{-\mathrm{i}\theta}}$), then we must be sure that we can still recover, $\Psi(b)$, in the limit $|a| \to 0$:

$$\lim_{|a|\to} \frac{1}{\nu}\int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{|a|\mathrm{e}^{-\mathrm{i}\frac{\theta}{2}}} S_2\left(\frac{x-b}{|a|\mathrm{e}^{-\mathrm{i}\frac{\theta}{2}}}\right)\Psi(x) = \Psi(b). \tag{168}$$

That is, we require that the effective scaling function, $S_{2;\theta}(z) \equiv \mathrm{e}^{\mathrm{i}\theta/2}S_2(z\mathrm{e}^{\mathrm{i}\theta/2})$, be bounded (asymptotically vanishing), as $\mathrm{Re}(z) \to \pm\infty$, for fixed θ.

For the Mexican hat wavelet and dual functions, from the analysis by HM (1998), the corresponding $S_2(z)$, will have a Gaussian character (in Fourier space). Let us assume that $S_2(z)$ is of a Gaussian form, and we can use $\mathrm{e}^{-z^2/2}$ as a guide. Then, $\mathrm{e}^{-z^2\mathrm{e}^{\mathrm{i}\theta}}$, is bounded, in the above manner, so long as $\cos(\theta) > 0$.

Combining this with the condition in equation (167), we see that $\frac{\pi}{2} < 5\theta < \frac{3\pi}{2}$ satisfies both the scalet (regulating) condition, as well as the boundedness of the $S_{2;\theta}$ scaling function.

For $\sigma = \mathrm{e}^{-\mathrm{i}\frac{\theta}{2}}$, the complex scale DCWT signal-wavelet inversion formula is (refer to appendix D)

$$\Psi(b) = \frac{1}{3.427}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty} \mathcal{D}_{mh}\left(\frac{b - j\sigma 2^l - \delta_l[b]}{\sigma 2^l}\right)\frac{1}{\sqrt{\sigma 2^l}}\underline{W_{mh}\Psi}(\sigma 2^l,\, j\sigma 2^l + \delta_l[b]) \tag{169}$$

where

$$b = n_l[b](\sigma\ 2^l) + \delta_l[b]. \tag{170}$$

Note that $\sigma\ 2^l$ is the complex scale, and $\delta_l[b]$ is the residual value, for given (complex) b, after determining the optimal integer $n_l[b]$.

We will take θ to be the mid-point of the interval $\frac{\pi}{10} < \theta < \frac{3\pi}{10}$, or $\theta = \frac{\pi}{5}$. In general, for this problem, the smaller the θ value taken ($\frac{\pi}{10} < \theta$), the more dominant the exponentially explosive mode in equation (165) will become. The larger θ becomes ($\theta < \frac{3\pi}{10}$), the slower the zero scale, asymptotic convergence to $\Psi(b)$ will become (requiring integration of the corresponding scalet equation to smaller scales), since the effective, underlying, scaling function becomes less compactly supported (i.e. $S_2(\frac{x}{e^{-i\theta/2}})$, refer to appendix D). Numerical integration of the scalet equation, for $\theta \approx 0.628$, could only be done up to $a = \frac{1}{2}$. At this scale, TPQ-DCWT was unable to clearly discern any estimates for the (low-lying) discrete state energies.

It is interesting to note that for the quartic anharmonic oscillator case, the exponentially decaying mode in equation (150), $\mu_0(\gamma, b) \rightarrow f_2(b)\exp\left(-\frac{4\epsilon}{3g}\gamma^3\right)$, would appear to be the algebraic counterpart to the mode in equation (165). We can also rotate in the γ-complex plane and check the viability of the preceding formalism. Although the TPQ-DCWT identification of discrete state energies is more difficult in the γ-complex plane (because of the appearance of increased oscillatory behaviour on the part of the generated determinant), we could, nevertheless, identify clearly recognizable roots corresponding to the ground energy state of the quartic potential $V(x) = x^4$. As indicated above, a similar analysis for the $V(x) = \mathrm{i}x^3$ problem proved more difficult. What is required is either greater computational capacity (increased precision), or an alternate strategy for removing (suppressing) the explosive mode altogether (which still remains significant, even after complex rotation).

In light of the ϵ dependence of the asymptotic mode in equation (165), we attempted to work with sufficiently small $\epsilon \approx \mathrm{O}(10^{-3})$ values so as to suppress the contributions of this explosive mode. Indeed, the other two modes (i.e. equation (163)) are algebraic in $\gamma^{-1/2}$ and ϵ; therefore, a significant reduction in ϵ will have the desired effect of suppressing the exponentially explosive mode, while not significantly diminishing the more physical modes, which are numerically moderate in magnitude. Our numerical experiments confirm this, and we were able to work with smaller scales, $a = \frac{1}{4}$; however, we were still unable to detect any discrete state energy values.

7. Conclusion

Given the comprehensive nature of this paper, we briefly summarize the main points developed in this work.

We have defined the *scalet equation* which can be used to generate the wavelet transform coefficients in terms of a reduced set of linear variables. For arbitrary, one-dimensional, bound-state rational fraction potentials, the number of these linear variables is identical to the total number of all complex turning points. This representation for the wavelet transform coefficients is then used to implement a turning point quantization procedure for generating the eigenenergies and wavefunction.

Unlike the (multidimensional) TPQ-MRF formulation of Handy *et al* (HMBB 2000), where many spurious solutions were generated, the present scalet-wavelet analysis generates no, or substantially fewer, spurious solutions; as discussed in the contexts of the double-well

quartic anharmonic oscillator, and the quartic potential, respectively. This is in keeping with the basic wavelet philosophy which makes them appropriate for analysing transient, short-scale features. This was the original motivation for this paper.

Although we did not discuss how to optimally select the mother wavelet, so as to reduce the number of spurious solutions, we did show that even the simplest use of a wavelet formalism (i.e. the *Mexican hat* mother wavelet), within a TPQ framework, can improve upon the TPQ-MRF analysis. In a forthcoming work, we will show how a moment quantization analysis can suggest optimal mother wavelets.

One important distinguishing feature about the TPQ strategy adopted in this, and other cited works, is that we emphasize all of the complex turning points, not just the real ones (as is the case in conventional JWKB analysis). Semiclassical methods, such as JWKB, are not too accurate for low-lying states. It has been conjectured that any method, such as ours, that emphasizes all of the (complex) turning points, should be able to generate very accurate results for the low-lying states. Our results are consistent with this.

We gave a detailed asymptotic analysis of the scalet equation, proving that for any energy parameter value, E, there will be scalet modes that converge to the corresponding (physical or unphysical) Schrödinger equation solution, at least in the neighbourhood of the turning points. When used in this manner, a pure scalet representation (i.e. solving numerically for the scalet equation solutions) cannot distinguish between physical and unphysical solutions, and must be used within the context of a wavelet representation for the wavefunction; wherein unphysical (unbounded) Schrödinger equation solutions are represented in terms of bounded (L^2) configurations.

The asymptotic analysis of the scalet equation was derived for the generic quartic anharmonic oscillator problem (including the double-well problem, and the pure quartic case). It was also presented for the non-Hermitian case of the complex potential $-\mathrm{i}x^3$, recently studied by Bender and Boettcher (1998). For this problem, the underlying numerical analysis revealed the inability of a scalet–wavelet TPQ ansatz to yield any results, even when introducing a complex scale. By way of contrast, the application of the MRF-TPQ analysis of HMBB, yields very good results (Handy *et al* 2001). This one example underscores the practical utility of TPQ methods in general.

The scalet equation is analytic in ϵ, the kinetic energy expansion parameter. We derived the zeroth-order form of the scalet configuration, within the ϵ expansion framework. In a forthcoming work, we derive the matrix-Green function analysis that generates all of the higher-order (in ϵ) configurations. It was argued that within an ϵ expansion framework, the scalet representation may be able to circumvent having to work with wavelets. Indeed, the ϵ-scalet expansion is very similar (and more rigorous) than the high-temperature lattice expansion formalism of Bender and Sharp (1981) and Handy (1981), simply because it avoids having to define a lattice model representation for the continuum problem.

Given all of the above, we believe that the present formalism, particularly as derived from a moment quantization perspective, should enhance the appreciation for, and relevancy of, wavelet analysis to quantum physics.

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Appendix A. Convergence of DCWT representation within the complex x-plane

Assume that the only singularities bounding $\mathcal{S}_{\mathcal{A}}$ are isolated poles, $\Psi(z) \approx \frac{1}{(z-z_0)^p}$. For turning points outside this strip, $\tau_\ell \notin \mathcal{S}_{\mathcal{A}}$, that also satisfy $\lim_{a\to 0} a^{-p}\partial_\xi^{p-1} S_2(\xi)|_{\frac{z_0-\tau_\ell}{a}} = 0$, then $\underline{S_2\Psi}(a,\tau_\ell)$ will converge to $\Psi(\tau_\ell)$. This follows upon rewriting the relevant scaling transform as

$$\underline{S_2\Psi}(a,b) = \frac{1}{\nu}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x}{a}S_2\left(\frac{x}{a}\right)\Psi(x+b)$$

which readily follows by analytic continuation for any $b \in \mathcal{S}_{\mathcal{A}}$. This integral representation can then be analytically continued into the regime $b \to \tau_\ell$. This implicitly requires a deformation of the real x-axis contour, $\Re \to \mathcal{C}$, so that (a subset of) the corresponding set of points, $\{z+b|z \in \mathcal{C}\}$, encircle the singularity as $b \to \tau_\ell$:

$$\underline{S_2\Psi}(a,\tau_\ell) = \frac{1}{\nu}\int_{\mathcal{C}}\frac{\mathrm{d}z}{a}S_2\left(\frac{z}{a}\right)\Psi(z+\tau_\ell).$$

The additional contour integral around the singularity corresponds to $z+\tau_\ell = z_0 + r\mathrm{e}^{\mathrm{i}\theta}$, for $0 \leqslant \theta < 2\pi$. The associated integral becomes

$$\frac{1}{a\nu}\mathrm{i}r\int_0^{2\pi}\mathrm{d}\theta\,\mathrm{e}^{\mathrm{i}\theta}S_2\left(\frac{z_0-\tau_\ell+r\mathrm{e}^{\mathrm{i}\theta}}{a}\right)\frac{1}{(r\mathrm{e}^{\mathrm{i}\theta})^p}.$$

This becomes

$$\frac{2\pi\mathrm{i}}{(p-1)!\nu a^p}\partial^{p-1}S_2\left(\frac{z_0-\tau_\ell}{a}\right).$$

Thus

$$\underline{S_2\Psi}(a,\tau_\ell) = \frac{2\pi\mathrm{i}}{(p-1)!\nu a^p}\partial^{p-1}S_2\left(\frac{z_0-\tau_\ell}{a}\right) + \frac{1}{\nu}\int_{-\infty}^{+\infty}\frac{\mathrm{d}x}{a}S_2\left(\frac{x}{a}\right)\Psi(x+\tau_\ell). \tag{A1}$$

In the zero-scale limit, the first term vanishes, under the above assumptions, and the integral expression yields $\Psi(\tau_\ell)$ (i.e. perform the change of variables $y = x/a$, and then expand $\Psi(ay+b)$, around b).

Since our ultimate objective is to use the above analysis for evaluating the second-order derivative, at the turning point (i.e. $\partial_\tau^2 = a^{-2}\partial_{\tau/a}^2$), one can choose dual-wavelet pairs so that the corresponding S_2 satisfy the above conditions (i.e. $\lim_{a\to 0} a^{-(p+2)}\partial^{p+1}S_2(\frac{z_0-\tau_\ell}{a}) = 0$).

If the singularity is a branch point, and Ψ's discontinuity is finite along the chosen cut, then a similar analysis follows. We are assuming that $\Psi(x)$ is well behaved, and sufficiently bounded along the real x-axis, so that $\underline{S_2\Psi}(a,b)$ is analytic both in $\alpha = \frac{1}{a}$ and b. As such, the analytic continuation of $\underline{S_2\Psi}(a,b)$, as $b \to \tau_\ell (\notin \mathcal{S}_{\mathcal{A}})$, cannot depend on how Ψ's cut is chosen. However, we will find that the analysis is simplified if the cut is taken in a particular manner, as clarified below.

Let $C_{z_0} \equiv \{z_0 + \xi|0 \leqslant \mathrm{Im}(\xi) \leqslant \mathrm{Im}(\tau_\ell)\}$ represent the locus of points defining the cut. Even though the cut may be infinite in extent, we are only interested in it over the finite range specified. This is implicitly assumed. The cut intersects the infinite line $\mathcal{L}_{\tau_\ell} \equiv \{x+\tau_\ell|x \in \Re\}$, at the point $\mathcal{L}_{\tau_\ell} \bigcap C_{z_0} = \{x_c + \tau_\ell\}$, where x_c is real.

As $b \to \tau_\ell$, the original real axis contour (i.e. $x \in \Re$) must be deformed into a new contour, $\Re \to \mathcal{C}$, so that the new set of points $\{z + \tau_\ell | z \in \mathcal{C}\}$ includes a subset that hugs the cut on both sides:

$$\mathcal{C} = (-\infty, x_c^{(-)}) \bigcup \{z | z + \tau_\ell = z_0 + \xi \pm 0^{(+)}, z_0 + \xi \in C_{z_0}\} \bigcup (x_c^{(+)}, +\infty). \tag{A2}$$

We refer to the middle set of points as the $\mathcal{C}_{cut}$ contour.

Although there are infinitely many ways of choosing the cut, they will be of two types. Assume that $\mathrm{Re}(\tau_\ell) \geqslant \mathrm{Re}(z_0)$ and $\mathrm{Im}(\tau_\ell) > 0$, for specificity. The cut will be either to the right or left of τ_ℓ. If it is to the right, then at some point along the cut we will have $\mathrm{Re}(z_0 + \xi) = \mathrm{Re}(\tau_\ell)$. If the cut is to the left, then there will be no such point.

The part of the deformed contour surrounding the cut, $\mathcal{C}_{cut}$, corresponds to an integral expression of the form:

$$\int_{\mathcal{C}_{cut}} \frac{\mathrm{d}\xi}{a} S_2\left(\frac{z_0 + \xi - \tau_\ell}{a}\right)(\Psi(z_0 + \xi + 0^+) - \Psi(z_0 + \xi - 0^+)).$$

If the cut is to the right of the turning point, then such integrals will usually involve infinite integrands, as $a \to 0$, making the ensuing analysis complicated (i.e. there will be cancellations of very large, positive/negative, terms). This is because, since $S_2(w)$ is bounded along the $\mathrm{Re}(w)$-axis, it has to become infinite along some direction in the complex $w = |w|\mathrm{e}^{\mathrm{i}\theta}$-plane, for $\theta_{min} < \theta < \theta_{max}$ (i.e. $|w| \to \infty$). Along the indicated contour, under the assumption that the cut is to the right of τ_ℓ, for $\tan^{-1}(\theta) = \frac{\mathrm{Im}(\tau_\ell - (z_0 + \xi))}{\mathrm{Re}(\tau_\ell - (z_0 + \xi))}$, we have that θ will vary over an interval that includes $\pi/2$, and should intersect the interval $(\theta_{min}, \theta_{max})$.

In order to avoid having to deal with the infinite intricacies of the above representation, it is preferable to choose the cut to be to the left of τ_ℓ. For this case, the analytically continued scaling transform becomes

$$\begin{aligned}\underline{S_2\Psi}(a, \tau_\ell) = {} & \frac{1}{\nu}\int_{C_{cut}} \frac{\mathrm{d}\xi}{a} S_2\left(\frac{z_0 + \xi - \tau_\ell}{a}\right)(\Psi(z_0 + \xi + 0^+) - \Psi(z_0 + \xi - 0^+)) \\ & + \frac{1}{\nu}\int_{-\infty}^{x_c^-} \frac{\mathrm{d}x}{a} S_2\left(\frac{x}{a}\right)\Psi(x + \tau_\ell) + \frac{1}{\nu}\int_{x_c^+}^{+\infty} \frac{\mathrm{d}x}{a} S_2\left(\frac{x}{a}\right)\Psi(x + \tau_\ell).\end{aligned} \tag{A3}$$

The last two integrals correspond to integrations with respect to the left and right cut contributions (i.e. $\Psi(x_c^- + \tau_\ell) \neq \Psi(x_c^+ + \tau_\ell)$), respectively. If the variation of the angle θ, as previously defined, satisfies $\theta < \theta_{min}$, then the first integral will vanish, in the small-scale limit. For these cases, the zero-scale limit of the $\underline{S_2\Psi}(a, \tau_\ell)$ scaling transform would recover $\Psi(\tau_\ell)$ for that turning point value corresponding to the Riemannian sheet satisfying the above conditions. If not, and no other cut orientation can be found satisfying these conditions, then the zero-scale limit for $\underline{S_2\Psi}(a, \tau_\ell)$ will be infinite.

It should be noted that if all of the preceding analysis is done with respect to $\partial_z^2\Psi(z)$, and not $\Psi(z)$, then $\partial_z^2\Psi(\tau_\ell) = 0$, on all the Riemannian sheets, since the analytic continuation of the Schrödinger equation preserves the definition of the turning point, on all the Riemannian surfaces.

Appendix B. The quantization scale and the extremal wavelet contributions to $\Psi(\tau)$

We now derive certain relations that automatically follow from the definition of the scaling transform, and certain minimal conditions on the choice of scaling function. These play an important role within the HMBB analysis, although not fully developed by them in their work.

As has been noted in equation (19), the scaling transform, $\underline{S\Psi}(a, x)$, evaluated at scale a, and position x, represents the sum over the wavelet transform decomposition of $\Psi(x)$, summed

over all scales $a_v \geqslant a$, and translation values $-\infty < b < +\infty$. However, $-\partial_a \underline{S\Psi}(a, x)$, is the sum over the wavelet transform decomposition of $\Psi(x)$, at fixed scale $a_v = a$, summed *only* over the translation values.

We are particularly interested in those cases where $x = \tau_\ell$, a (complex) turning point. At a given position, τ_ℓ, we focus on the extremal values of $\partial_a \underline{S\Psi}(a, \tau_\ell)$, as a function of a. These are denoted by $a_e(\tau_\ell)$, and satisfy

$$\partial_a^2 \underline{S\Psi}(a_e(\tau_\ell), \tau_\ell) = 0. \tag{B1}$$

They define the important *wavelet* scales contributing to the system, at point τ_ℓ. The global maximum wavelet contribution, at point τ_ℓ, is denoted by $a_w(\tau_\ell)$, and is one of the extremal scales: $a_w(\tau_\ell) \in \{a_e(\tau_\ell)\}$. At $a_w(\tau_\ell)$ we have

$$|\partial_a \underline{S\Psi}(a_w(\tau_\ell), x)| \geqslant |\partial_a \underline{S\Psi}(a, x)| \qquad 0 < a < \infty. \tag{B2}$$

Since $\lim_{a\to 0} \underline{S\Psi}(a, x) = \Psi(x)$, it naturally follows that the same holds for any derivative with respect to x. In particular, from a TPQ perspective, one is interested in $\lim_{a\to 0} \partial_x^2 \underline{S\Psi}(a, x) = \partial_x^2 \Psi(x)$. The natural question is, for $x = \tau_\ell$, at what scale value does this asymptotic limit manifest itself? That is, at what scale, $a_Q(\tau_\ell)$, do we have $\partial_\tau^2 \underline{S\Psi}(a, \tau_\ell) \approx 0$, for $a \leqslant a_Q(\tau_\ell)$? From the TPQ perspective, this would define the 'quantization scale', for the turning point τ_ℓ. It turns out that the zero-scale limit for $\partial_x^2 \underline{S\Psi}(a, x)$ and $\partial_a^2 \underline{S\Psi}(a, x)$ are very much related. However, the latter is the more natural expression to consider, within the context of scaling transform theory. We do so below, in defining the quantization scale.

The zero-scale asymptotic expansion for the scaling transform,

$$\underline{S\Psi}(a, x) = \frac{1}{\nu_0} \int \frac{\mathrm{d}b}{a}\, S\left(\frac{b-x}{a}\right) \Psi(b)$$

is given by (i.e. perform the change of variables $y = \frac{b-x}{a}$, and expand around x, within the representation $\underline{S\Psi}(a, x) = \frac{1}{\nu_0} \int \mathrm{d}y\; S(y)\Psi(ay + x)$) is

$$\underline{S\Psi}(a, x) = \Psi(x) + \frac{1}{\nu_0} \sum_{n=1}^{\infty} \frac{a^n \nu_n}{n!} \partial_x^n \Psi(x). \tag{B3}$$

Assuming $\nu_1 = 0$, we have in the zero-scale limit

$$\underline{S\Psi}(a, x) = \Psi(x) + \frac{\nu_2}{2\nu_0} a^2 \partial_x^2 \Psi(x) + \mathrm{O}(a^3) \tag{B4}$$

$$\partial_x^2 \underline{S\Psi}(a, x) = \partial_x^2 \Psi(x) + \mathrm{O}(a^2) \tag{B5}$$

and

$$\partial_a^2 \underline{S\Psi}(a, x) = \frac{\nu_2}{\nu_0} \partial_x^2 \Psi(x) + \mathrm{O}(a). \tag{B6}$$

Thus, under the simple assumption that $\nu_1 = 0$ and $\nu_2 \neq 0$, we find that both $\partial_x^2 \underline{S\Psi}(a, x)$ and $\partial_a^2 \underline{S\Psi}(a, x)$ converge, in the zero-scale limit, to $\partial_x^2 \Psi(x)$ (up to a proportionality factor).

If $\nu_3 \neq 0$, then $\partial_x^2 \underline{S\Psi}(a, x)$ converges faster than $\partial_a^2 \underline{S\Psi}(a, x)$; however, if $\nu_3 = 0$ (i.e. the scaling function, S, is symmetric), then both converge at the same rate (i.e. $\mathrm{O}(a^2)$). Under this assumption, we prefer to work with the latter.

The turning points of the physical wavefunction correspond to points of inflection where the second derivative is zero, $\partial_\tau^2 \Psi(\tau_\ell) = 0$. The zero-scale limit of the scaling transform converges fastest at the inflection points. This follows readily from the above expansion, since $\underline{S\Psi}(a, \tau_\ell) = \Psi(\tau_\ell) + \mathrm{O}(a^3)$. However, the same does not apply for the second-order derivative expressions. They converge at the same rate, $\mathrm{O}(a^2)$, regardless of whether or not the point x is an inflection point.

Defining the extremal scales at the turning points. We have the following, important relations, at $a = \infty$ and 0:

$$\partial_a \underline{S\Psi}(a, x) \to \begin{cases} 0, \text{ as } a \to \infty & \text{by definition of } \underline{S\Psi}(a, x) \\ 0, \text{ as } a \to 0 & \text{from equation (177)} \end{cases} \tag{B7}$$

also,

$$\partial_a^2 \underline{S\Psi}(a, \tau_\ell) \to \begin{cases} 0, \text{ as } a \to \infty & \text{by definition of } \partial_a \underline{S\Psi}(a, \tau_\ell) \\ 0, \text{ as } a \to 0 & \text{from equation (179).} \end{cases} \tag{B8}$$

Therefore, $\partial_a \underline{S\Psi}(a, \tau_\ell)$ must have local extrema on the positive real axis, $a \in (0, \infty)$; so too for $\partial_a^2 \underline{S\Psi}(a, \tau_\ell)$. In the former case, the local extrema define the *extremal wavelet* scales, $a_e(\tau_\ell)$, and the global extremal wavelet scale, $a_w(\tau_\ell)$.

Let us designate the smallest of these extremal scales by

$$a_\sigma(\tau_\ell) \equiv \text{Min}\{a_e(\tau_\ell)\}. \tag{B9}$$

At both endpoints of the interval $(0, a_\sigma(\tau_\ell))$, the function $\partial_a^2 \underline{S\Psi}(a, \tau_\ell)$ becomes zero. It cannot have any other zero inside this interval, by definition of a_σ. Thus, it must have extremal values within this interval. The smallest of these defines the quantization scale, $a_Q(\tau_\ell)$. Starting at $a = a_Q(\tau_\ell)$, and proceeding to zero, $a \to 0$, the function $\partial_a^2 \underline{S\Psi}(a, \tau_\ell)$ monotonically converges to zero, in accordance with equation (181). Therefore, we define the quantization scale, at turning point τ_ℓ, to be the smallest scale satisfying

$$\partial_a^3 \underline{S\Psi}(a_Q(\tau_\ell), \tau_\ell) = 0. \tag{B10}$$

It is evident from the above that

$$a_Q(\tau) < a_w(\tau). \tag{B11}$$

This relation is the main criterion used by HMBB to discriminate between physical solutions and spurious solutions generated through their particular turning point quantization approach.

We emphasize that all of the preceding analysis did not make any assumptions specific to the physical problem. All that was assumed is that $\Psi(x)$ is a bounded, integrable configuration, and that the turning points can be taken to be any of the inflection points of the configuration.

Appendix C. Turning-point quantization within the multiscale reference function representation

In their work, HMBB do not directly solve the scalet equation. Instead, they investigate the extent to which another moment-dependent, wavefunction representation yields approximate scalet solutions. Specifically, from the wavefunction representation developed within the work by Handy (1996), and Tymczak *et al* (1998a, b), one has

$$\Psi_{MRF}(x) = \sum_{n=0}^{\infty} a_n[E, \epsilon, \mu_0, \ldots, \mu_{m_s}](-\partial_x)^n R(x) \tag{C1}$$

involving an arbitrary (within certain restrictions) *reference* function, $R(x)$, and readily obtainable coefficients, a_n, linearly dependent on the missing moments

$$a_n[E, \epsilon, \mu_0, \ldots, \mu_{m_s}] = \sum_{\ell=0}^{m_s} D_{n,\ell}(E, \epsilon)\mu_\ell. \tag{C2}$$

We refer to the above representation as the multiscale reference function (MRF) representation. In their work, Tymczak *et al* argue that the MRF basis, $\{(-\partial_x)^n R(x)\}$, when properly chosen, will recover the physical solution (particularly in the momentum representation).

Interestingly, the MRF representation is formally analogous to the distributed approximating functionals (DAFs) of Hoffman and Kouri (1993). This is because it can be formally rederived from the simple identity

$$\frac{1}{\sqrt{2\pi}} = \hat{H}^{-1}(k)\hat{H}(k) \tag{C3}$$

where $\hat{H}(k)$ is a bounded, Fourier transform expression, with an analytic inverse. It must also have a bounded, inverse Fourier transform, $H(x)$. Expanding $\hat{H}^{-1}(k) = \sum_{n=0}^{\infty} a_n(\mathrm{i}k)^n$, and implementing an inverse Fourier transform yields $\delta(x) = \sum_{n=0}^{\infty} a_n(\partial_x)^n H(x)$, which can be translated

$$\delta(x-b) = \sum_{n=0}^{\infty} a_n(\partial_x)^n H(x-b). \tag{C4}$$

Integrating with respect to $\Psi(x)$ then yields $\Psi(b) = \sum_{n=0}^{\infty} a_n(-\partial_b)^n \int \mathrm{d}x\, \Psi(x)\, H(x-b)$, which reduces to the MRF representation upon identifying $\int \mathrm{d}x\, \Psi(x)\, H(x-b) \equiv R(b)$.

At a given expansion order, N, HMBB imposed the TPQ conditions

$$\partial_x^2 \Psi_{MRF}^{(N)}(\tau_\ell(E)) = 0 \qquad 0 \leqslant \ell \leqslant m_s \tag{C5}$$

or

$$\sum_{n=0}^{N} a_n[E, \epsilon, \mu_0, \ldots, \mu_{m_s}](-\partial_x)^{n+2} R(\tau_\ell(E)) = 0. \tag{C6}$$

Substituting the a_n-missing moment relation (i.e. equation (186)) defines a determinantal equation of dimension $1 + m_s$:

$$\mathrm{Det}\left(\Delta_{\ell_1,\ell_2}^{(N)}(E,\epsilon)\right) = 0 \tag{C7}$$

where

$$\Delta_{\ell_1,\ell_2}^{(N)}(E,\epsilon) \equiv \sum_{n=0}^{N} D_{n,\ell_2}(E,\epsilon)(-\partial_{\tau_{\ell_1}})^{n+2} R(\tau_{\ell_1}(E)) = 0. \tag{C8}$$

Upon determining the energy roots, one can recover the missing moments, subject to a convenient normalization (i.e. $\mu_0 = 1$). This in turn determines the MRF configuration.

C.1. DCWT analysis for identifying the physical TPQ-MRF solutions

The above TPQ-MRF approach yielded excellent results for various one- and two-dimensional problems; however, many spurious solutions were also generated. In order to define a multiscale procedure for discriminating between the physical and unphysical (spurious) solutions, HMBB implemented a wavelet-based analysis.

It is to be emphasized that the scalet equation will be satisfied to all scales only for the physical solution.

For a given TPQ-MRF solution, denoted by $\Psi_{MRF}^{(N)}(x)$, HMBB determined the smallest (critical) scale, $a_c(\tau_\ell)$, up to which the approximate solution would satisfy the scalet equation.

This critical scale measures the physical content of the generated TPQ-MRF configuration (whether it is an actual valid physical approximation or a spurious configuration).

Thus, one calculates the generalized moments, $\mu_\ell(\alpha, b) = \int \mathrm{d}x\, x^p S(\alpha x)\Psi^{(N)}_{MRF}(x+b)$, from the Nth-order, MRF-generated configuration, $\Psi^{(N)}_{MRF}$, and determines the smallest scale, $a_c(\tau_\ell)$, at turning point τ_ℓ, up to which they satisfy the scalet equation:

$$\partial_\alpha \overrightarrow{\mu}(\alpha, \tau_\ell) \approx \mathcal{M}(\alpha, \tau_\ell, E, \epsilon)\overrightarrow{\mu}(\alpha, \tau_\ell) \tag{C9}$$

(i.e. $0 \leqslant \alpha \leqslant 1/a_c(\tau_\ell)$).

Utilizing the Mexican hat mother wavelet kernel, one can compute the wavelet transform

$$W_{mh}\Psi_{MRF}(a, b) = \frac{1}{\sqrt{a}} \int \mathrm{d}x\, \mathcal{W}_{mh}\left(\frac{x-b}{a}\right) \Psi^{(N)}_{MRF}(x). \tag{C10}$$

We can then define $\Psi^{(N)}_{MRF}$'s Mexican hat dual-wavelet decomposition, as given in equation (23). The summation of this expansion, over all terms corresponding to $L \leqslant l < \infty$, is the scaling transform $\underline{S_2\Psi_{MRF}}(2^L, \tau)$, for a particular scaling function, S_2, derived by Handy and Murenzi (1999).

The extremal scale values of the generated wavelet transform, $W_{mh}\Psi_{MRF}(a, \tau_\ell(E))$, essentially define the extremal wavelet scales corresponding to $\partial_a \underline{S_2\Psi_{MRF}}(a, \tau_\ell(E))$, as discussed in the previous subsection. The global extremal wavelet scale, $a_w(\tau_\ell(E))$, can then be identified.

The important question is then, what is the relationship between $a_w(\tau_\ell(E))$ and the critical scale $a_c(\tau_\ell(E))$?

This is easier to address if we first assume that Ψ_{MRF} is a spurious solution. For this case, small-scale errors ('noise') in the MRF representation conspire to generate a false solution to the TPQ-MRF conditions (i.e. equation (190)). The scale at which these significant errors contribute, $a_w(\tau_\ell(E)$, must be smaller than the scale that measures the (minimal) possible physical content of these spurious configurations (as manifested by the corresponding a_c). In other words, for the spurious solutions we must have $a_w(\tau_\ell(E)) < a_c(\tau_\ell(E))$.

If Ψ_{MRF} is a good physical approximation, then there must be consistency between a_c and a_w. That is, the support of the wavelet transform (as measured by the scale a_w) must lie within the scale interval that measures the physical content of the MRF solution. That is, $a_w \in (a_c, \infty)$.

Thus, within the TPQ-MRF formalism, the discriminating relation for distinguishing between physical and spurious solutions corresponds to

$$\begin{cases} a_w(\tau_\ell(E)) < a_c(\tau_\ell(E)) & \text{for unphysical (spurious) } \Psi_{MRF} \\ a_c(\tau_\ell(E)) < a_w(\tau_\ell(E)) & \text{for physical } \Psi_{MRF}. \end{cases} \tag{C11}$$

Appendix D. DCWT representation for complex scales

We consider the scaling transform for complex scales, $a = \sigma|a|$, and $\sigma = \mathrm{e}^{-\mathrm{i}\theta/2}$:

$$\underline{S\Psi}(a, x) = \frac{1}{\nu_0} \int_{-\infty}^{+\infty} \frac{\mathrm{d}b}{\sigma|a|} S\left(\frac{b-x}{\sigma|a|}\right)\Psi(b). \tag{D1}$$

We assume that $S(\frac{b}{\sigma})$ is a bounded configuration (asymptotically vanishing faster than any exponential $\mathrm{e}^{-\gamma|b|}$) along the real b-axis, provided $\theta_{min} < \theta < \theta_{max}$ (which includes $\theta = 0$). Under these conditions, the scaling transform exists for all $|a|$ and x, and will converge to $\Psi(x)$ (assuming that Ψ is an entire function), in the zero-scale limit $|a| \to 0$.

Indeed, the new function $S_\sigma(x) \equiv \frac{1}{\sigma} S(\frac{x}{\sigma})$, can be regarded as the new scaling function; and its zeroth-order moment is σ independent, $\int_{-\infty}^{+\infty} \mathrm{d}x\, S_\sigma(x) = \nu_0 = \int_{-\infty}^{+\infty} \mathrm{d}x\, S(x)$.

We can now repeat the DCWT analysis developed in the work by Handy and Murenzi (1998), with respect to the scaling function, $S_1 \equiv S$. In terms of the Fourier transform, $\hat{S}(k) \equiv \frac{1}{\sqrt{2\pi}} \int \mathrm{d}y\, \mathrm{e}^{-\mathrm{i}ky} S(y)$, we have that $\hat{S}_\sigma(k) = \hat{S}_1(\sigma k)$.

The DCWT analysis of Handy and Murenzi uses the following defining relationship between the scaling function and the dual-wavelet configurations:

$$\hat{S}(k) - \hat{S}(\rho k) = \left[\sum_{j=-\infty}^{+\infty} \mathcal{D}(j)\, \mathrm{e}^{\mathrm{i}fjk} \right] \hat{\mathcal{W}}\left(\frac{k}{a_0}\right). \tag{D2}$$

This can be analytically continued into the complex k-plane, yielding

$$\hat{S}_\sigma(k) - \hat{S}_\sigma(\rho k) = \left[\sum_{j=-\infty}^{+\infty} \mathcal{D}(j)\, \mathrm{e}^{\mathrm{i}fj\sigma k} \right] \hat{\mathcal{W}}_\sigma\left(\frac{k}{a_0}\right) \tag{D3}$$

where $\hat{\mathcal{W}}_\sigma(\frac{k}{a_0}) = \hat{\mathcal{W}}(\frac{\sigma k}{a_0})$. The corresponding inverse Fourier transform expressions are $\mathcal{W}_\sigma(x) = \frac{1}{\sigma}\mathcal{W}(\frac{x}{\sigma})$.

The inverse Fourier transform expansion of the former identity yields the DCWT reconstruction formula

$$\Psi(x) = \frac{1}{\nu_0} \sum_{l=-\infty}^{+\infty} \sum_{j=-\infty}^{+\infty} \mathcal{D}\left(\frac{x - fa_0 j\rho^l - \delta_l[x]}{fa_0\rho^l} \right) \frac{1}{\sqrt{\rho^l}} \underline{W\Psi}(\rho^l,\, fa_0 j\rho^l + \delta_l[b]) \tag{D4}$$

where

$$\underline{W\Psi}(a, x) = \frac{1}{\sqrt{a}} \int \mathrm{d}\xi\, \mathcal{W}\left(\frac{\xi - x}{a}\right) \Psi(\xi) \tag{D5}$$

and $\delta_l[x]$ is the residual amount, at scale ρ^l, satisfying

$$x = n_l[x] fa_0\rho^l + \delta_l[x]. \tag{D6}$$

The generalization of this, for the case $\sigma \neq 1$ (i.e. $f \to f\sigma$, and $\mathcal{W} \to \mathcal{W}_\sigma$, except we redefine the $\frac{1}{\sqrt{a}}$ factor) is then

$$\Psi(b) = \frac{1}{\nu_0} \sum_{l=-\infty}^{+\infty} \sum_{j=-\infty}^{+\infty} \mathcal{D}\left(\frac{b - f\sigma a_0 j\rho^l - \delta_l[b]}{f\sigma a_0\rho^l} \right) \frac{1}{\sqrt{\sigma\rho^l}} \underline{W_\sigma\Psi}(\rho^l,\, f\sigma a_0 j\rho^l + \delta_l[b]) \tag{D7}$$

where

$$\underline{W_\sigma\Psi}(a, b) = \frac{1}{\sqrt{\sigma a}} \int \mathrm{d}\xi\, \mathcal{W}\left(\frac{\xi - b}{\sigma a}\right) \Psi(\xi) \tag{D8}$$

and $\delta_l[b]$ is the residual amount, at scale $\sigma\rho^l$, satisfying

$$b = n_l[b] fa_0\sigma\rho^l + \delta_l[b]. \tag{D9}$$

For the Mexican hat wavelet and dual case, $\mathcal{W}_{mh}(x) = \mathcal{D}_{mh}(x)$, with $f = a_0 = 1$, the crucial question is whether the corresponding scaling function, $S(\frac{y}{\sigma})$, is sufficiently bounded, for real values of y. However, this has to be influenced by the extent to which the dual-wavelet expansion is definable for such complex scales. This is our assumption.

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