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Moment-wavelet quantization and (complex) multiple turning point contributions

C R Handy, R Murenzi, K Bouyoucef and H A Brooks

Department of Physics and Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, GA 30314, USA

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Abstract. Wavelet transform theory is an efficient multiscale formalism for analysing local structures. This philosophy, when incorporated within quantum mechanics, demands that there be a naturally corresponding, localized quantization theory, in contrast to the variational formalisms in the literature. Through the recently established equivalency formalism between moment quantization theory and continuous wavelet transform theory (Handy C R and Murenzi R 1998 *J. Phys. A: Math. Gen.* **31** 9897 and Handy C R and Murenzi R 1999 *J. Phys. A: Math. Gen.* **32** 8111), we argue that a new quantization prescription can be defined in which the kinetic energy term is set to zero at the (complex) turning points (or turning hypersurfaces). We establish this, both for one- and two-dimensional systems, and clarify the relevancy of multiscale wavelet analysis in this quantization process.

1. Introduction

Nearly two decades ago, Handy (1981) emphasized the importance of a moment quantization strategy in defining an efficient multiscale formalism for analysing (scale related) transient effects in singular perturbation/strong coupling problems.

Moment quantization (MQ) refers to all methods for solving the configuration space quantum system by transforming it into an extensive (non-local) representation involving the moments, $\mu(p) \equiv \int \mathrm{d}x\, x^p \Psi(x)$, of the (unknown) wavefunction, Ψ, as represented in the works by Blankenbeckler *et al* (1980), Killingbeck *et al* (1985), Handy and Bessis (1985), Handy *et al* (1988a, b), and Fernandez and Ogilvie (1993). This perspective led to fundamentally new energy-quantization methods, based on the classic *moment problem* within pure mathematics (Shohat and Tamarkin 1963), for solving difficult, singular perturbation-type problems, such as the quadratic Zeeman effect for strong magnetic fields (Handy and Bessis 1985, Handy *et al* 1988a, b).

More recently, a significiant vindication of the MQ philosophy has been achieved through Handy and Murenzi's (HM) work establishing the equivalence between MQ and continuous wavelet transform (CWT) analysis (HM 1998a, b). This unified analysis leads to the multiscale generation of the configuration space wavefunction.

Consistent with Handy's original formulation, the unification of MQ and CWT required the use of the generalized moments, $\mu_{a,b}(p) \equiv \int \mathrm{d}x\, x^p \mathcal{S}(\frac{x}{a})\Psi(x+b)$, dependent on the scale and translation variables, a and b, respectively. The *scaling function*, $\mathcal{S}$, is generally arbitrary, although limiting it to the form $\mathcal{S}(x) = \mathrm{e}^{-Q(x)}$, where $Q(x)$ is an appropriate polynomial, leads to certain advantages.

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The *scaling transform* of a function, $F(x)$, is defined as $SF(a,b) \equiv \frac{1}{\nu}\int \frac{\mathrm{d}x}{a}\mathcal{S}(\frac{x-b}{a})F(x)$, where $\nu \equiv \int \mathrm{d}x\, \mathcal{S}(x)$. Thus the scaled and translated moments, $\mu_{a,b}(p)$, are essentially linear superpositions of the scaling transform for the functions $\{x^p\Psi(x)|p \geqslant 0\}$.

In a subsequent work HM extended the equivalence between MQ and CWT to a particular (exact) discretization of CWT, referred to as DCWT (HM 1999). As is well known, CWT and its discretized (a-adic) formulation, DCWT, define efficient, simultaneous space–scale, or time–frequency, localized representations of a given signal or wavefunction (Daubechies 1991). They are well suited for studying transient effects, a characteristic feature of (strong coupling) singular perturbation-type problems.

For future reference, in this work we shall consider wavelet transforms (Grossmann and Morlet 1984),

$$W\Psi(a,b) \equiv \frac{1}{\sqrt{a}}\int \mathrm{d}x\, \mathcal{W}\left(\frac{x-b}{a}\right)\Psi(x) \tag{1}$$

where the *mother wavelet* is given by $\mathcal{W}(x) = \mathcal{N}\partial_x^I \mathrm{e}^{-Q(x)}$, $I \geqslant 1$, and $Q(x)$ is a suitable polynomial. For such cases, we have that the wavelet transform corresponds to a finite superposition of the scaled and translated moments:

$$W\Psi(a,b) = \sum_{p=0}^{P} C(a,b;\,p)\mu_{a,b}(p) \tag{2}$$

where the coefficient functions are readily obtainable.

One of the more impressive results of the MQ-CWT/DCWT equivalency formalism is the straightforward derivation of the *signal-wavelet* inversion formula(s). For the continuous case (CWT) we have (HM 1998b)

$$\Psi(b) = \frac{1}{\nu}\int_0^{+\infty}\frac{\mathrm{d}a}{a^{\frac{5}{2}}}\int_{-\infty}^{+\infty}\mathrm{d}\xi\, \mathcal{D}\left(\frac{\xi-b}{a}\right)W\Psi(a,\xi) \tag{3}$$

where $\mathcal{D}$ corresponds to a suitable dual function which must satisfy, in terms of the Fourier transforms, a three-way relation involving the scaling function and the mother wavelet

$$-k\partial_k\hat{\mathcal{S}}(k) = \sqrt{2\pi}\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k). \tag{4}$$

For real configurations, we also have

$$\int \mathrm{d}b\, \Psi(b)^2 = \int_0^{+\infty}\int_{-\infty}^{+\infty}\frac{\mathrm{d}a\,\mathrm{d}\xi}{\nu a^{\frac{5}{2}}}D\Psi(a,\xi)W\Psi(a,\xi) \tag{5}$$

where

$$D\Psi(a,\xi) = \int \mathrm{d}b\, \mathcal{D}\left(\frac{\xi-b}{a}\right)\Psi(b). \tag{6}$$

For the discrete case (DCWT), the corresponding signal-wavelet inversion formula is (HM 1999)

$$\Psi(b) = \frac{1}{\nu}\sum_{l=-\infty}^{+\infty}\sum_{j=-\infty}^{+\infty}\mathcal{D}\left(\frac{b - fa_0 j\rho^l - \delta_l[b]}{fa_0\rho^l}\right)\times\frac{1}{\sqrt{\rho^l}}W\Psi(\rho^l,\, fa_0 j\rho^l + \delta_l[b]). \tag{7}$$

For this case, one assumes an (a-adic) discretization of the scale ($a_0\rho^l$) and translation ($fa_0\rho^l j$) parameter space ($\rho > 1$). In addition, at each scale value, the point of reconstruction, b, assumes a decomposition

$$b = n_l[b]fa_0\rho^l + \delta_l[b] \tag{8}$$

where $n_l[b]$ is the optimal integer translation value, and $\delta_l[b]$ the ensuing remainder term.

The dual function, also satisfies a three-way relation of the form

$$(\hat{\mathcal{S}}(k) - \hat{\mathcal{S}}(\rho k)) = \left[\sum_{j=-\infty}^{\infty} \mathcal{D}(j) \mathrm{e}^{ijfk} \right] \hat{\mathcal{W}} \left(\frac{k}{a_0} \right) \tag{9}$$

where the scaling function is different from that in the CWT case.

The preceding signal (Ψ)-wavelet reconstruction formulae suggest a multiscale, pointwise, reconstruction ansatz at each point, b. This is better appreciated within the context of their derivation, as reviewed in section 2. This interpretation defines the basic motivation for this work: to determine the corresponding local quantization formalism that naturally complements the multiscale, pointwise reconstruction character inherent to the above inversion formulae. We argue in this paper that a (complex) turning point quantization strategy is the most relevant.

This work is an attempt at better understanding the significance of CWT/DCWT in quantum mechanics. We are not satisfied with its present, widespread, use as only providing a convenient localized basis on which to implement variational calculations (Cho *et al* 1993, Wei and Chou 1996, and Tymczak and Wang 1997). Based on the underlying MQ formalism, we believe that the real importance of CWT/DCWT is in its implicit emphasis on understanding the contribution of all (complex) turning points (hypersurfaces) to the quantization problem.

In this work we limit our analysis to the bound state problem for linear quantum operators, as defined in terms of the Schrodinger Hamiltonian representation

$$\mathcal{H}\Psi(x) = E\Psi(x) \tag{10}$$

where $\mathcal{H} \equiv -\epsilon \partial_x^2 + V(x)$, for rational fraction potentials (which includes many important physical processes)

$$V(x) = \frac{\mathcal{P}_N(x)}{\mathcal{P}_D(x)} \tag{11}$$

where $\mathcal{P}_N(x) \equiv \sum_{j=0}^{T} N(j)x^j$ and $\mathcal{P}_D(x) \equiv \sum_{j=0}^{B} D(j)x^j$. In terms of their respective degrees, we define $m_s + 1 = \mathrm{Max}\{T, B\}$. The multidimensional extension of the above is implicitly assumed as well, and will be used in a specific case later on. The extension of the present formalism to scattering states will be discussed in a future work.

The turning points, τ_ℓ, satisfy

$$V(\tau_\ell(E)) = E \tag{12}$$

for $0 \leqslant \ell \leqslant m_s$. Thus, there are $m_s + 1$, (complex) turning point root solutions, for arbitrary values of the energy parameter variable, E.

In terms of the scaling transform representation the (equivalent) Schrodinger equation problem $\mathcal{P}_D(x)(\mathcal{H} - E)\Psi(x) = 0$, is transformed into

$$S_H\Psi(a, b) \equiv \int \mathrm{d}x\, \mathcal{S}\left(\frac{x-b}{a} \right) \mathcal{P}_D(x)(\mathcal{H} - E)\Psi(x) = 0 \tag{13}$$

for all a and b values. Since the scaling function becomes (up to a factor) the Dirac measure in the zero-scale limit, the scaling transform equation is equivalent to the original Schrodinger equation.

In principle, taking $S_H\Psi(a, b) = 0$ at fixed a, b does not guarantee that Ψ will be a solution to the Schrodinger equation. If all the moments of a 'well behaved' function are zero, $\mu(p) = \int \mathrm{d}x\, x^p f(x) = 0$, then $f(x) = 0$. Accordingly, we should also consider expanding the above set of constraints by working with

$$\int \mathrm{d}x\, (x-b)^p \left(\mathcal{S}\left(\frac{x-b}{a} \right) \mathcal{P}_D(x)(\mathcal{H} - E)\Psi(x) \right) = 0 \tag{14}$$

for arbitrary $p \geqslant 0$.

This set of relations is demanding that Ψ satisfy the Schrodinger equation both locally ($a \to 0$) and globally (extensively), with regards to the p dependence. The former is an attribute of configurations space, whereas the latter corresponds to momentum space. Thus, a simultaneous space–scale quantization is implicitly defined by these relations.

These integral equations generate the $\mu_{a,b}(p)$ *moment equation*, which is equivalent to the configuration space Schrodinger equation.

For systems of the above type, if the scaling function is of the form $\mathcal{S}(x) = \mathrm{e}^{-Q(x)}$, where $Q(x)$ is an appropriate polynomial (i.e. $Q(0) = 0$), the scaled ($a \geqslant 0$) and translated ($|b| < \infty$) moments of the (unknown) wavefunction ($\alpha \equiv \frac{1}{a}$)

$$\mu_{\alpha,b}(p) = \int \mathrm{d}x\, x^p \mathrm{e}^{-Q(\alpha x)} \Psi(x + b) \tag{15}$$

convert the scaling tranform moment expressions into an infinite set of coupled moment equations of the form

$$\mu_{\alpha,b}(p) = \sum_{\ell=0}^{m_s} M_{E,\alpha,b}(p, \ell) \mu_{\alpha,b}(\ell) \tag{16}$$

$p \geqslant 0$, explained subsequently (Handy and Bessis 1985, Handy *et al* 1988a, b).

All of the scaled and translated moments, $\mu_{\alpha,b}(p)$, depend on the first $1 + m_s$ moments. The latter in turn, satisfy a finite, linear, set of coupled differential moment equations (CDME) of first order in the inverse scale variable, α:

$$\partial_\alpha \vec{\mu}_{\alpha,b} = \mathcal{M}(\alpha, b, E, \epsilon) \vec{\mu}_{\alpha,b} \tag{17}$$

where $\vec{\mu}_{\alpha,b} \equiv (\mu_{\alpha,b}(0), \ldots, \mu_{\alpha,b}(m_s))$. The $\mathcal{M}(\alpha, b, E, \epsilon)$ matrix is readily obtainable, and depends on the energy parameter, E. These equations reveal how the large-scale ($a = \infty, \alpha = 0$) structure impacts the local behaviour ($a = 0, \alpha = \infty$) of the problem. As such, they define an important multiscale representation (HM 1996, 1997, 1998a, b, 1999).

As mentioned previously, many important wavelet transforms can be written as superpositions of the above moments (i.e. $\{\mu_{\alpha,b}(\ell) | 0 \leqslant \ell \leqslant m_s\}$). Thus we can regard the CDME equations as the *wavelet transform* equation of the Schrodinger equation.

The scaled and translated moments have several important properties. For physical solutions, they are regular in b (i.e. $\mu_{\alpha,b}(p) = \int \mathrm{d}x\, (x - b)^p \mathrm{e}^{-Q(\frac{x-b}{a})} \Psi(x)$). As long as the asymptotic form of $Q(x)$ does not grow faster than the corresponding JWKB representation (i.e. $\Psi(x) = \mathrm{e}^{-T(x)}$, and $\lim_{|x| \to \infty} \frac{Q(x)}{T(x)} = \text{const}$), then they are also analytic at $\alpha = 0$.

In general, as required by the underlying dependence on Ψ, we restrict the form of the 'initial', $\alpha = 0$, configuration to be an arbitrary polynomial, in b, of the form

$$\mu_{0,b}(\ell) = \sum_{j=0}^{\ell} \binom{\ell}{j} (-b)^{\ell - j} \mu_{0,0}(j) \tag{18}$$

where, $0 \leqslant \ell \leqslant m_s$, $\binom{\ell}{j} \equiv \frac{\ell!}{(\ell - j)! j!}$, and the $\mu_{0,0}(j)$ are arbitrary.

From the above polynomial representation, we see that the infinite-scale ($a = \infty, \alpha = 0$) moments are linear superpositions of the infinite-scale, zero-translation moments $\mu_{0,0}(\ell) \equiv \mu(\ell)$, which are referred to as the *missing moments*. We shall also use the notation $\mu_\ell \equiv \mu(\ell)$.

There are three distinct ways of solving the CDMEs in equation (17).

(1) In all of the previous studies by HM (1996, 1997, 1998a, b, 1999), they utilized MQ methods different from those presented here (i.e. the eigenvalue moment method (EMM), Handy *et al* (1988a, b)) in order to determine the physical values for the energy and missing moments (and in turn the $\mu_{0,b}(\ell)$). These physical values are then used to integrate the

initial value problem defined by the CDME, up to sufficiently small scales, $\frac{1}{\alpha} = a \to 0$. This procedure led to the pointwise recovery (reconstruction) of the physical wavefunction based on using either: (i) the asymptotic moment relations

$$\lim_{\alpha\to\infty} \alpha^{1+p}\mu_{\alpha,b}(p) = \nu(p)\Psi(b) \tag{19}$$

(provided $\nu(p) \equiv \int \mathrm{d}y\, y^p \mathrm{e}^{-Q(y)} \neq 0$); or, (ii) reconstructing $\Psi(b)$ through the relevant signal-wavelet inversion formula which depends on the computed $\mu_{\alpha,b}(p)$.

Although this approach has proven to be effective for many strong coupling/singular perturbation problems, in the case of extremely singular problems the use of EMM theory may be too slowly converging since large moment expansion orders are required. We can circumvent this difficulty by incorporating the quantization procedure within the analysis of the CDME. This is the focus of approaches 2 and 3, described below.

(2) One can study the CDME directly and generate $m_s + 1$ independent solutions, for each E:

$$\partial_\alpha \mathcal{B}^{(j)}_{\ell_1}(\alpha, b, E, \epsilon) = \sum_{\ell_2=0}^{m_s} \mathcal{M}_{\ell_1,\ell_2}(\alpha, b, E, \epsilon)\mathcal{B}^{(j)}_{\ell_2}(\alpha, b, E, \epsilon) \tag{20}$$

where $0 \leqslant j, \ell_1 \leqslant m_s$, and

$$\mathcal{B}^{(j)}_{\ell}(0, b, E, \epsilon) = \begin{cases} \binom{\ell}{j}(-b)^{\ell-j}, & \text{for} \quad \ell \geqslant j \\ 0, & \text{if} \quad \ell < j. \end{cases} \tag{21}$$

The general CDME solution is given by the superposition

$$\mu_{\alpha,b}(\ell) = \sum_{j=0}^{m_s} \mu_j \mathcal{B}^{(j)}_{\ell}(\alpha, b, E, \epsilon) \tag{22}$$

for arbitrary μ_j. As previously noted, a large class of wavelet transforms, $W\Psi(a, b)$, can be written as a superposition of the $\mu_{\alpha,b}(\ell)$. As argued in this work, if a_s is a sufficiently small-scale value, we can then quantize by imposing the condition

$$W\Psi(a_s, \tau_\ell(E)) = 0 \tag{23}$$

at each of the $m_s + 1$ (complex) turning points. For mother wavelets of the form $\mathcal{W}(x) = \partial_x^2 \mathrm{e}^{-Q(x)}$, the $a_s \to 0$ limit of the above quantization condition becomes $\partial_x^2 \Psi(\tau_\ell(E)) = 0$.

Since there are as many turning points as there are missing moments, the quantization condition defined by equation (23) leads to a set of $m_s + 1$ linear equations in $m_s + 1$ unknowns, resulting in a determinantal equation for determining the physical energy roots. This (exact) approach, is discussed in a forthcoming work (Handy and Brooks 2000). It involves the numerical determination of the functions $\mathcal{B}^{(j)}_{\ell}$, which is beyond the scope of this paper. Also, the extension of this formalism to the multidimensional case, although possible, poses a difficult analytical problem which has not been solved as yet.

Despite the above difficulties, it is possible to analytically implement the essence of the above procedure (in a manner extendable to the multidimensional case as well) through a non-orthogonal basis representation described in the works by Tymczak, Japaridze, Handy, and Wang (TJHW 1998a, b). This is the focus of this work.

(3) In the two recent works by TJHW (1998a, b) they showed that the wavefunction can be expressed in terms of the representation

$$\Psi(x) = \sum_{n=0}^{\infty} A_n(E, \mu_0, \ldots, \mu_{m_s})(-\partial_x)^n R(x) \tag{24}$$

(to be referenced as Ψ_{TJHW}) for some appropriate *reference function*, $R(x)$. The A_n coefficients are linearly dependent on the missing moments, μ_ℓ. The TJHW quantization condition, $A_{N-\ell}(E, \mu_0, \ldots, \mu_{m_s}) = 0$, for $N \to \infty$ and $0 \leqslant \ell \leqslant m_s$, yielded impressive results for a wide assortment of one- and two-dimensional quantum problems.

In this paper, we investigate the suitability of the TJHW representation from the perspective of moment-wavelet turning point quantization, as defined below.

One important feature of the TJHW representation is that because it is derived from a resummation of the Fourier space power series expansion, it is intrinsically a multiscale expansion as well. Therefore, the scaled and translated power moments, $\mu_{\alpha,b}(p) = \int \mathrm{d}x\, x^p \mathrm{e}^{-Q(\alpha x)} \Psi_{\mathrm{TJHW}}(x + b)$, should satisfy the CDME at large scale values ($a \to \infty$) for a wide range of energy parameter values. It is only for the physical solution that the moments of the Ψ_{TJHW} representation will satisfy the CDME for all scale values ($0 \leqslant a < \infty$).

Let

$$\Psi^{(N)}(x) \equiv \sum_{n=0}^{N} A_n(E, \mu_0, \ldots, \mu_{m_s})(-\partial_x)^n R(x) \tag{25}$$

define the Nth-order TJHW representation. Because the $\{(-\partial_x)^n R(x)\}$ define a non-orthogonal complete basis set, the TJHW representation is complete and therefore capable of accurately generating the true solution, for some sufficiently large order, N. Instead of the TJHW quantization conditions, we investigate the effectiveness of the turning point quantization (TPQ) conditions (utilizing mother wavelets of the form $\mathcal{W}(x) = \mathcal{N}\partial_x^2 \mathrm{e}^{-Q(x)}$)

$$W\Psi^{(N)}(a_s, \tau_\ell(E)) = 0 \tag{26}$$

for $0 \leqslant \ell \leqslant m_s$, and some suitably small a_s.

The legitimacy of this quantization condition is established in section 4. There we argue that if the mother wavelet is modelled after the form of the kinetic energy operator, then the signal-wavelet inversion formula converges fastest to $\Psi(b)$ at the turning points, $b = \tau_\ell(E)$. At the turning points, the kinetic energy term is zero. Since the wavelet transform converges asymptotically to the kinetic energy term (up to a scale-dependent factor), in the zero-scale limit, the motivation for equation (26) becomes readily apparent.

The TJHW solution to the TPQ condition in equation (26) is denoted by $\Psi_{a_s}^{(N)}(x)$. Most of the following discussion adopts a general formalism with respect to a_s; however, in practice, we will usually take $a_s = 0$. For this case, the TPQ condition simply becomes

$$\partial_x^2 \Psi^{(N)}(\tau_\ell(E)) = 0. \tag{27}$$

Due to the linear dependence of the A_n on the μ, the TPQ condition corresponds to a set of $m_s + 1$ linear equations, yielding a determinantal equation for approximating the physical root solutions, $E_r^{(N)}(a_s)$, and the corresponding missing moments, $\{\mu_\ell^{(N)}(a_s)\}$. The energy roots corresponding to the case $a_s = 0$ are denoted by $E_r^{(N)} \equiv E_r^{(N)}(0)$.

Imposing the TPQ conditions not only yields highly accurate estimates for the physical energies, but also (non-converging) spurious, unphysical values as shown in figure 1, for $N = 40$ (refer to table 1, for the $E_r^{(N)}(0)$ estimates corresponding to $N = 20, 30, 40$). In order to discriminate between the physical and unphysical solutions, one could check the accuracy of the generated TPQ configuration solution by measuring the extent to which it satisfies

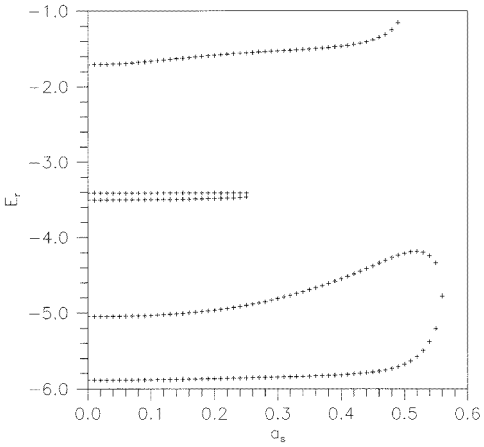

Figure 1. TPQ roots $W\Psi(a_s, \tau_\ell(E)) = 0$.

Table 1. Results for $V(x) = -5x^2 + x^4$ (* physical roots).

N	E_{gr}	N	E_{gr}	N	E_{gr}
20	−5.551 8649	30	−5.827 0575	40	−5.887 4918
	−3.410 7938*		−4.452 3274		−5.048 7046
	−3.357 3571		−3.410 1404*		−3.503 0771
	−1.623 2814		−2.540 7367		−3.410 1428*
	−0.259 2104		−1.315 0128		−1.708 8318
			−0.187 3868		−0.679 9603
					−0.112 5330

the Schrodinger equation. However, within the present multiscale analytical framework, one should establish consistency with the Schrodinger equation, scale by scale (proceding from the largest scale). The fact that the CDME equations are a space–scale representation of the Schrodinger equation becomes important in this regard.

The moments generated from the TPQ solution $\Psi^{(N)}_{a_s}(x)$, will satisfy the CDME equations up to a critical scale, $a_c(a_s, N)$. For the physical solution, particularly as $N \to \infty$, one expects $a_c \approx a_s$ as $a_s \to 0$. In our calculations, particularly for the double-well quartic anharmonic oscillator, at order $N = 40$, we find that the TPQ estimates for the physical ground state energy yields $a_s \to 0$ and $a_c \to 0.4$. Nevertheless, the TPQ generated wavefunction satisfies the Schrodinger equation very well. Likewise, for the spurious roots (also at $N = 40$), we find that even as $a_s \to 0$, the critical scale value a_c stays essentially unchanged at $a_c = \mathrm{O}(0.8)$. While these numerical behaviours are consistent with the expected behaviour, we prefer a more emphatic criterion for discriminating between the physical and unphysical TPQ roots.

At finite order, N, let us decompose the TPQ solution (physical or unphysical) into the representation

$$\Psi^{(N)}_{a_s}(x) = \mathcal{R}(x) + \mathcal{A}(x) \tag{28}$$

where $\Psi^{(N)}_{a_s}$ is the TJHW configuration obtained by imposing the TPQ condition at scale a_s. The configuration $\mathcal{A}(x)$ denotes all the terms or integrand, from the DCWT or CWT signal-wavelet inversion formulae, respectively, corresponding to scale $a \geqslant a_c$ (i.e. the projection of $\Psi^{(N)}_{a_s}$ onto the wavelet space with scale $a \geqslant a_c$); whereas $\mathcal{R}$ is the remainder. The $\mathcal{A}(x)$ configuration will satisfy the CDME equations up to scale a_c (i.e. will be a solution to the

Schrodinger equation up to that scale). The remainder configuration, $\mathcal{R}(x)$, will be made up of wavelet space terms corresponding to scale values $a < a_c$.

If the configuration $\Psi_{a_s}^{(N)}(x)$ is to correspond to a physical state, then a_s should be close to a_c. By 'close', we mean that the remainder configuration, $\mathcal{R}(x)$, must be small. One way of assessing this is to compare the wavelet transform $W\Psi_{a_s}^{(N)}(a,\tau)$ (for fixed a_s, and any relevant turning point, τ) for $a \in (0, a_c)$ and $a \in [a_c, \infty)$. We emphasize that $\mathcal{A}$ corresponds to the projection onto the wavelet space defined by scale values in the second interval, $[a_c, \infty)$.

If $W\Psi_{a_s}^{(N)}(a,\tau)$ assumes significant values on the interval $(0, a_c)$, as compared with the interval $[a_c, \infty)$, it indicates that $\mathcal{R}(x)$ is likewise significant and thus $\Psi_{a_s}^{(N)}(x)$ does not represent a good (approximate) solution to the Schrodinger equation (since it significantly differs from $\mathcal{A}(x)$, which is a solution to the Schrodinger equation, to scale a_c).

If $W\Psi_{a_s}^{(N)}(a,\tau)$ assumes no significant values on $(0, a_c)$, as compared with its values on $[a_c, \infty)$, then both $\Psi_{a_s}^{(N)}$ and $\mathcal{A}(x)$ are sufficiently close to each other (i.e. $\mathcal{R}(x)$ is negligible), and thus $\Psi_{a_s}^{(N)}$ (approximately) solves the Schrodinger equation, to scale a_c.

The preceding analysis defines a process for distinguishing between physical and unphysical TPQ solutions. We use this as an effective criteria in discriminating between the physical and unphysical solutions.

In the following sections we present a more comprehensive analysis of the preceding formalism, together with numerical examples for several representative problems in one and two space dimensions. Only the double-well quartic anharmonic oscillator is discussed in detail. We first define the necessary moment-wavelet expressions.

2. The wavelet transform

In this section we clarify why the preceding signal-wavelet inversion formulae really correspond to a multiscale analysis of the local behaviour of Ψ. Consider the scaling transform

$$\mathcal{S}\Psi(a,b) \equiv \frac{1}{\nu}\int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{a} \mathrm{e}^{-Q(\frac{x-b}{a})}\Psi(x) \tag{29}$$

where $\mathcal{S}(x) \equiv \mathrm{e}^{-Q(x)}$, $\nu = \int \mathrm{d}x\, \mathrm{e}^{-Q(x)} \neq 0$, Ψ is a physical (wavefunction) configuration, and a and b are arbitrary scale and translation variables, respectively. In the zero-scale limit, we recover the wavefunction

$$\operatorname*{Lim}_{a\to 0} \mathcal{S}\Psi(a,b) = \Psi(b). \tag{30}$$

Thus $\mathcal{S}\Psi(a,b)$ represents the multiscale dependence of Ψ at the scale value a.

Through some simple substitutions we can transform $\mathcal{S}\Psi(a,b)$ into the signal (Ψ)-wavelet inversion formula (HM 1998a, b)

$$\mathcal{S}\Psi(a,b) = \frac{1}{\nu}\int_{a}^{+\infty} \frac{\mathrm{d}a_v}{a_v^{\frac{5}{2}}} \int \mathrm{d}\xi\, \mathcal{D}\left(\frac{\xi - b}{a_v}\right) W\Psi(a_v,\xi) \tag{31}$$

where the wavelet transform, $W\Psi$, is given by

$$W\Psi(a_v,\xi) = \frac{1}{\sqrt{a_v}}\int \mathrm{d}x\, \mathcal{W}\left(\frac{x-\xi}{a_v}\right)\Psi(x). \tag{32}$$

The kernel, $\mathcal{W}$, corresponds to a suitable *mother wavelet*, where $\mathcal{D}$ is its dual. The mother wavelet, dual function, and scaling function, $\mathcal{S}(x) \equiv \mathrm{e}^{-Q(x)}$, constrain each other through relations given in terms of their Fourier transforms (i.e. $\hat{\mathcal{W}}(k) \equiv \frac{1}{\sqrt{2\pi}}\int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}\mathcal{W}(x)$)

$$-k\partial_k \hat{\mathcal{S}}(k) = \sqrt{2\pi}\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k). \tag{33}$$

We stress that the scaling transform in equation (29), which corresponds to an averaging sampling process, is equivalent to integrating over all scale values of the signal-wavelet

inversion formula ($a_v \geqslant a$). An analogous result also holds for the discrete case, discussed below.

From the MQ perspective, an exact discretization of the above two-dimensional integration can be readily obtained. Two versions of this are (HM 1999)

$$\mathcal{S}\Psi(\rho^L, b) = \frac{1}{\nu} \sum_{j=-\infty}^{+\infty} \sum_{l=L}^{+\infty} \mathcal{D}\left(\frac{b - j\rho^l - \delta_l[b]}{\rho^l}\right) \times \frac{1}{\sqrt{\rho^l}} W\Psi(\rho^l, j\rho^l + \delta_l[b]) \tag{34}$$

and

$$\mathcal{S}\Psi(\rho^L, b) = \frac{1}{\nu} \sum_{j=-\infty}^{+\infty} \sum_{l=L}^{+\infty} \frac{\mathcal{D}(j)}{\sqrt{(\rho^l)}} W\Psi(\rho^l, b - j\rho^l) \tag{35}$$

where $W\Psi(\rho^l, b - j\rho^l) = \frac{1}{\sqrt{(\rho^l)}} \int \mathrm{d}x\, \mathcal{W}(\frac{x-(b-j\rho^l)}{\rho^l})\Psi(x)$. Note that $\rho > 1$, $L \to -\infty$, and $\operatorname{Lim}_{L\to-\infty} \mathcal{S}\Psi(\rho^L, b) = \Psi(b)$. The expression $\delta_l[b]$, for arbitrary b, is defined by the decomposition $b = n_l[b]\rho^l + \delta_l[b]$, where n_l is the optimal integer, at scale index l, satisfying the relation. We have $\operatorname{Lim}_{l\to-\infty} \delta_l[b] = 0$, and $\operatorname{Lim}_{l\to+\infty} \delta_l[b] = b$.

The $\mathcal{W}$ mother-wavelet and $\mathcal{D}$ satisfy (for a different scaling function to that given in equation (33))

$$\hat{\mathcal{S}}(k) - \hat{\mathcal{S}}(\rho k) = \sum_{j=-\infty}^{+\infty} [\mathcal{D}(j)\mathrm{e}^{ijk}]\hat{\mathcal{W}}(k). \tag{36}$$

In this paper we will adopt the dyadic ($\rho = 2$) scale, 2^l, and translation, $j2^l$, values, as well as the Mexican hat wavelet and dual functions

$$\mathcal{W}_{MH}(x) = -\mathcal{N}_{MH}\partial_x^2 \mathrm{e}^{-\frac{x^2}{2}} \tag{37}$$

$$D(j) = \mathcal{N}_{MH}(1 - j^2)\mathrm{e}^{-\frac{j^2}{2}} \tag{38}$$

where $\mathcal{N}_{MH} \equiv \frac{2}{3^{\frac{1}{2}}\pi^{\frac{1}{4}}}$, and $\nu = 3.44$. The preceeding discretized wavelet transform analysis is referred to as (a-adic) discrete continuous wavelet transform (DCWT) analysis.

From the above formalism, it is clear that either CWT or DCWT defines a multiscale formulation (involving the contributions from all scales) for understanding the local structure of the configuration at point b. Because of this interpretation, the application of CWT/DCWT to quantum mechanics should be focused on identifying important localized features of a physical solution which serve to determine it. The most natural localized features of a wavefunction are its characteristics near the turning points (or hypersurfaces). The focus on turning points is, in fact, quite natural within both MQ and CWT analyses. We show this in the next two sections.

3. Turning points and moment quantization

The original motivation for MQ analysis (Handy 1981) was that it provided a representation in which kinetic energy term perturbation (i.e. singular perturbation theory) was manifestly more regular than that provided by a configuration space analysis. Thus consider the time-independent, Schrodinger equation problem

$$-\epsilon\partial_x^2\Psi(x) + V(x)\Psi(x) = E\Psi(x) \tag{39}$$

where ϵ is a 'small' kinetic energy perturbation parameter, $V(x)$ is the potential function, and E the energy. In this paper we limit the potential function to be a (multidimensional) rational fraction

$$V(x) = \frac{\sum_{j=0}^{T} N(j)x^j}{\sum_{j=0}^{B} D(j)x^j}. \tag{40}$$

Within configuration space, the singular perturbation character of ϵ-expansions makes it an undesirable representation. That is, the order of the Schrodinger differential equation abruptly changes for $\epsilon = 0$ and 0^+. This is not the case if one transforms the Schrodinger equation into a moment representation defined by

$$\mu(p) = \int \mathrm{d}x\, x^p \Psi(x) \tag{41}$$

where $p \geqslant 0$.

The corresponding *moment equation* (i.e. multiply both sides of equation (39) by $x^p \sum_{j=0}^{B} D(j)x^j$ and perform the necessary integration by parts)

$$-\epsilon\left(\sum_{j=0}^{B} D(j)(p+j)(p+j-1)\mu(p+j-2)\right) + \sum_{j=0}^{T} N(j)\mu(p+j) = E\left(\sum_{j=0}^{B} D(j)\mu(p+j)\right) \tag{42}$$

for $p \geqslant 0$, is of effective order $m_s + 1 = \mathrm{Max}\{T, B\}$, since the initialization (i.e. missing) moments $\{\mu(\ell)|0 \leqslant \ell \leqslant m_s\}$ must be specified before all the other moments can be determined. The energy, E, appears as a variable parameter.

The order of the finite-difference moment equation does not change for any value of ϵ. This is one immediate manifestation of the relevance of such moment representations in addressing singular perturbation problems corresponding to kinetic energy perturbation. In a moments' representation, such expansions are more regular than in a configuration representation.

The linear dependence of the $\{\mu(p)|p > m_s\}$ moments, with respect to the missing moments, can be expressed through the relation

$$\mu(p) = \sum_{\ell=0}^{m_s} M_E(p, \ell)\mu(\ell) \tag{43}$$

where the readily obtainable M_E-coefficients satisfy $M_E(\ell_1, \ell_2) = \delta_{\ell_1,\ell_2}$.

In the zero-order limit, $\epsilon = 0$, the moment equation has the exact solution

$$\mu_0(p) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell \tau_\ell^p(E) \tag{44}$$

where the $\mathcal{A}_\ell$ are arbitrary, and the $\tau_\ell(E)$ correspond to all the $m_s + 1$ turning point roots of the defining equation

$$V(\tau_\ell(E)) = E \tag{45}$$

for $0 \leqslant \ell \leqslant m_s$. We emphasize that we regard the turning points as known (computable) functions of the energy variable. Furthermore, we will be working with all of them. Some of these may be complex functions, depending on the potential.

The zero-order moment solution corresponds to an atomic distribution defined by

$$\Psi_{\epsilon=0}(x) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell \delta(x - \tau_\ell(E)). \tag{46}$$

We have implicitly derived all the preceding relations assuming that the moments correspond to the physical configuration. This is because the unphysical solutions to the Schrodinger equation do not admit finite moments. However, within the context of the moment equation, we see that for arbitrary E one can generate a moment space solution which is finite. Clearly then, the moment equation defines a finite extension of the problem, even for the unphysical regime.

There are many quantization methods based on the use of the moment equation representation. The works by Handy and Bessis (1985), and Handy *et al* (1988a, b) emphasized the importance of this representation with regards to strong coupling/singular perturbation-type problems. These methods generated very good estimates for the discrete state energies; however, they did not pursue the issue of wavefunction reconstruction.

The recent works by HM (1996, 1997, 1998a, b, 1999) focused on this problem. Central to their analysis is the use of the generalized, scale- and translation-dependent, moments ($\alpha \equiv \frac{1}{a}$)

$$\mu_{\alpha,b}(p) = \int \mathrm{d}x\, x^p \mathrm{e}^{-Q(\alpha x)} \Psi(x+b) \tag{47}$$

where $Q(x) = \sum_{n=0}^{2N} \Xi(n) x^n$, $\Xi(0) = 0$, and $\Xi(2N) > 0$.

The function $\Phi(x) \equiv \mathrm{e}^{-Q(\alpha x)}\Psi(x+b)$ satisfies the corresponding Schrodinger equation

$$-\epsilon(\partial_x^2 + 2\alpha Q'(\alpha x)\partial_x + \alpha^2[Q''(\alpha x) + (Q'(\alpha x))^2])\Phi(x) + V(x+b)\Phi(x) = E\Phi(x). \tag{48}$$

So long as

$$\operatorname*{Lim}_{|x|\to\infty} \frac{Q'(x)}{\sqrt{V(x)}} = \text{const} \tag{49}$$

the order of the moment equation satisfied by the $\mu_{\alpha,b}(p)$ (i.e. $\mu_{\alpha,b}(p) = \int \mathrm{d}x\, x^p \Phi(x)$) is unchanged, $m_s + 1$. This leads to the representation

$$\mu_{\alpha,b}(p) = \sum_{\ell=0}^{m_s} M_{\alpha,b,E,\epsilon}(p,\ell)\mu_{\alpha,b}(\ell) \tag{50}$$

(similarly derived as in equation (42)) where $M_{\alpha,b,E,\epsilon}(\ell_1,\ell_2) = \delta_{\ell_1,\ell_2}$, as before.

In general,

$$\partial_\alpha \mu_{\alpha,b}(p) = -\int \mathrm{d}x\, x^{p+1} Q'(\alpha x)\mathrm{e}^{-Q(\alpha x)}\Psi(x+b). \tag{51}$$

From the assumed polynomial structure of Q, as well as the dependence of all the moments on the (initialization) moments $\{\mu_{\alpha,b}(\ell)|0 \leqslant \ell \leqslant m_s\}$ a finite, coupled, set of first-order equations in the inverse scale variable, α, is obtained:

$$\partial_\alpha \begin{pmatrix} \mu_{\alpha,b}(0) \\ \cdot \\ \cdot \\ \cdot \\ \mu_{\alpha,b}(m_s) \end{pmatrix} = \begin{pmatrix} \mathcal{M}_{0,0}(\alpha,b,E,\epsilon)\ldots\mathcal{M}_{0,m_s}(\alpha,b,E,\epsilon) \\ \cdots \\ \cdots \\ \cdots \\ \mathcal{M}_{m_s,0}(\alpha,b,E,\epsilon)\ldots\mathcal{M}_{m_s,m_s}(\alpha,b,E,\epsilon) \end{pmatrix} \begin{pmatrix} \mu_{\alpha,b}(0) \\ \cdot \\ \cdot \\ \cdot \\ \mu_{\alpha,b}(m_s) \end{pmatrix}. \tag{52}$$

The $\mathcal{M}(\alpha,b,E,\epsilon)$ matrix is readily obtainable. It is also regular in b.

So long as equation (49) is satisfied, the CDME (i.e. equation (52)) is analytic at $\alpha = 0$. Viewed as an initial value problem, as indicated earlier, the specification of the physical energy, E, and infinite-scale moments, $\{\mu_{0,b}(\ell)|0 \leqslant \ell \leqslant m_s\}$, leads to the asymptotic recovery of the wavefunction through the relations

$$\operatorname*{Lim}_{\alpha\to\infty} \alpha^{\ell+1+\sigma_\ell}\mu_{a,b}(\ell) = \frac{\nu(\ell+\sigma_\ell)}{\sigma_\ell!}\partial_b^{\sigma_\ell}\Psi(b) \tag{53}$$

where $\nu(\ell) \equiv \int \mathrm{d}y\, y^\ell \mathrm{e}^{-Q(y)}$, and $\nu(\ell+\sigma_\ell)$ is the first non-zero moment starting from order ℓ (i.e. $\nu(\ell) = \nu(\ell+1) = \cdots = \nu(\ell+\sigma_\ell-1) = 0$, and $\nu(\ell+\sigma_\ell) \neq 0$).

As outlined in the previous section, these asymptotic relations represent the integration (summation) of the signal-wavelet inversion formulae over all scale and translation values.

If equation (49) is not satisfied, the asymptotic relations still hold; however, the coupled moment differential equations are singular at $\alpha = 0$ and require other methods for their analysis (i.e. the 'Bohr' atom, as investigated in HM (1997)). These complications also arise in the extension of the present formalism to the case of scattering problems.

The $\mathcal{M}(\alpha, b, E, \epsilon)$ matrix is regular in ϵ. Setting $\epsilon = 0$, the integration of equation (52) will yield the atomic distribution in equation (46), for arbitrary E, through the above $\alpha \to \infty$ asymptotic relations (Handy and Brooks 2000).

The above analysis betrays the importance of turning points within a MQ formalism. Turning points are also relevant within CWT analysis.

4. Turning points and continuous wavelet transforms

Within CWT theory, turning points are important because they define the b values where the pointwise convergence of equation (52) is the fastest. That is, in terms of the scaling function definition in equation (29), upon performing the change of variables $y = \frac{x-b}{a}$, and expanding the ensuing configuration $\Psi(ay + b)$, with respect to a, we obtain

$$\mathcal{S}\Psi(a, b) = \frac{1}{\nu} \sum_{q=0}^{\infty} \frac{a^q \nu(q)}{q!} \partial_b^q \Psi(b) \tag{54}$$

where $\nu(q) \equiv \int \mathrm{d}x\, x^q \mathrm{e}^{-Q(x)}$ and $\nu = \nu(0)$. If we assume $\nu(0) \neq 0$ and $\nu(1) = 0$ (i.e. symmetric scaling function), then

$$\mathcal{S}\Psi(a, b) = \Psi(b) + a^2 \frac{\nu(2)}{2\nu(0)} \partial_b^2 \Psi(b) + \mathrm{O}(a^3). \tag{55}$$

Furthermore, at the turning point values, τ_ℓ, we have (i.e. $\partial_b^2 \Psi(\tau_\ell) = 0$)

$$\mathcal{S}\Psi(a, \tau_\ell) = \Psi(\tau_\ell) + \mathrm{O}(a^3). \tag{56}$$

Thus, the convergence to the wavefunction, by the multiscale configuration in equation (29), is fastest at the turning points, in the zero-scale limit. Clearly, this also holds for any other inflection point; however, we do not know these (zeros of the wavefunction) as functions of the energy. This is why we restrict our analysis only to the turning points.

An important alternate way of expressing the above is in terms of the wavelet transform itself. Performing the same change of variables and a-expansion on equation (1), with respect to mother wavelets of the form $\mathcal{W}(x) = \mathcal{N}\partial_x^2 \mathrm{e}^{-Q(x)}$ (because of the second-order nature of the Schrodinger equation), one obtains

$$W\Psi(a, b) = \sqrt{a} \sum_{q=0}^{\infty} \frac{a^q \omega(q)}{q!} \partial_b^q \Psi(b) \tag{57}$$

where $\omega(q) \equiv \mathcal{N} \int \mathrm{d}y\, y^q \partial_y^2 \mathrm{e}^{-Q(y)}$, yielding (i.e. $\omega(0) = \omega(1) = 0$)

$$W\Psi(a, b) = \sqrt{a} \left(\frac{a^2 \omega(2)}{2} \partial_b^2 \Psi(b) + \mathrm{O}(a^3) \right). \tag{58}$$

The zero-scale limit will always be zero, $\lim_{a \to 0} W\Psi(a, b) = 0$, for any b value. However, at the turning points (i.e. $\partial_b^2 \Psi(\tau_\ell) = 0$), the convergence to zero is much faster

$$W\Psi(a, \tau_\ell) = \mathrm{O}(a^{\frac{7}{2}}) \qquad a \to 0. \tag{59}$$

Therefore, at moderately small-scale values, a_s, we have

$$W\Psi(a_s, \tau_\ell) \simeq 0. \tag{60}$$

The rapid convergence to zero, exhibited by the wavelet transform at the turning points, makes them suitable for defining a TPQ strategy as defined by the conditions in equation (23) or (26).

5. Turning point quantization

Although the essence of the TPQ procedure has been described in the previous sections (particularly in the introduction), in this section we want to summarize the conspiring factors that argue in favour of its natural role as the one and only logical quantization prescription within a moment-wavelet analytical framework.

Firstly, we have established that for mother wavelets modelled after the kinetic energy operator (of the multidimensional) Schrodinger equation, the wavelet transform converges to zero fastest at all of the turning points. The manifestly non-wavelet equivalent to this is the expression in equation (19). Such moment limits converge fastest to the wavefunction (pointwise) at the turning points. We established that such limits are identical to the signal-wavelet inversion/reconstruction formulae in equations (30), (31).

Secondly, for any one-dimensional, rational fraction (bound state) potential Schrodinger-Hamiltonian, the number of turning points is identical to the number of missing moments, $1 + m_s$.

Finally, for a large assortment of mother wavelet kernels, the wavelet transform is linearly dependent on the missing moments.

It then follows that the TPQ condition in equation (23) is the natural choice which can readily produce a determinantal equation for finding the energy root values.

In addition, because of the underlying dependence on a moment formulation, and the proven effectiveness of MQ methods in addressing strongly coupled singular perturbation-type problems, the TPQ condition should be effective for these types of systems as well. Indeed, MQ analysis, particularly as developed in Handy *et al* EMM analysis (1988a, b), corresponds to a conformally invariant variational procedure (HM 1998b) capable of yielding impressive results, as in the case of the notoriously difficult (and highly singular) quadratic Zeeman effect for strong magnetic fields (Handy *et al* 1988b).

Given all the above, the most natural implementation of the TPQ condition is to explicitly solve the CDME relations directly. We outline this procedure below, for completeness. It provides an important contrast to the procedure developed in the following sections, based on the TJHW representation for the wavefunction.

We should emphasize that the manifestly wavelet-dependent TPQ condition in equation (23) is really minimally dependent on wavelet analysis. Afterall, what equation (23) represents is an approximation to the kinetic energy condition at the turning points.

As previously noted, the works by HM generated the wavefunction configuration by regarding the CDME, $\partial_\alpha \overrightarrow{\mu}_{\alpha,b} = \mathcal{M}(\alpha, b, E, \epsilon)\overrightarrow{\mu}_{\alpha,b}$, as an initial value problem dependent on the infinite-scale ($\alpha = 0$) moment relations

$$\mu_{0,b}(\ell) = \sum_{j=0}^{\ell} \binom{\ell}{j} (-b)^{\ell-j} \mu(j) \tag{61}$$

where $\mu(j) \equiv \mu_{0,0}(j)$, and $\binom{\ell}{j} = \frac{\ell!}{(\ell-j)!\,j!}$. Through moment equation based quantization methods (Handy and Bessis 1985, Handy *et al* 1988a, b), they were able to determine the physical energy and missing moment values, enabling the integration of the CDME; thereby leading to the pointwise recovery of the wavefunction through equation (19).

We can express the general solution to the CDME as

$$\overrightarrow{\mu}_{\alpha,b} = \mathcal{G}(\alpha, b, E, \epsilon)\overrightarrow{\mu} \tag{62}$$

$\overrightarrow{\mu} = (\mu(0), \ldots, \mu(m_s))$. The generating matrix, $\mathcal{G}$, is computable, for arbitrary E.

Since, in many cases, the wavelet transform is a superposition of the (missing) moments

$$W\Psi(a,b) = \sum_{\ell=0}^{m_s} C_\ell(\alpha, b, E, \epsilon)\mu_{\alpha,b}(\ell) \tag{63}$$

(involving readily determinable coefficients, C_ℓ) we can make the appropriate substitution and obtain a linear relation between the wavelet transform and the (infinite-scale, zero-translation) missing moments:

$$W\Psi(a,b) = \sum_{\ell=0}^{m_s} \mathcal{K}_\ell(\alpha, b, E, \epsilon)\mu(\ell) \tag{64}$$

where

$$\mathcal{K}_\ell(\alpha, b, E, \epsilon) = \sum_{\ell_v=0}^{m_s} C_{\ell_v}(\alpha, b, E, \epsilon)\mathcal{G}_{\ell_v,\ell}(\alpha, b, E, \epsilon). \tag{65}$$

Given that there are as many turning points as there are missing moments, a TPQ strategy is identifiable upon imposing equation (23). The pertinent equations are (i.e. $\alpha_s = \frac{1}{a_s}$)

$$\sum_{\ell_2=0}^{m_s} \mathcal{K}_{\ell_2}(\alpha_s, \tau_{\ell_1}(E), E, \epsilon)\mu(\ell_2) = 0 \tag{66}$$

or

$$\det(\Delta(a_s, E, \epsilon)) = 0 \tag{67}$$

where

$$\Delta_{\ell_1,\ell_2}(a_s, E, \epsilon) = \mathcal{K}_{\ell_2}(\alpha_s, \tau_{\ell_1}(E), E, \epsilon). \tag{68}$$

There is an important, recently discovered, result (Handy and Brooks 2000), that dramatically clinches the need for the inclusion of a wavelet basis expansion in the above formalism. It turns out that the CDME equations, for any E value, and any starting (infinite-scale, zero-translation) missing moment values, $\overrightarrow{\mu}$, will always converge (as given by equation (19)) to solutions to the configuration-space Schrodinger equation (physical or unphysical). Therefore, equation (23), will always hold, for any E, since both bounded and unbounded solutions to the Schrodinger equation have turning points (where the kinetic energy term is always zero). Thus, if equation (63) is used exclusively within a CDME-TPQ context, then equation (67) will not generate physical energy values, because it is satisfied by any E value.

What is required is another version of equation (63) that associates bounded configurations for both unphysical and physical E values. However, this is exactly what the DCWT representation provides. Thus, for an appropriately truncated DCWT representation (equation (7), $f = a_0 = 1$) we have

$$\tilde{\Psi}(b) \equiv \sum_{l\in\mathcal{L}} \sum_{j\in\mathcal{J}} \mathcal{D}\left(\frac{b - j\rho^l - \delta_l[b]}{\rho^l}\right) \times \frac{1}{\sqrt{\rho^l}} W\Psi(\rho^l, j\rho^l + \delta_l[b]). \tag{69}$$

We can express the wavelet transform factor, $W\Psi(\rho^l, j\rho^l + \delta_l[b])$, in terms of the representation in equation (64). However, it is the wavelet transform of $\tilde{\Psi}(b)$, at scale a_s, which must be used in imposing the TPQ condition: $W\tilde{\Psi}(a_s, \tau_\ell(E)) = 0$. Excellent results have been obtained through such a procedure. The details are presented in the forthcoming work by Handy and Brooks (2000).

As indicated in the introduction, implementation of the TPQ condition within a purely CDME context (i.e. directly solving it and generating equation (62)) is not possible, at this time, for multidimensional systems. As such, in the following sections we implement a different

strategy applicable to multidimensional systems which, nevertheless, adheres to the spirit of the present analysis. That is, working within the TJHW wavefunction representation, we will impose the TPQ conditions and discriminate between spurious and physical configurations by assessing how well they satisfy the CDME relations (scale by scale).

6. A convenient implementation of TPQ

The preceding formalism defines an exact wavelet analysis for quantizing physical systems based on the generation of all the CDME basic solutions. As noted, this is particularly difficult to implement for multidimensional problems. Fortunately, an alternate approach exists which adheres to the underlying theoretical framework defined in the previous section. Specifically, we will utilize the wavefunction representation developed within the moment space quantization formulation of TJHW (1998a, b).

The TJHW (multidimensional) analysis tells us that the wavefunction can be expressed as

$$\Psi(x) = \sum_{n=0}^{\infty} A_n[E; \overrightarrow{\mu}](-\partial_x)^n R(x) \tag{70}$$

where $R(x)$ is some convenient reference function (i.e. Gaussian, etc). The A_n coefficients are linearly dependent on the (infinite-scale, zero-translation) missing moments, $\{\mu(0), \ldots, \mu(m_s)\}$, previously defined:

$$A_n[E; \overrightarrow{\mu}] = \sum_{\ell=0}^{m_s} D_{n,\ell}(E)\mu(\ell). \tag{71}$$

The $D_{n,\ell}(E)$ are determinable, algebraically, as follows. From the Fourier transform for the wavefunction

$$\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}x\, \mathrm{e}^{-\mathrm{i}kx}\Psi(x) \tag{72}$$

the ensuing k-power series becomes

$$\hat{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \sum_{p=0}^{\infty} \frac{\mu(p)}{p!}(-\mathrm{i}k)^p. \tag{73}$$

From the underlying moment equation for the $\mu(p)$, we have

$$\mu(p) = \sum_{\ell=0}^{m_s} M_{E,\epsilon}(p, \ell)\mu(\ell) \tag{74}$$

where $p \geqslant 0$ and $M_{E,\epsilon}(\ell_1, \ell_2) = \delta_{\ell_1,\ell_2}$, for $0 \leqslant \ell_1, \ell_2 \leqslant m_s$.

We can transform the Fourier power series expansion into

$$\hat{\Psi}(k) = \left(\sum_{n=0}^{\infty} A_n[E; \overrightarrow{\mu}](-\mathrm{i}k)^n \right) \hat{R}(k) \tag{75}$$

for an appropriate $\hat{R}(k)$, with an analytic inverse at $k = 0$. The functions $\{k^n \hat{R}(k) | n \geqslant 0\}$ are required to be complete within the Fourier representation. Upon expanding $\frac{\hat{\Psi}(k)}{\hat{R}(k)}$, one obtains the A_n as linear functions of the missing moments; thereby generating equation (71). The inverse Fourier transform of the above representation gives us the configuration space expansion in equation (70).

Let us define the truncated TJHW representation,

$$\Psi^{(N)}(x) \equiv \sum_{n=0}^{N} A_n[E, \overrightarrow{\mu}](-\partial_x)^n R(x). \tag{76}$$

An important property of the truncated representation is that it yields, exactly, all the moments up to order N (i.e. $\mu(p) = \int \mathrm{d}x\, x^p \Psi^{(N)}(x)$, for $p \leqslant N$):

$$\mu(p) = \sum_{n=0}^{p} A_n[E, \overrightarrow{\mu}] \frac{p!}{(p-n)!} \sigma(p-n) \tag{77}$$

where $\sigma(j) = \int \mathrm{d}x\, x^j R(x)$.

We can compute its wavelet transform according to

$$W\Psi^{(N)}(a,b) = \frac{1}{\sqrt{a}} \int \mathrm{d}x\, \mathcal{W}\left(\frac{x-b}{a}\right) \Psi^{(N)}(x) \tag{78}$$

$$= \sum_{n=0}^{N} A_n[E; \overrightarrow{\mu}](-1)^n W R^{(n)}(a,b) \tag{79}$$

where

$$WR^{(n)}(a,b) = \frac{1}{\sqrt{a}} \int \mathrm{d}x\, \mathcal{W}\left(\frac{x-b}{a}\right) \partial_x^n R(x). \tag{80}$$

Imposing the TPQ condition, we obtain

$$W\Psi^{(N)}(a_s, \tau_\ell(E)) = 0 \tag{81}$$

or (substituting equation (71))

$$\det(\Delta[E; N, a_s]) = 0 \tag{82}$$

where

$$\Delta_{\ell_1,\ell_2}[E; N, a_s] = \sum_{n=0}^{N} D_{n,\ell_2}(E)(-1)^n W R^{(n)}(a_s, \tau_{\ell_1}(E)). \tag{83}$$

We shall use the notation $\Psi^{(N)}(x)$ to denote the Nth-order TJHW representation, while $\Psi^{(N)}_{a_s}(x)$ denotes the specific configuration resulting from solving the above TPQ equations at scale a_s.

When $a_s = 0$, equation (81) is equivalent to (i.e. implicitly assuming $\mathcal{W}(x) = -\mathcal{N}\partial_x^2 \mathrm{e}^{-Q(x)}$)

$$\partial_\tau^2 \Psi^{(N)}(\tau_\ell(E)) = 0 \tag{84}$$

or

$$\det(\tilde{\Delta}[E; N]) = 0 \tag{85}$$

where

$$\tilde{\Delta}_{\ell_1,\ell_2}[E; N] = \sum_{n=0}^{N} D_{n,\ell_2}(E)(-\partial_\tau)^{n+2} R(\tau_{\ell_1}(E)). \tag{86}$$

7. The double-well quartic anharmonic oscillator

Consider the quartic anharmonic double-well oscillator,

$$-\epsilon\partial^2\Psi(x) + (Z^2x^2 + x^4)\Psi(x) = E\Psi(x). \tag{87}$$

The associated (infinite-scale, zero-translation) moment equation is

$$\mu(p+4) = -Z^2\mu(p+2) + E\mu(p) + p(p-1)\epsilon\mu(p-2) \tag{88}$$

for $p \geqslant 0$. This corresponds to 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. In general, all the moments are linearly dependent on the missing moments. This is expressible as

$$\mu(p) = \sum_{\ell=0}^{m_s} M_{E,\epsilon}(p,\ell)\mu(\ell) \tag{89}$$

where

$$M_{E,\epsilon}(\ell_1,\ell_2) = \delta_{\ell_1,\ell_2} \tag{90}$$

for $0 \leqslant \ell_1, \ell_2 \leqslant m_s$. In this work, we do not have to specify a normalization condition (although in previous works we adopted $\sum_{\ell=0}^{m_s} \mu(\ell) = 1$).

The $M_{E,\epsilon}(p,\ell)$ satisfy the moment equation with respect to the p index, for fixed ℓ. Combined with the initial conditions given above, the $M_{E,\epsilon}$ can be easily generated.

The fourth-order nature of the finite-difference moment equation is not affected by the value of ϵ. Thus, when $\epsilon = 0$, the finite-difference equation becomes

$$\mu_0(p+4) = -Z^2\mu_0(p+2) + E\mu_0(p) \tag{91}$$

and has the general solution

$$\mu_0(p) = \sum_{\ell=0}^{m_s} \mathcal{A}_\ell(\tau_\ell(E))^p \tag{92}$$

where the $\mathcal{A}_\ell$ are arbitrary and the turning point, energy-dependent functions satisfy

$$(\tau_\ell(E))^4 = -Z^2(\tau_\ell(E))^2 + E \tag{93}$$

(i.e. $V(\tau_\ell(E)) = E$), resulting in

$$\tau_\ell^2 = -\frac{Z^2}{2} \pm \sqrt{E - V_{\min}} \tag{94}$$

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

$$\tau_\ell(E) = \begin{cases} -\sqrt{-\dfrac{Z^2}{2} + \sqrt{E - V_{\min}}}, & \ell = 0 \\ -\sqrt{-\dfrac{Z^2}{2} - \sqrt{E - V_{\min}}}, & \ell = 1 \\ +\sqrt{-\dfrac{Z^2}{2} - \sqrt{E - V_{\min}}}, & \ell = 2 \\ +\sqrt{-\dfrac{Z^2}{2} + \sqrt{E - V_{\min}}}, & \ell = 3. \end{cases} \tag{95}$$

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.

We now derive the structure of the moment equation, for the generalized moments $\mu_{\alpha,b}(p) = \int \mathrm{d}x\, x^p \mathrm{e}^{-Q(\alpha x)}\Psi(x+b)$, recall $\alpha \equiv \frac{1}{a}$. Upon translating the corresponding Schrodinger equation by an amount b, we obtain

$$-\epsilon\partial_x^2\Psi(x+b) + (Z^2(x+b)^2 + (x+b)^4)\Psi(x+b) = E\Psi(x+b). \tag{96}$$

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

$$\begin{aligned} &-\epsilon(\partial_x^2 + 2\alpha Q'(\alpha x)\partial_x + \alpha^2[Q''(\alpha x) + (Q'(\alpha x))^2])\Phi(x) \\ &\quad +(Z^2(x+b)^2 + (x+b)^4)\Phi(x) = E\Phi(x). \end{aligned} \tag{97}$$

So long as Q is an asymptotically positive polynomial, and equation (49) is satisfied, the ensuing $\mu_{\alpha,b}(p)$-moment equation will be analytic in ϵ. From JWKB analysis, we know that

the asymptotic form for the physical states is $\Psi(x) \to \mathrm{e}^{-\frac{1}{3}|x|^3}$. Therefore, taking $Q(x) = \frac{x^2}{2}$, satisfies equation (49). The corresponding generalized moment equation is

$$\begin{aligned}\mu_{\alpha,b}(p+4) = &-4b\mu_{\alpha,b}(p+3)\\ &-[6b^2 + Z^2 - \epsilon\alpha^4]\mu_{\alpha,b}(p+2) - [4b^3 + 2Z^2 b]\mu_{\alpha,b}(p+1)\\ &+[E - b^4 - Z^2b^2 - \epsilon\alpha^2(2p+1)]\mu_{\alpha,b}(p) + \epsilon p(p-1)\mu_{\alpha,b}(p-2) \end{aligned} \tag{98}$$

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

$$\mu_{\alpha,b}(p) = \sum_{\ell=0}^{m_s=3} M_{\alpha,b,E,\epsilon}(p,\ell)\mu_{\alpha,b}(\ell) \tag{99}$$

involving readily derivable M function coefficients which are analytic in all the dependent variables.

The corresponding set of coupled moment differential equations is obtained by recognizing that

$$\partial_\alpha \mu_{\alpha,b}(p) = -\alpha\mu_{\alpha,b}(p+2) \tag{100}$$

or

$$\partial_\alpha \mu_{\alpha,b}(p) = \sum_{\ell=0}^{m_s=3} \mathcal{M}_{p,\ell}(\alpha, b, E, \epsilon)\mu_{\alpha,b}(\ell) \tag{101}$$

where $\mathcal{M}_{p,\ell}(\alpha, b, E, \epsilon) = -\alpha M_{\alpha,b,E,\epsilon}(p+2, \ell)$.

Since all the moments are linearly dependent on the $\{\mu_{\alpha,b}(\ell)|0 \leqslant \ell \leqslant 3\}$, we can limit the above differentiation to these generalized missing moments:

$$\partial_\alpha \begin{pmatrix} \mu_{\alpha,b}(0)\\ \mu_{\alpha,b}(1)\\ \mu_{\alpha,b}(2)\\ \mu_{\alpha,b}(3)\end{pmatrix} = \begin{pmatrix} 0, 0, -\alpha, 0\\ 0, 0, 0, -\alpha\\ \mathcal{M}_{2,0}, \mathcal{M}_{2,1}, \mathcal{M}_{2,2}, \mathcal{M}_{2,3}\\ \mathcal{M}_{3,0}, \mathcal{M}_{3,1}, \mathcal{M}_{3,2}, \mathcal{M}_{3,3}\end{pmatrix} \begin{pmatrix} \mu_{\alpha,b}(0)\\ \mu_{\alpha,b}(1)\\ \mu_{\alpha,b}(2)\\ \mu_{\alpha,b}(3)\end{pmatrix}. \tag{102}$$

The Mexican hat wavelet transform

$$W_{MH}\Psi(a,b) \equiv \int \mathrm{d}x\, \mathcal{W}_{MH}\left(\frac{x-b}{a}\right)\Psi(x) \tag{103}$$

where $\mathcal{W}_{MH}(x) = -\mathcal{N}_{MH}\partial_x^2 \exp(-\frac{x^2}{2})$, can be written in terms of the generalized moments:

$$W_{MH}\Psi(a,b) = \mathcal{N}_{MH}(\mu_{\alpha,b}(0) - \alpha^2\mu_{\alpha,b}(2)). \tag{104}$$

In order to implement the TJHW/TPQ analysis, we adopt the reference function

$$\hat{R}(k) = \mathrm{e}^{-\beta k^2} \qquad \beta = \tfrac{1}{2} \tag{105}$$

with a configuration space counterpart

$$R(x) = \frac{1}{\sqrt{2\beta}} \exp\left(-\frac{x^2}{4\beta}\right). \tag{106}$$

It should be noted that the choice of R is not dictated by the choice of scaling function, Q. We adopt the above reference function because of its convenience. Also, although β will be taken to be $\frac{1}{2}$, the TJHW formalism allows for variable β values; therefore, we make explicit the reference to this parameter.

The generation of the required TJHW representation procedes as follows. We first equate the k-expansion of the Fourier transform of Ψ with the general TJHW representation:

$$\frac{1}{\sqrt{2\pi}} \sum_{p=0}^{\infty} \frac{\mu(p)}{p!}(-\mathrm{i}k)^p = \sum_{n=0}^{\infty} A_n[E;\mu](-\mathrm{i}k)^n \hat{R}(k) \tag{107}$$

yielding (note that $\frac{1}{\hat{R}(k)} = \mathrm{e}^{-\beta(-\mathrm{i}k)^2}$)

$$A_n[E;\mu] = \frac{1}{\sqrt{2\pi}} \sum_{2j+p=n} \frac{(-\beta)^j}{j!} \frac{\mu(p)}{p!}. \tag{108}$$

Upon inserting equation (89) we obtain

$$A_n[E;\mu] = \frac{1}{\sqrt{2\pi}} \sum_{\ell=0}^{m_s} D_{n,\ell}(E)\mu(\ell) \tag{109}$$

where

$$D_{n,\ell}(E) = \sum_{2j+p=n} \frac{(-\beta)^j}{j!} \frac{M_{E,\epsilon}(p,\ell)}{p!}. \tag{110}$$

Since the TJHW representation, for some sufficiently large-order N, is capable of representing the physical solution, we can impose the TPQ conditions. This requires that we evaluate the appropriate wavelet transform for the Nth-order TJHW representation:

$$W\Psi^{(N)}(a,b) = \sum_{n=0}^{N} A_n[E;\mu](-1)^n WR^{(n)}(a,b). \tag{111}$$

For the case of the Mexican wavelet transform we have

$$WR^{(n)}(a,b) = -(2\beta)^{-\frac{1}{2}} \frac{\sqrt{\pi}a^2}{\gamma} \partial_b^{(n+2)} \exp\left(-\frac{b^2}{4\beta + 2a^2}\right) \tag{112}$$

where $\gamma^2 = \frac{1}{2a^2} + \frac{1}{4\beta}$.

Since the convergence of the signal-wavelet inversion relation is fastest at the turning points, the TPW condition is applied at moderately small a_s scale values:

$$W\Psi^{(N)}(a_s, \tau_\ell(E)) = 0 \tag{113}$$

which becomes

$$\sum_{\ell_2=0}^{m_s=3} \left(\sum_{n=0}^{N} D_{n,\ell_2}(E)(-1)^n WR^{(n)}(a_s, \tau_{\ell_1}(E)) \right) \mu(\ell_2) = 0 \tag{114}$$

for $0 \leqslant \ell_1 \leqslant m_s = 3$. The determinantal equation is

$$\det(\Delta(a_s, E; N)) = 0 \tag{115}$$

where

$$\Delta_{\ell_1,\ell_2}(a_s, E; N) = \sum_{n=0}^{N} D_{n,\ell_2}(E)(-1)^n WR^{(n)}(a_s, \tau_{\ell_1}(E)). \tag{116}$$

The E-root solutions to these equations, for given N, will be denoted by $E_r(a_s)$. The corresponding (infinite-scale, zero-translation) missing moments will be denoted by $\mu_{E_r(a_s)}(\ell)$.

In the case $a_s = 0$, the corresponding asymptotic form for the wavelet transform expression shows that $WR^{(n)}(a_s = 0, b) \propto \partial_b R^{(n+2)}(b)$. The preceding formalism then takes on the simple structure

$$\partial_\tau^2 \Psi^{(N)}(\tau_\ell(E)) = 0 \tag{117}$$

for $0 \leqslant \ell \leqslant m_s$, or

$$\sum_{\ell_2=0}^{m_s=3} \tilde{\Delta}_{\ell_1,\ell_2}(E; N)\mu(\ell_2) = 0 \tag{118}$$

corresponding to

$$\det(\tilde{\Delta}(E; N)) = 0 \tag{119}$$

where

$$\tilde{\Delta}_{\ell_1,\ell_2}(E; N) = \sum_{n=0}^{N} D_{n,\ell_2}(E)(-1)^n \partial_\tau^{(n+2)} R(\tau_{\ell_1}(E)). \tag{120}$$

The energy roots to these equations, $E_r(0)$, will be referred to as E_r.

8. Numerical results for the double-well quartic anharmonic potential

We limit our numerical analysis to the ground state problem only, for simplicity. We investigate the Hamiltonian parameter case defined by $\epsilon = 1$ and $Z^2 = -5$.

In table 1 we show the results of the TPQ strategy corresponding to (i.e. $a_s = 0$) $\partial_\tau^2 \Psi^{(N)}(\tau_\ell(E)) = 0$. At each of the respective orders, $N = 20, 30, 40$, spurious solutions appear, in addition to the correct physical ground state energy value $E_r = -3.410\,1428$ ($N = 40$). Even though the spurious solutions show no clear convergence pattern (as opposed to the relatively rapid convergence of the physical energy value), we focus on implementation of the previous theory in order to confirm the identification of the ground state energy.

In figure 1, we plot all the root branches ensuing from implementing the basic TPQ equation $W\Psi^{(N)}(a_s, \tau_\ell(E)) = 0$. We take $N = 40$. By themselves, these plots do not allow us to judge which is the physical root. Indeed, the spurious roots appear at scales larger than the scale at which the true physical branch first appears. In order to select the physical branch, we must determine the extent to which the underlying TJHW configurations satisfy the CDME relations in equation (102). As explained earlier, this analysis corresponds to a scale by scale verification (proceeding from the largest to the smallest possible scale) that the Schrodinger equation is being satisfied.

At the scale value a_s, the corresponding energy roots, $E_r(a_s)$, and associated missing moment values generate the TJHW configuration ($\Psi^{(N)}_{E_r(a_s)} \equiv \Psi^{(N)}_{a_s}$)

$$\Psi^{(N)}_{E_r(a_s)}(x) = \sum_{n=0}^{N} A_n[E_r(a_s), \overrightarrow{\mu}_{E_r(a_s)}](-\partial_x)^n R(x). \tag{121}$$

Using this configuration, we can numerically generate the moments

$$\mu_{\alpha,b,E_r(a_s)}(\ell) = \int \mathrm{d}x\, x^\ell \mathrm{e}^{-\frac{1}{2}(\frac{x}{a})^2} \Psi^{(N)}_{E_r(a_s)}(x) \tag{122}$$

and determine the critical (minimum) scale, $a_c(N, r, a_s)$, for which these moments (or equivalently $\Psi^{(N)}_{E_r(a_s)}(x)$) satisfy equation (102) at any one of the turning points $\tau_{\ell_v}(E_r(a_s))$. This in turn allows us to implement the discrimination procedure explained in the introduction.

In order to determine $a_c(N, r, a_s)$, we procede as follows. Since

$$\partial_\alpha \mu_{\alpha,b,E_r(a_s)}(\ell) = -\alpha \mu_{\alpha,b,E_r(a_s)}(\ell + 2) \tag{123}$$

all we must check is if

$$\mu_{\alpha,b,E_r(a_s)}(p) = \sum_{\ell_v=0}^{3} M_{\alpha,b,E_r(a_s),\epsilon}(p, \ell_v)\mu_{\alpha,b,E_r(a_s)}(\ell_v) \tag{124}$$

for $p = 4, 5$, at both (positive) turning points $b = \tau_{2,3}(E_r(a_s))$. Because of the underlying symmetry we have $\tau_0(E) = -\tau_3(E)$, and $\tau_1(E) = -\tau_2(E)$. Thus, we do not have to check these.

Let

$$R(p, \alpha, b, E_r(a_s)) \equiv 1 - \frac{\sum_{\ell_v=0}^{3} M_{\alpha,b,E_r(a_s),\epsilon}(p, \ell_v)\mu_{\alpha,b,E_r(a_s)}(\ell_v)}{\mu_{\alpha,b,E_r(a_s)}(p)}. \tag{125}$$

Define

$$\delta(a, E_r(a_s)) = \sum_{\ell=2}^{3}\sum_{p=4}^{5}\left(R\left(p, \frac{1}{a}, \tau_\ell(E_r(a_s)), E_r(a_s)\right)\right)^2. \tag{126}$$

We define $a_c(N, r, a_s)$ by determining the smallest scale, a, satisfying $\delta(a, E_r(a_s)) \leqslant 10^{-4}$. That is, this inequality is satisfied for $a_c \leqslant a < \infty$.

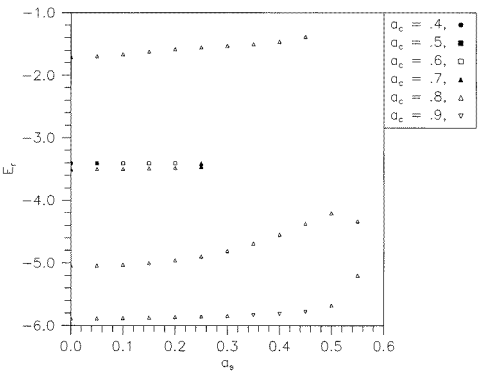

Figure 2. The critical scale, a_c, up to which the TJHW/TPQ solutions satisfy the CDME: $\Psi_{\mathrm{TJHW}}(x) = \mathcal{R}(x) + \mathcal{A}_{a_c}(x)$. The projected configurations, $\mathcal{R}(x)$ and $\mathcal{A}_{a_c}(x)$, each involve a DCWT multiscale representation with scale contributions in the range $0 < a < a_c$ and $a_c \leqslant a < \infty$, respectively.

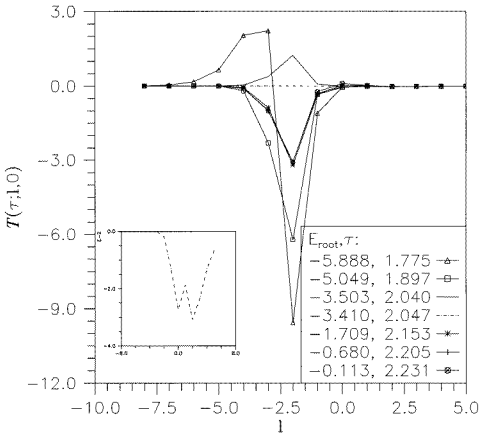

Figure 3. The dyadic DCWT terms for the TJHW/TPQ (ground state) solutions corresponding to the potential function $V(x) = -5x^2 + x^4$. The support interval for the spurious (unphysical) solutions ($2^{-7} < a < 2^0$) does not significantly overlap with the critical scale interval $[a_c \approx 0.8, \infty)$ determined in figure 2; therefore the remainder, 'noise', configuration $\mathcal{R}(x)$, is significant. The support interval for the physical solution, given in the inset ($2^{-2} < a < 2^6$), does significantly overlap with the critical scale interval $[a_c = 0.4, \infty)$ given in figure 2; therefore the corresponding $\mathcal{R}(x)$ is small, and $\Psi_{\mathrm{TJHW}}(x) \approx \mathcal{A}_{a_c}(x)$, confirming the correct physical representation.

In figure 2 we give the approximate a_c value for various TPQ roots. We see that along the physical branch (that leading to the correct physical value $E_r(0) = -3.410\,1428$) the a_c critical values become progressively smaller, although we obtain $a_c \to \mathrm{O}(0.4)$ as $a_s \to 0$. Instead, for each of the other unphysical branches, a_c remains approximately constant, $a_c \approx \mathrm{O}(0.8)$, even as $a_s \to 0$. In principle, as $N \to \infty$, for physical solutions, one expects $a_c \to a_s$, particularly as $a_s \to 0$.

As noted in the introduction, we can decompose the TPQ generated configuration (for $a_s = 0$)

$$\Psi_0^{(N)}(x) = \mathcal{R}(x) + \mathcal{A}(x) \tag{127}$$

where $\mathcal{A}(x)$ is the DCWT wavelet projection corresponding to scales greater than, or equal to, a_c. $\mathcal{R}(x)$ is made up of wavelet transform contributions for scale $0 < a < a_c$. In figure 3 we plot the expression (from equation (35)),

$$\mathcal{T}(\tau_\ell(E_r); l, 0) = \frac{1}{\nu}\frac{\mathcal{D}(0)}{\sqrt{\rho^l}} W\Psi(\rho^l, \tau_\ell(E_r)) \tag{128}$$

involving the wavelet transform for each of the TPQ generated configurations at the larger of the two positive turning points, $\tau_3(E)$ (i.e. $W\Psi^{(N)}(a, \tau_3(E_r))$).

We see that for the unphysical branches, the DCWT transform evaluated at $a = 2^l$, peaks around $a = 2^{-2} = \frac{1}{4}$. This is much smaller than the typical a_c value for the unphysical branches, $a_c \approx 0.8$. Thus the corresponding $\mathcal{R}(x)$ is significantly large, making $\Psi_0^{(N)}(x)$ not be a solution to the Schrodinger equation.

In contrast, the $W\Psi^{(N)}(a, \tau_3(E_r))$ for the physical TPQ configuration, peaks around $a = \mathrm{O}(2^2)$, which lies within the interval $(a_c = 0.4, \infty)$. Consequently, the corresponding

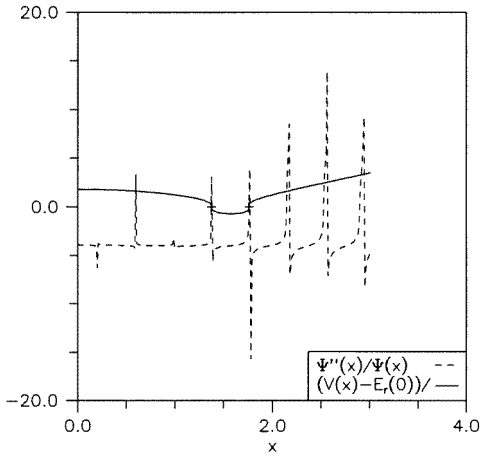

Figure 4. (Spurious) TJHW/TPQ solution, Ψ, for $E_r(0) = -5.888$: comparison of $\frac{\Psi''(x)}{\Psi(x)}$ with $(V(x) - E_r(0))$.

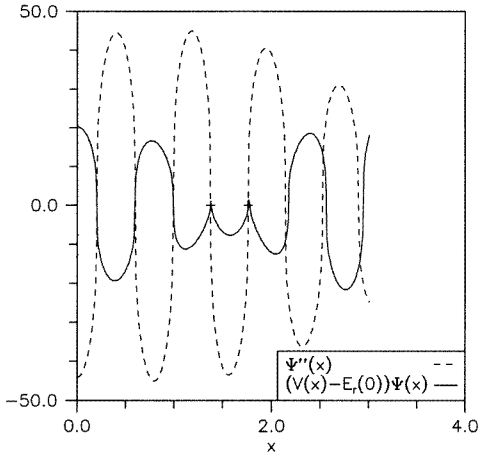

Figure 5. (Spurious) TJHW/TPQ solution, Ψ, for $E_r(0) = -5.888$: comparison of $\Psi''(x)$ with $(V(x) - E_r(0))\Psi(x)$.

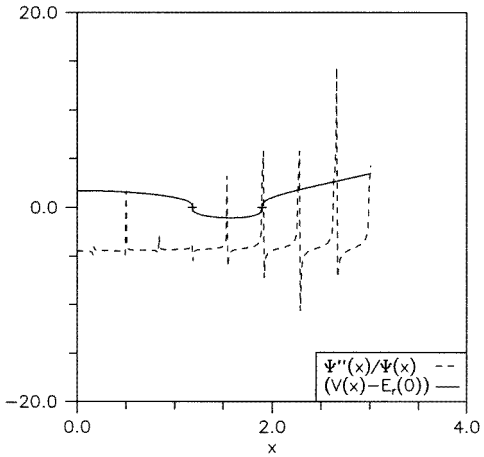

Figure 6. (Spurious) TJHW/TPQ solution, Ψ, for $E_r(0) = -5.049$: comparison of $\frac{\Psi''(x)}{\Psi(x)}$ with $(V(x) - E_r(0))$.

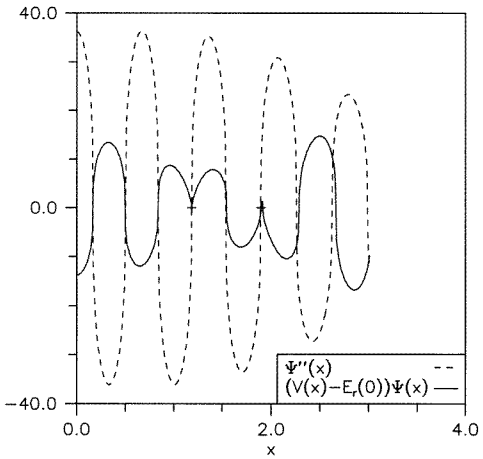

Figure 7. (Spurious) TJHW/TPQ solution, Ψ, for $E_r(0) = -5.049$: comparison of $\Psi''(x)$ with $(V(x) - E_r(0))\Psi(x)$.

remainder configuration, $\mathcal{R}(x)$, does not contain any (relatively) significant DCWT wavelet components (i.e. it is a small remainder configuration), and thus $\Psi_0^{(N)}(x)$ is close to $\mathcal{A}(x)$, which satisfies the Schrodinger equation up to the scale a_c.

The above behaviour is also repeated if we generate the DCWT relative to the smaller of the two positive turning points, τ_2.

In figures 4–13 we check the accuracy to which the TPQ configurations, $\Psi_0^{(N)}(x)$, satisfy the Schrodinger equation by comparing $\frac{\partial_x^2 \Psi_0^{(N)}(x)}{\Psi_0^{(N)}(x)}$ and $(V(x) - E_r)$. We also compare $\partial_x^2 \Psi_0^{(N)}(x)$ with $(V(x) - E_r)\Psi_0^{(N)}(x)$. This is done for both physical and spurious solutions. It is very clear that only for the physical solution is there agreement with the Schrodinger equation. The spurious solutions deviate significantly.

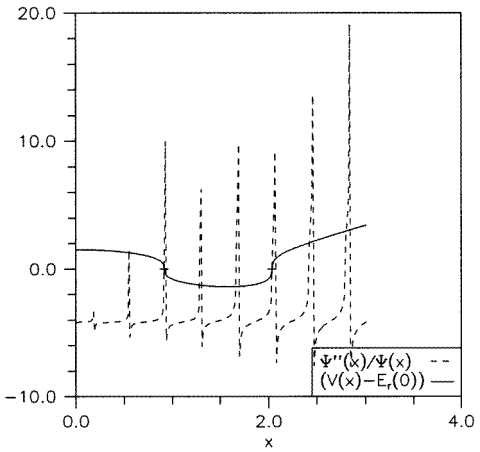

Figure 8. (Spurious) TJHW/TPQ solution, Ψ, for $E_r(0) = -3.503$: comparison of $\frac{\Psi''(x)}{\Psi(x)}$ with $(V(x) - E_r(0))$.

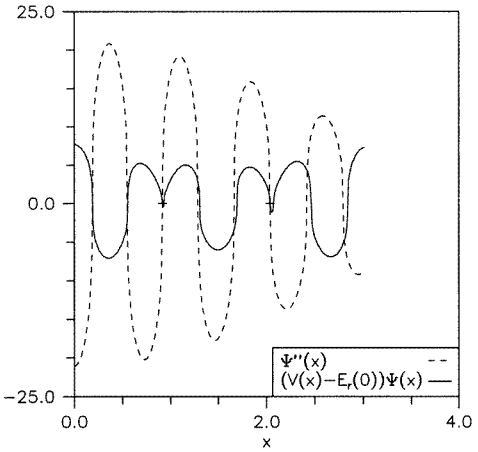

Figure 9. (Spurious) TJHW/TPQ solution, Ψ, for $E_r(0) = -3.503$: comparison of $\Psi''(x)$ with $(V(x) - E_r(0))\Psi(x)$.

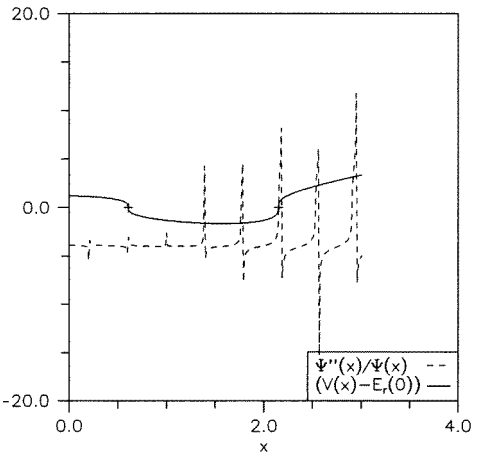

Figure 10. (Spurious) TJHW/TPQ solution, Ψ, for $E_r(0) = -1.709$: comparison of $\frac{\Psi''(x)}{\Psi(x)}$ with $(V(x) - E_r(0))$.

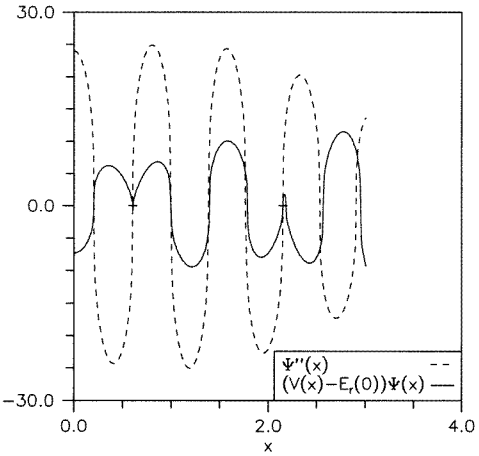

Figure 11. (Spurious) TJHW/TPQ solution, Ψ, for $E_r(0) = -1.709$: comparison of $\Psi''(x)$ with $(V(x) - E_r(0))\Psi(x)$.

The preceding analysis serves to discriminate between the physical and unphysical (spurious) solutions. We are also interested in identifying modifications to the TPQ prescription that only generate physical approximants (no spurious states generated).

9. 'Noise' filtering and CWT/DCWT

As detailed in the previous section, the numerical implementation of the TPQ strategy, within the TJHW representation, yields excellent physical energy values and configurations, in addition to spurious, unphysical, results.

Despite the effectiveness of the described, wavelet-based, procedure for discriminating between physical and unphysical solutions, it is preferable to have a TPQ-based quantization

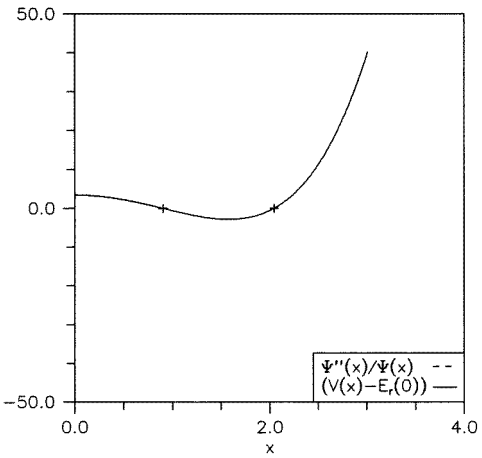

Figure 12. (Physical) TJHW/TPQ solution, Ψ, for $E_r(0) = -3.410$: comparison of $\frac{\Psi''(x)}{\Psi(x)}$ with $(V(x) - E_r(0))$.

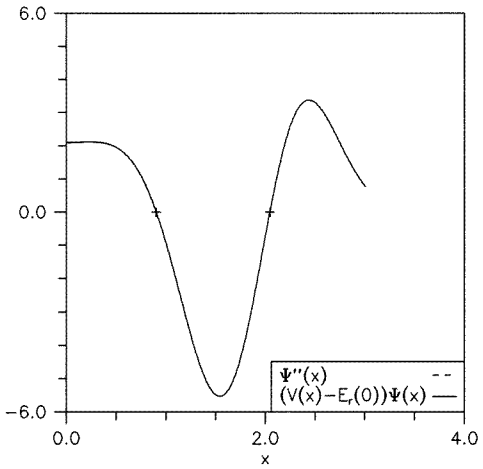

Figure 13. (Physical) TJHW/TPQ solution, Ψ, for $E_r(0) = -3.410$: comparison of $\Psi''(x)$ with $(V(x) - E_r(0))\Psi(x)$.

method that does not generate any spurious solutions. To put this in proper perspective, reconsider the previously defined decomposition

$$\Psi_{a_s}^{(N)}(x) = \mathcal{R}(x) + \mathcal{A}(x). \tag{129}$$

The configuration $\mathcal{A}(x)$ corresponds to the wavelet space projection (for the smallest possible scale, a_c) that satisfies the CDMEs. As previously noted, the CDMEs are equivalent to a wavelet transformation of the Schrodinger equation. The remainder, $\mathcal{R}(x)$, may be considered as 'noise'.

Whereas $\Psi_{a_s}^{(N)}(x)$ satisfies $W\Psi(a_s, \tau_\ell) = 0$ (which is an approximation to $\partial_\tau^2 \Psi_{a_s}^{(N)}(\tau_\ell) = 0$), this may not be the case (even approximately) for $\mathcal{A}(x)$. It will, however, if the noise is small. The analysis previously described, in the context of figure 3, uses wavelet transforms to assess whether the noise is small or not. If the noise is small, then $\Psi_{a_s}^{(N)}(x)$ defines a physically consistent approximation (including the associated energy), because it will both satisfy the Schrodinger equation (to scale a_c) and approximately satisfy the TPQ condition.

In the case of unphysical TPQ configurations, significant short-scale noise contributions generate unphysical $\Psi_{a_s}^{(N)}(x)$ which do not satisfy the Schrodinger equation. We would like to modify the TPQ strategy so that these solutions do not appear from the outset.

In the following discussion, all references to E will implicitly refer to $E_r(a_s)$.

From the numerical results presented in the previous section, for both physical and unphysical $\Psi_{a_s}^{(N)}(x)$ configurations, $\partial_x^2 \Psi_{a_s}^{(N)}(x)$ is proportional to $x - \tau_\ell(E)$, in the neighbourhood of the turning point(s), $\tau_\ell(E)$. Refer to figures 5, 7, 9, 11 and 13. This is precisely what the TPQ condition $W\Psi(a_s, \tau_\ell(E)) = 0$ suggests. That is

$$\int \mathrm{d}x\, \mathrm{e}^{-\frac{(x-\tau_\ell(E))^2}{2a^2}} \partial_x^2 \Psi_{a_s}^{(N)}(x) = 0 \tag{130}$$

or

$$\int \mathrm{d}x\, \partial_x^2 \mathrm{e}^{-\frac{(x-\tau_\ell(E))^2}{2a^2}} \Psi_{a_s}^{(N)}(x) = 0 \tag{131}$$

(a arbitrarily small, a_s fixed) which is equivalent to $W_{MH}\Psi_{a_s}^{(N)}(a, \tau_\ell(E)) = 0$, in terms of the Mexican hat mother wavelet.

Also, as previously noted, for these same configurations the expression $(V(x)-E)\Psi_{a_s}^{(N)}(x)$ will be proportional to $x-\tau_\ell(E)$ only for the physical solution (refer to figures 5, 7, 9, 11 and 13, for the case $a_s=0$). Therefore,

$$\int \mathrm{d}x\, \mathrm{e}^{-\frac{(x-\tau_\ell(E))^2}{2a^2}}(V(x)-E)\Psi_{a_s}^{(N)}(x)=0 \tag{132}$$

only for the physical configuration.

From the above general discussion, it would appear that a suitable modification of the TPQ conditions, capable of removing (*ab initio*) the unphysical, spurious, solutions, is

$$\int \mathrm{d}x\, \mathrm{e}^{-\frac{(x-\tau_\ell(E))^2}{2a^2}}(\mathcal{H}-E)\Psi^{(N)}(x)=0 \tag{133}$$

for each of the m_s+1 turning points, and moderately small scale parameter values. (If the Hamiltonian contains a rational fraction potential, $V=\frac{\mathcal{P}_N}{\mathcal{P}_D}$, then these equations would be modified by the denominator polynomial, $(\mathcal{H}-E)\rightarrow \mathcal{P}_D(\mathcal{H}-E)$.) Clearly, if a is very small, the above conditions become the previous TPQ conditions.

However, these modified TPQ equations also lead to different types of spurious solutions (besides also generating the physical solutions). Indeed, there is nothing unique about the turning points in satisfying equation (133). The only way of defining a TPQ condition that filters out the unphysical solutions is to combine the above with the original TPQ conditions.

Specifically, for the double-well quartic anharmonic oscillator, imposing

$$W_{MH}\Psi^{(N)}(a_s,\tau)=0 \tag{134}$$

and

$$\int \mathrm{d}x\, \mathrm{e}^{-\frac{1}{2}(\frac{x-\tau}{a})^2}(V(x)-E)\Psi^{(N)}(x)=0 \tag{135}$$

for τ restricted to the set $\{\pm\tau_2(E))\}$ or the set $\{\pm\tau_3(E)\}$, filters out the spurious energies and only generates physical approximants. The results duplicate those in table 1, with respect to the physical energy. Clearly, both of these equations are demanding that around each of the turning points, for sufficiently small scales, the scaling transform for the kinetic energy and the $(V-E)$ terms be zero.

10. Other examples

The double-well quartic anharmonic oscillator, for the Hamiltonian parameter values reported, involve real value turning points. That is, for the ground state ($Z^2=-5$), we could restrict E to the interval $E>V_{\min}$ and $-\frac{Z^2}{2}>\sqrt{E-V_{\min}}$. For the pure quartic anharmonic oscillator, $V(x)=x^2+x^4$, and the rational fraction potential $V(x)=x^2+\frac{0.1x^2}{1+0.1x^2}$, one must work with complex turning point functions, $\tau_\ell(E)$. We implemented the TJHW/TPQ analysis with respect to the ($a_s=0$) formulation given in equations (117)–(120). In all cases, spurious energies were detected; however, as exhibited in table 1, the physical state energy values (including excited states) exhibited rapid convergence properties. These are reported in table 2. The results are consistent with values reported by TJHW (1998a, b).

In addition to the preceding three one-dimensional problems, we also addressed the case of the two-dimensional problem (Vrscay and Handy 1989) $V(x,y)=x^2+y^2+(xy)^2$. Clearly, multidimensional systems involve turning hypersurfaces. We briefly outline the essential procedures for implementing the TPQ prescription for this system. As in the one-dimensional cases, spurious states were also detected. The rapid convergence of the physical ground state value (as the order of the calculation increase), allowed us to identify the physical solution as well. This is given in table 2.

Table 2. Quantization results for various potentials.

V	$N(L^*)$	E_{gr}	E_{exc}
$x^2 + x^4$	40	1.392 351 642	8.655 049 961
$x^2 + \frac{0.1x^2}{1+0.1x^2}$	40	1.043 173 726	5.181 094 75
$x^2 + y^2 + (xy)^2$	11^{*a}, 13^{*b}	2.195 917[a]	7.031 248[b]

We outline the basic steps for the two-dimensional problem,

$$-\nabla^2\Psi + (x^2 + y^2 + (xy)^2)\Psi = E\Psi. \tag{136}$$

The corresponding moment equation (for ground state symmetry solutions) is

$$\begin{aligned} u(p+1, q+1) = {} & Eu(p, q) - u(p+1, q) - u(p, q+1) \\ & +[2p(2p-1)]u(p-1, q) + [2q(2q-1)]u(p, q-1) \end{aligned} \tag{137}$$

where $u(p, q) = \int \mathrm{d}x\, \mathrm{d}y\, x^{2p} y^{2q} \Psi(x, y)$. The missing moments correspond to the infinite set $(\{u(\ell, 0)|0 \leqslant \ell < \infty\})$, although at any given order a finite number are required. A more detailed discussion of the missing moment structure of this problem can be found in the references.

Within our TJHW/TPQ formalism, the turning points become 'turning hypersurfaces' $(\mathcal{T}_{\mathcal{H}}(E))$, defined by $V(\overrightarrow{\tau}) = E$. Since the two-dimensional version of the TJHW representation converges to the physical solution, we are free to impose $\nabla^2\Psi(\overrightarrow{\tau}_\ell) = 0$ on a reasonable ('multiscale') distribution of points, $\overrightarrow{\tau}_\ell(E) \in \mathcal{T}_{\mathcal{H}}(E)$.

Let

$$\overrightarrow{\tau}_\ell = |\tau(E, \theta_\ell)|(\cos(\theta_\ell), \sin(\theta_\ell)). \tag{138}$$

Implementing our analysis to Lth order (i.e. involving the $L+1$ missing moments: $\{u(\ell, 0)|0 \leqslant \ell \leqslant L\}$), we evenly divide the angular interval $[0, \frac{\pi}{4}]$ (because of the implicit $x \leftrightarrow y$ symmetry) into L subintervals whose endpoints define the θ_ℓ.

For arbitrary E, at each θ_ℓ we determine the $|\tau(E, \theta_\ell)|$ that intersects $\mathcal{T}_{\mathcal{H}}(E)$. We then solve the determinantal condition ensuing from taking $\nabla^2\Psi(\overrightarrow{\tau_\ell}(E)) = 0$, on the appropriate TJHW (two-dimensional) representation. As L increases, we can identify the physical values quoted in table 2.

For this problem, $\mathcal{T}_{\mathcal{H}}$, is bounded. As $L \to \infty$ the density of turning points chosen, on the turning hypersurface, increases. Clearly, a better selection strategy for distributing the $\overrightarrow{\tau_\ell}$ on $\mathcal{T}_{\mathcal{H}}(E)$ should improve the convergence rate. This is beyond the scope of this paper.

11. Conclusion

We have defined a TPQ formalism which makes use of a recently developed wavefunction representation (i.e. TJHW analysis). This procedure, while generating accurate physical values, also generates spurious, unphysical solutions. By applying wavelet based methods (within the context of the HM moment-wavelet formalism) we are able to discriminate between the physical and unphysical solutions. The importance of the method presented is that because it involves a multiscale formalism for analysing localized structures (i.e. turning point behaviours) it is the natural complementing quantization prescription that can take advantage of what wavelet analysis was designed to do: address the multiscale behaviour of localized structures.

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