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On the equivalence of moment quantization and continuous wavelet transform analysis

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Abstract. The space of polynomials maps onto itself under affine transformations, $x \to \frac{x-b}{a}$. This suggests that a moment reformulation of continuous wavelet transform (CWT) theory (the affine convolution, $W\Psi(a,b) = \frac{\mathcal{N}}{\sqrt{a}}\int_{-\infty}^{\infty} \mathrm{d}x\, \mathcal{W}(\frac{(x-b)}{a})\Psi(x)$, of a signal, or wavefunction, $\Psi(x)$) should lead to significant simplifications in its implementation. We present a comprehensive formalism, with numerical examples, that inextricably links moment quantization (MQ) and CWT theory. For rational fraction potential problems and mother wavelets of the form $\mathcal{W}(x) = \partial_x^i \mathrm{e}^{Q(x)}$ ($Q(x)$ an appropriate polynomial), MQ permits a more efficient and accurate (in a pointwise convergent sense) CWT implementation; whereas, CWT broadens the scope of applicability for MQ methods, and is its natural extension when a more global approximation is desired. Our formalism also gives one justification for the empirical superiority manifested by previous MQ studies, as compared with dyadic wavelet reconstruction methods. We implement our formalism in the context of the quartic, sextic and octic anharmonic oscillator potentials, and demonstrate the flexibility of the method by treating both the Mexican hat wavelet transform, as well as that based on the mother wavelet $\mathcal{W}(x) = \partial_x^2 \mathrm{e}^{-x^4}$.

1. Introduction

The space of polynomials of degree N, $\mathcal{P}_N(x)$, maps onto itself under the affine transformation, $x \to \frac{x-b}{a}$. This simple observation underlies the theoretical simplicity that a moment-based analysis can bring to important problems such as the inverse (map) problem for affine, self-similar fractals (Handy and Mantica 1990, Bessis and Demko 1991), or the continuous wavelet transform (CWT) analysis of one-dimensional Sturm–Liouville problems in quantum mechanics (Handy and Murenzi 1996, 1997).

In several recent works, Handy and Murenzi (HM) have shown that moment quantization (MQ) methods, involving properly scaled and translated power moments, $\mu_{\alpha,b}(p) \equiv \int \mathrm{d}x\, x^p \mathrm{e}^{Q(\alpha x)}\Psi(x+b)$, can be used to generate the associated CWT (Grossmann and Morlet 1984, Mallat 1989)

$$W\Psi(a,b) = \frac{\mathcal{N}}{\sqrt{a}}\int_{-\infty}^{\infty} \mathrm{d}x\, [\partial_{\frac{x}{a}}^i \mathrm{e}^{Q(\frac{(x-b)}{a})}]\Psi(x) \tag{1.1}$$

of one-dimensional discrete states, $\Psi(x)$, without the need for any theoretical approximations ($\alpha \equiv \frac{1}{a}$, the inverse scale parameter). That is, one does not have to approximate the Schrödinger equation through a discretized, Galerkin-wavelet, type of analysis, as has been done in many other (numerical analysis) works (Gomes 1997). Instead, one can transform the Schrödinger equation exactly into a finite set of first-order (in α) coupled differential equations for the $\mu_{\alpha,b}(p)$'s. The numerical integration of these equations generates $W\Psi(a,b)$, since it is linearly dependent on a finite subset of the moments. One can then use dyadic frame (CWT formulae, refer to equation (2.2)) to reconstruct the desired wavefunction (Daubechies 1991).

Alternatively, the asymptotic ($\alpha \to \infty$) behaviour of the numerically integrated moments can also be used to directly recover the wavefunction (equation (2.3)). This approach has been shown by HM to yield superior (pointwise) results to those based on CWT-dyadic frame reconstruction. One of the important results of this work (section 3) is the proof that the asymptotic reconstruction approach is equivalent to a CWT analysis which integrates over all scales and translations (equation (3.6*b*)), in contrast to the dyadic formula which samples over dyadic scale and translation parameter values. Although this involves a straightforward analysis (which is nevertheless not widely known within the quantum physics community), in the present context of MQ, it is a very important result because it clearly demonstrates that the development of a $\mu_{\alpha,b}$-moment wavefunction reconstruction theory directly leads to one of the more important (group theory based) formulae in signal/continuous wavelet reconstruction. This is widely unappreciated, despite the fact that it yields an important and different perspective on the general concern of the classic moment problem: the reconstruction of a function from its moments (Shohat and Tamarkin 1963, Akhiezer 1965).

Accordingly, this work presents a complete MQ formalism (for determining the energy and wavefunction), in one dimension, and establishes the unequivocal equivalence between MQ and CWT theory within the context of Schrödinger problems with rational polynomial potential functions; and wavelet kernels, $\partial^i_{\frac{x}{a}} \mathrm{e}^{Q(\frac{(x-b)}{a})}$, for which $Q(x)$ is a polynomial and $\int \mathrm{d}x\, \mathrm{e}^{Q(x)} < \infty$. Despite these restrictions, they still define a broad class of interesting physics problems.

It should be stressed that although CWT has been applied to many physical and mathematical systems, relatively little has been done with respects to quantum mechanics. The few existing works, other than those of HM, have either been highly specialized or involved a variational analysis utilizing discrete wavelet bases (Paul 1984, Plantevin 1992, Cho *et al* 1993, Wei and Chou 1996, Tymczak and Wang 1997). Other than the cited works by HM, and the present effort, no other researchers have investigated the direct (and exact) transformation of the Schrödinger equation into a CWT representation (or an equivalent one), its resolution therein, and the requisite inversion to recover the solution. As noted, this work presents such a complete analysis for the class of problems defined above.

Until now, the investigations by HM have been limited solely to the *Mexican hat* wavelet, corresponding to $Q(x) = -\frac{1}{2}x^2$. We extend this analysis to other choices of wavelet functions, such as $Q(x) = -\frac{1}{2}x^4$. Also, we present a simpler formalism allowing the extension of the HM method to excited states.

Finally, our numerical examples focus on the important problems corresponding to the quartic, sextic and octic anharmonic oscillator potentials. In each case, we examine the first three symmetric states. The extension to other states is immediate, but not presented here for reasons of simplicity of presentation. The previous investigations by HM have focused on the ground and second excited states for the quartic anharmonic oscillator, $V(x) = mx^2 + gx^4$; the ground state of the rational polynomial potential $V(x) = \frac{gx^6}{1+\lambda x^2}$; and the ground state of the Bohr atom, $V(r) = 1/r$. The restriction to the *ground state* for the latter two cases was only for simplicity. The numerical examples presented in this work broaden the scope of applicability of the HM method.

2. Essentials of the moment-wavelet quantization formalism

We highlight some of the salient features of the HM formalism essential to this work. A fuller discussion may be found in the cited references.

Under the aforementioned conditions (rational potentials and polynomial $Q(x)$'s), the wavelet transform is a finite superposition

$$W\Psi(a,b) = \sum_{i=1}^{I} D_i[a]\mu_{\alpha,b}[i] \tag{2.1a}$$

of the scaled (a, $\alpha \equiv \frac{1}{a}$) and translated ($b$) moments,

$$\mu_{\alpha,b}(p) = \int_{-\infty}^{\infty} \mathrm{d}x\, x^p \mathrm{e}^{Q(\alpha x)}\Psi(x+b) \qquad p \geqslant 0. \tag{2.1b}$$

For the class of Hamiltonians being considered, all of the $\mu_{\alpha,b}(p)$ moments are linearly dependent on a finite subset, $\{\mu_{\alpha,b}(l) | 0 \leqslant l \leqslant m_s\}$, referred to as the *missing moments* (m_s is problem dependent). We show in the context of deriving equation (2.8) how the underlying Schrödinger equation can be transformed into a finite set of coupled differential moment equations, first order in α, for arbitrary translation parameter value. This allows one to relate the missing moments at a given scale to those at another scale. Note that the $\mu_{0,b}(p)$ moments have a trivial 'b' dependence and are simple linear superpositions of the $\mu_{0,0}(p)$ moments (refer to equation (2.10)).

Once the infinite scale, zero translation, moments are determined ($a = \infty$ and $b = 0$), as well as the physical energy value, E, it is a simple matter to (numerically) integrate the referenced equations in order to obtain the $\mu_{\alpha,b}(p)$ moments for all a, b values, thereby generating $W\Psi(a,b)$ as well. This defines a multiscale process in which infinite scale information enables the generation of the small-scale structure, all the way to $a \to 0$.

Given $W\Psi(a,b)$ for all scale and translation parameter values, one may use it to recover the corresponding discrete state wavefunction through dyadic reconstruction formulae of the type (for the Mexican hat wavelet (Daubechies 1991))

$$\Psi(x) \approx \frac{2}{6.819} \sum_{m,n} \mathcal{W}_{m,n} \frac{1}{\sqrt{2^m}} \mathcal{W}\left(\frac{(x - n2^m)}{2^m}\right) \tag{2.2}$$

where $\mathcal{W}_{m,n} \equiv W\Psi(2^m, n2^m)$, $\mathcal{W}(x) \equiv \mathcal{N}\partial_x^2 \mathrm{e}^{Q(x)}$, $Q(x) = -\frac{x^2}{2}$, and $\mathcal{N} = -\frac{2}{\sqrt{3}}\pi^{-\frac{1}{4}}$.

Alternatively, one can use the asymptotic relations (Handy and Murenzi 1996, 1997)

$$\mathrm{Lim}_{a\to 0}\left(\frac{\mu_{\frac{1}{a},b}(p)}{a^{1+p}\nu(p)}\right) = \Psi(b) \tag{2.3}$$

provided $\nu(p) = \int_{-\infty}^{+\infty} \mathrm{d}y\, y^p \mathrm{e}^{Q(y)} \neq 0$. The HM numerical results show the latter to be more effective than the dyadic formula, for the cases studied. We will return to this point shortly.

2.1. Moment quantization

An implicit, key component, of the preceding formalism is the determination of the infinite scale moments, $\{\mu_{0,0}(l)\}$, and the physical energy value, E. This is accomplished through the general procedure of MQ. MQ of the Schrödinger equation involves transforming the configuration space representation into a moment equation and solving for the physical energy and corresponding $\mu_{0,0}(l)$ moments.

For the class of Hamiltonians being considered, the moments satisfy a homogeneous, finite difference relation (moment equation) of the generic form (assuming no anomalous singular behaviour in the coefficients):

$$\mu_{\alpha,b}(n+m_s+1) = \sum_{l=0}^{m_s} C_{\alpha,b,E}[n,l]\mu_{\alpha,b}(n+l) \qquad n \geqslant 0 \tag{2.4}$$

where m_s is problem dependent (the *missing moment* order), and the coefficients, $C_{\alpha,b,E}[n,l]$ are algebraically or numerically determinable as functions of the energy variable, E.

It follows that all of the moments, $\mu_{\alpha,b}(p)$, corresponding to $p \geqslant m_s+1$ are linearly dependent on the first m_s+1 moments, $\{\mu_{\alpha,b}(l)|0 \leqslant l \leqslant m_s\}$, the missing moments:

$$\mu_{\alpha,b}(p) = \sum_{l=0}^{m_s} M_{\alpha,b,E}(p,l)\mu_{\alpha,b}(l) \qquad p \geqslant 0. \tag{2.5}$$

Self-consistency requires $M_{\alpha,b,E}(i,j) = \delta_{i,j}$, for $0 \leqslant i, j \leqslant m_s$.

The missing moments, at some convenient set of values for the scale and translation variables (usually: $a_* = \infty$, $\alpha_* = 0$ and $b_* = 0$), must satisfy some appropriate normalization condition. We usually take it to be

$$\sum_{l=0}^{m_s} \mu_{\alpha_*,b_*}(l) \equiv 1. \tag{2.6}$$

At a fixed set of values for the scale and translation parameters (a^*, b^*), one can use MQ techniques to determine the physical values for the associated moments and energy. Of course, since quantization is a global problem, the larger the scale ($a \to \infty$, $\alpha \to 0$) the better the moments correspond to extensive (nonlocal) objects. As such, the available MQ schemes are only suitable for sufficiently large-scale values, preferably $a = \infty$, and (essentially) arbitrary b values.

Various MQ prescriptions have been developed by several groups (Blankenbeckler *et al* 1980, Killingbeck *et al* 1985, Handy and Bessis 1985, Fernandez and Ogilvie 1993, Tymczak *et al* 1998a, b); however, the eigenvalue moment method (EMM) by Handy and Bessis (1985) and Handy *et al* (1988a, b) is particularly relevant to this work for two reasons. First, it is one of the few that emphasizes the role of the missing moments. Secondly, its quantization prescription for determining the energy and missing moments, as described the appendix, underscores the importance of polynomials with respects to forming an invariant set under scalings and translations. This is reviewed in the appendix. The work of Tymczak *et al* (1998) also solves for the missing moments and can be used in place of the EMM approach.

2.2. Generating the missing moments at all scales

We can use the preceding relations to generate the missing moments at all scales, based on knowledge of the missing moments at a predetermined (large) scale. Let $\Phi_{\alpha,b}(x) \equiv \mathrm{e}^{Q(\alpha x)}\Psi(x+b)$. From $Q(x)$'s (assumed) polynomial structure, $Q(x) = \sum_{i=0}^{I_Q} d_i x^i$, it follows that

$$\partial_\alpha \mu_{\alpha,b}(l) = \int \mathrm{d}x\, x^{1+l} Q'(\alpha x)\Phi_{\alpha,b}(x) \tag{2.7a}$$

or

$$\partial_\alpha \mu_{\alpha,b}(l) = \sum_{i=0}^{I_Q} i d_i \alpha^{i-1} \mu_{\alpha,b}(l+i) \tag{2.7b}$$

for $0 \leqslant l \leqslant m_s$.

Through equation (2.5), the r.h.s. of equation (2.7b) can be transformed into a sum over the missing moments. There then ensues a coupled set of $1 + m_s$ first-order differential equations relevant in determining the moments for all scales.

$$\frac{\partial}{\partial\alpha}\begin{pmatrix}\mu_{\alpha,b}(0)\\ \cdot\\ \mu_{\alpha,b}(i)\\ \cdot\\ \mu_{\alpha,b}(m_s)\end{pmatrix} = \begin{pmatrix}\mathcal{M}_{0,0}[\alpha,b,E] & \cdot & \mathcal{M}_{0,j}[\alpha,b,E] & \cdot & \mathcal{M}_{0,m_s}[\alpha,b,E]\\ \cdot & \cdot & \cdot & \cdot & \cdot\\ \cdot & \cdot & \mathcal{M}_{i,j}[\alpha,b,E] & \cdot & \cdot\\ \cdot & \cdot & \cdot & \cdot & \cdot\\ \mathcal{M}_{m_s,0}[\alpha,b,E] & \cdot & \mathcal{M}_{m_s,j}[\alpha,b,E] & \cdot & \mathcal{M}_{m_s,m_s}[\alpha,b,E]\end{pmatrix}$$
$$\times\begin{pmatrix}\mu_{\alpha,b}(0)\\ \cdot\\ \mu_{\alpha,b}(j)\\ \cdot\\ \mu_{\alpha,b}(m_s)\end{pmatrix}. \tag{2.8}$$

Knowledge of the physical energy value, E, and missing moments at a fixed b value and $a = \infty$ ($\alpha = 0$) will allow the integration of the above equations. However, a fortunate simplification arises in that at $a = \infty$, the $\{\mu_{0,0}(l)|0 \leqslant l \leqslant m_s\}$ moments determine all the moments: $\{\mu_{0,b}(l)|0 \leqslant l \leqslant m_s\}$. This follows from the simple relation

$$\mu_{0,b}(p) = \int_{-\infty}^{+\infty} x^p \Psi(b+x)\,\mathrm{d}x = \int_{-\infty}^{+\infty} (x-b)^p \Psi(x)\,\mathrm{d}x \tag{2.9}$$

or (expanding)

$$\mu_{0,b}(p) = \sum_{q=0}^{p} \binom{p}{q} (-b)^{p-q} \mu_{0,0}(q). \tag{2.10}$$

As previously noted, E and $\{\mu_{0,0}(l)|0 \leqslant l \leqslant m_s\}$ are obtainable through MQ.

In some of the examples to be presented, particularly for the excited states, it will be necessary to integrate equation (2.8) in a different manner. Specifically, through an analogous set of first-order differential equations with respects to 'b', we can obtain the $\{\mu_{\frac{1}{a_s},b}(l)|0 \leqslant l \leqslant m_s\}$ moments corresponding to some (large) finite value for the scale variable, a_s. This is achieved by integrating the appropriate equations starting from the EMM determined values for $\{\mu_{\frac{1}{a_s},0}(l)|0 \leqslant l \leqslant m_s\}$. Once the $\{\mu_{\frac{1}{a_s},b}(l)|0 \leqslant l \leqslant m_s\}$ moments are known, for $|b| \leqslant B$, one can then use them to initialize the integration of equation (2.8) in both directions: $a \to 0$ and $a \to \infty$.

In HM's original work, their numerical experiments revealed that the asymptotic moment reconstruction approach (equation (2.3)) was far superior to the dyadic-frame reconstruction in equation (2.2). The details of their analysis are summarized below.

Let $-B \leqslant b \leqslant B$ define the range of b values considered in the context of integrating equation (2.8), and $a_{\min}(b)$ define the smallest a value that one can reach through numerical integration initiated at 'b'. Upon considering all the dyadic formula integer pairs (m, n) in equation (2.2) consistent with $a_{\min}(b) < 2^m$ and $-B \leqslant n2^m \leqslant B$, (i.e. $a = 2^m$ and $b = n2^m$), for which the wavelet transform $W\Psi(a, b)$ is numerically calculable, the resulting reconstructed configuration was worse than that obtained through equation (2.3) (for the Mexican hat wavelet case). One additional complication in implementing this is the fact that the case $n = 0$ and $m \to \infty$ can only be approximated. That is, in practice, one must take $m \leqslant M$.

Such numerical results might suggest that the use of wavelets is ineffective in recovering quantum states. However, this is erroneous since the asymptotic formula in equation (2.3) corresponds to an exact wavelet reconstruction ansatz wherein one is integrating over all scales and translation parameter values. This is presented in the following section.

3. Moment quantization reconstruction and CWT analysis

In this section we shall prove that the asymptotic limit reconstruction ansatz in equation (2.3) is a continuous wavelet analysis result. First, let us generalize it by working with

$$U_S[a,b] \equiv \frac{1}{\nu}\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{a}S\left(\frac{(x-b)}{a}\right)\Psi(x) \qquad a>0 \tag{3.1}$$

where $\nu = \int_{-\infty}^{\infty}\mathrm{d}y\, S(y) \neq 0$. The function $S(y)$ is arbitrary, provided ν is nonzero, and it is at least differentiable to first order. We also assume $\Psi(x)$ to be well behaved. It readily follows that $\mathrm{Lim}_{a\to 0}U_S[a,b] = \Psi(b)$. Intuitively, the expression $\frac{1}{a\nu}S(\frac{(x-b)}{a})$ is approximating the Dirac function, $\delta(x-b)$ as $a\to 0$. Clearly, better choices of S function will increase the rate of pointwise convergence to the underlying function, $\Psi(b)$.

This pointwise result in b may be rewritten as

$$-\int_{a_f}^{\infty}\mathrm{d}a\,\partial_a U_S[a,b] = U_S[a_f,b] \tag{3.2}$$

or $(a_f \to 0)$

$$-\int_{0}^{\infty}\mathrm{d}a\,\partial_a U_S[a,b] = \Psi(b) \tag{3.3}$$

assuming $U_S[\infty,b]\equiv 0$.

Combining the above results, there follows:

$$\Psi(b) = \frac{1}{\nu}\int_0^{\infty}\frac{\mathrm{d}a}{a^2}\int_{-\infty}^{\infty}\mathrm{d}x\,\mathcal{F}\left(\frac{x-b}{a}\right)\Psi(x) \tag{3.4a}$$

where

$$a^{-2}\mathcal{F}\left(\frac{x-b}{a}\right) = -\partial_a\left[\frac{1}{a}S\left(\frac{x-b}{a}\right)\right] = a^{-2}\left\{S\left(\frac{x-b}{a}\right)+\frac{x-b}{a}S'\left(\frac{x-b}{a}\right)\right\}$$

or

$$\mathcal{F}(z) = \partial_z[zS(z)]. \tag{3.4b}$$

The function $\mathcal{F}$ takes on the manifest form of a wavelet. Indeed, if $S(z) = \mathrm{e}^{-\frac{1}{2}z^2}$, then $\mathcal{F}(z) = -\partial_z^2\mathrm{e}^{-\frac{1}{2}z^2}$, the Mexican hat wavelet (up to a normalization constant); however, this is not the objective of the present analysis.

The relation in equation (3.3) only integrates over all scales. In order to obtain a result which also integrates over all translations, one must rewrite $\mathcal{F}$ as a convolution integral:

$$\mathcal{F}\left(\frac{x-b}{a}\right) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\xi}{a}\mathcal{W}\left(\frac{x-\xi}{a}\right)\mathcal{D}\left(\frac{\xi-b}{a}\right) \tag{3.5a}$$

(note r.h.s. $= \int_{-\infty}^{\infty}\frac{\mathrm{d}\xi}{a}\mathcal{D}(\frac{x-\xi}{a})\mathcal{W}(\frac{\xi-b}{a})$) for arbitrary $\mathcal{W}$ and $\mathcal{D}$, provided the respective Fourier transforms satisfy

$$\hat{\mathcal{F}}(k) = \sqrt{2\pi}\,\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k). \tag{3.5b}$$

Inserting equation (3.5a) into equation (3.4) results in

$$U_S[a_f,b] = \frac{1}{\nu}\int_{a_f}^{\infty}\frac{\mathrm{d}a}{a^{\frac{5}{2}}}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\mathcal{D}\left(\frac{\xi-b}{a}\right)W\Psi(a,\xi) \tag{3.6a}$$

or

$$\Psi(b) = \frac{1}{\nu}\int_0^\infty \frac{\mathrm{d}a}{a^{\frac{5}{2}}}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\mathcal{D}\left(\frac{\xi-b}{a}\right)W\Psi(a,\xi) \tag{3.6b}$$

where $W\Psi(a,\xi) \equiv \int_{-\infty}^{\infty}\frac{\mathrm{d}x}{\sqrt{a}}\mathcal{W}(\frac{x-\xi}{a})\Psi(x)$ will denote the wavelet transform of Ψ (if besides satisfying equation (3.8), one also has $\hat{\mathcal{W}}(0) = 0$).

Combining equations (3.4b) and (3.5b) one obtains

$$-k\partial_k\hat{S}(k) = \sqrt{2\pi}\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k). \tag{3.7}$$

One important observation is that if S is well behaved (i.e. $\hat{S}(k)$ differentiable and asymptotically vanishing, and $\partial_k\hat{S}(k)$ L^1 integrable), then not only is $\int \mathrm{d}k\,\frac{\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k)}{k} = 0$, but also

$$\int \mathrm{d}k\,\frac{|\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k)|}{|k|} < \infty \tag{3.8a}$$

which is the more general wavelet condition. The normalization constant ν is given by

$$\nu = \sqrt{2\pi}\hat{S}(0) = 2\pi\int_0^\infty \mathrm{d}k\,\frac{\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k)}{k} \tag{3.8b}$$

or

$$\nu = \sqrt{2\pi}\hat{S}(0) = -2\pi\int_{-\infty}^0 \mathrm{d}k\,\frac{\hat{\mathcal{W}}(k)\hat{\mathcal{D}}(k)}{k} \tag{3.8c}$$

where $\hat{S}(\pm\infty) = 0$.

The importance of the preceding derivation is that in those cases where $S(x) = \mathrm{e}^{Q(x)}$ and $Q(x)$ is a suitable polynomial (regardless of the choice of mother wavelet and dual functions, provided they satisfy equation (3.7)), then the integral in equation (3.6b) (or its approximation through equation (3.6a), for suitably small a_f) is equivalent to determining the asymptotic limit in equation (2.3) through MQ methods and (numerical) integration of the corresponding coupled first-order equations symbolized in equation (2.8).

Alternatively, $S(x)$ may not be of the aforementioned type; however, the adopted mother wavelet does involve such an exponential, $\mathcal{W} = \mathrm{e}^{Q(x)}$. One can then determine the wavelet transform through our moment analysis, and utilize equation (3.6) (together with a prespecified dual function) to reconstruct the desired solution.

In the various works by HM, they make repeated use of the Mexican hat wavelet transform corresponding to the mother wavelet function: $\mathcal{W}_h(x) = \mathcal{D}_h(x) = -\mathcal{N}_h\partial_x^2\mathrm{e}^{-\frac{x^2}{2}}$, $\mathcal{N}_h = \frac{2}{\sqrt{3\sqrt{\pi}}}$ (normalized according to $\int \mathrm{d}x\,|\mathcal{W}_h(x)|^2 = 1$). The Fourier transform is $\hat{\mathcal{W}}_h(k) = \mathcal{N}_h k^2\mathrm{e}^{-\frac{k^2}{2}}$. The corresponding $\hat{S}(k)$ is

$$-k\ \partial_k\hat{S}(k) = \sqrt{2\pi}\mathcal{N}_h^2k^4\mathrm{e}^{-k^2} \tag{3.9a}$$

or

$$\hat{S}(k) = \frac{\sqrt{2\pi}}{2}\mathcal{N}_h^2(1+k^2)\mathrm{e}^{-k^2} \tag{3.9b}$$

with configuration representation (designated as S_{02})

$$S_{02}(x) = \frac{\sqrt{2\pi}}{2^{\frac{3}{2}}}\mathcal{N}_h^2\left(\frac{3}{2}-\frac{1}{4}x^2\right)\mathrm{e}^{-\frac{x^2}{4}}. \tag{3.10}$$

This result is very different from what HM used in their various works. Their asymptotic limits for the moments (equation (2.3)) were based on using $S_0(x) = \mathrm{e}^{-\frac{x^2}{2}}$ and $S_2(x) = x^2\mathrm{e}^{-\frac{x^2}{2}}$. However, no significant disparity is possible between the moment asymptotic limits derived using S_{02} and those obtained by HM, since a simple linear superposition of the latter yields the former. Specifically, using self-explanatory notation, $U_{S_{02}}[0,b] = \frac{1}{2\sqrt{\pi}}[\frac{3\nu(0)}{\sqrt{2}}U_{S_0}[0,b] - \frac{\nu(2)}{\sqrt{2}}U_{S_2}[0,b]]$, which becomes ($\nu(0) = \nu(2) = \sqrt{2\pi}$) $U_{S_{02}}[0,b] = \frac{1}{2}[3\,U_{S_0}[0,b] - U_{S_2}[0,b]]$; however, this is an identity since $\Psi(b) = U_{S_{02}}[0,b] = U_{S_0}[0,b] = U_{S_2}[0,b]$.

For the unnormalized Mexican hat wavelet $\mathcal{W}(x) = -\partial_x^2\mathrm{e}^{-\frac{x^2}{2}}$ and the exponential dual, $\mathcal{D}(x) = \mathrm{e}^{-\frac{x^2}{2}}$, the corresponding S is $S(x) = \frac{\sqrt{\pi}}{2}\mathrm{e}^{-\frac{x^2}{4}}$ ($\hat{S}(k) = \sqrt{\frac{\pi}{2}}\mathrm{e}^{-k^2}$).

Upon choosing an appropriate $S(x)$, and a corresponding $\mathcal{W}, \mathcal{D}$ pair, it follows from equation (3.6a) that knowledge of the wavelet transform $W\Psi(a,\xi)$ within the strip $\mathcal{R}^2_{a_f} \equiv [a_f, \infty) \times (-\infty, +\infty)$ allows us to calculate the approximation to the wavefunction $\Psi_{\mathrm{approx.}}(b) = U_S[a_f, b]$ derived by numerically integrating equation (2.8) from $\alpha = 0$ to $\alpha_f = \frac{1}{a_f}$.

An interesting observation is that if $\hat{S}(k) = \mathrm{e}^{-\frac{k^2}{2}}$ and $\hat{\mathcal{D}}(k) = \frac{1}{1+k^2}$, then $\hat{\mathcal{W}}(k) = k^2(1+k^2)\mathrm{e}^{-\frac{k^2}{2}}$. The inverse Fourier transforms are $\mathcal{W}(x) = \partial_x^2(\partial_x^2 - 1)\mathrm{e}^{-\frac{x^2}{2}}$ and $\mathcal{D}(x) = \sqrt{\frac{\pi}{2}}\mathrm{e}^{-|x|}$. The corresponding wavefunction reconstruction formula is

$$\Psi(b) = \sqrt{\frac{\pi}{2}}\frac{1}{\nu}\int_0^\infty \frac{\mathrm{d}a}{a^3}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\mathrm{e}^{-|\frac{\xi-b}{a}|}W\Psi(a,\xi) \tag{3.11a}$$

where

$$W\Psi(a,\xi) = \int\frac{\mathrm{d}x}{\sqrt{a}}\left[\left(\frac{x-\xi}{a}\right)^4 - 7\left(\frac{x-\xi}{a}\right)^2 + 4\right]\mathrm{e}^{-\frac{(x-\xi)^2}{2a^2}}\Psi(x) \tag{3.11b}$$

$$= a^{-\frac{9}{2}}\mu_{\alpha,b}(4) - 7a^{-\frac{5}{2}}\mu_{\alpha,b}(2) + 4a^{-\frac{1}{2}}\mu_{\alpha,b}(0) \tag{3.11c}$$

and $\mu_{\alpha,b}(p) \equiv \int\mathrm{d}x\,x^p\mathrm{e}^{-\frac{x^2}{2a}}\Psi(x+\xi)$ (note that $\partial_x^2(\partial_x^2-1)\mathrm{e}^{-\frac{x^2}{2}} = (x^4 - 7x^2 + 4)\mathrm{e}^{-\frac{x^2}{2}}$). Equation (3.11) is reminiscent of Padé–Fourier reconstruction methods discussed by Handy (1981, 1986).

We may rewrite equation (3.5a) as $\mathcal{F}(z) = \partial_z[zS(z)] = \int\mathrm{d}x\,\mathcal{W}(z-x)\mathcal{D}(x)$, which becomes $\partial_z[zS(z)] = \partial_z^i\int\mathrm{d}x\,\mathrm{e}^{[-Q(z-x)-Q(x)]}$ for the case where $\mathcal{W}(x) = \partial_x^i\mathrm{e}^{-Q(x)}$ ($i \geqslant 0$) and $\mathcal{D}(x) = \mathrm{e}^{-Q(x)}$.

In the case that $Q(x) = x^{2N}$, we can readily determine the asymptotic form for $S(x)$. Consider the integral $\mathcal{I}(z) = \int\mathrm{d}x\,\mathrm{e}^{-[(z-x)^{2N}+x^{2N}]}$. Performing the successive change of variables ($z > 0$) $y = x - \frac{z}{2}$, and $s = \frac{2}{z}y$ yields

$$\mathcal{I}(z) = \frac{z}{2}\mathrm{e}^{-2(\frac{z}{2})^{2N}}\int\mathrm{d}s\,\exp\left[-2(\frac{z}{2})^{2N}\left(\sum_{\eta=1}^{N}\binom{2N}{2\eta}s^{2\eta}\right)\right] \tag{3.12}$$

where $\binom{p}{q} \equiv \frac{p!}{(p-q)!q!}$. Rescaling according to $\sigma = \frac{s}{\lambda}$, and defining $\lambda^2 = \frac{1}{2(\frac{z}{2})^{2N}}$, we transform the integral into

$$\mathcal{I}(z) = \frac{z\mathrm{e}^{[-2(\frac{z}{2})^{2N}]}}{2^{\frac{3}{2}}(\frac{z}{2})^N}\int\mathrm{d}\sigma\,\exp\left[-\left\{N(2N-1)\sigma^2 + \sum_{\eta=2}^{N}\binom{2N}{2\eta}\left(\frac{2^{(2N-1)(\eta-1)}\sigma^{2\eta}}{(z)^{2N(\eta-1)}}\right)\right\}\right]. \tag{3.13a}$$

Table 1. $S(x)$, $\mathcal{W}(x)$, and $\mathcal{D}(x)$.

$S(x)$	$\mathcal{W}(x)$	$\mathcal{D}(x)$
$\frac{\sqrt{\pi}}{2}(\frac{3}{2} - \frac{1}{4}x^2)\mathrm{e}^{-\frac{x^2}{4}}$	$-\partial_x^2\mathrm{e}^{-\frac{x^2}{2}}$	$-\partial_x^2\mathrm{e}^{-\frac{x^2}{2}}$
$\frac{\sqrt{\pi}}{2}\mathrm{e}^{-\frac{x^2}{4}}$	$-\partial_x^2\mathrm{e}^{-\frac{x^2}{2}}$	$\mathrm{e}^{-\frac{x^2}{2}}$
$\mathrm{e}^{-\frac{x^2}{2}}$	$\partial_x^2(\partial_x^2 - 1)\mathrm{e}^{-\frac{x^2}{2}}$	$\sqrt{\frac{\pi}{2}}\mathrm{e}^{-\|x\|}$
$\sim \frac{1}{x}\partial_x \frac{x\mathrm{e}^{[-2(\frac{x}{2})^{2N}]}}{2^{\frac{3}{2}}(\frac{x}{2})^N}\sqrt{\frac{\pi}{N(2N-1)}}$	$\partial_x^2\mathrm{e}^{-x^{2N}}$	$\mathrm{e}^{-x^{2N}}$

with asymptotic form

$$\mathcal{I}(z) \sim \Omega(z) \equiv \frac{z\mathrm{e}^{[-2(\frac{z}{2})^{2N}]}}{2^{\frac{3}{2}}(\frac{z}{2})^N}\sqrt{\frac{\pi}{N(2N-1)}} \qquad \text{as } z \to +\infty. \tag{3.13b}$$

We then have that $S(z) \sim \frac{1}{z}\partial_z\Omega(z)$, if $\mathcal{W}(z) = \partial_z^2\mathrm{e}^{-z^N}$. Note that if $S(z) \sim \frac{1}{z}[\text{constant} + \partial_z\Omega(z)]$, the requirement that $\nu \equiv \int \mathrm{d}z\, S(z) < \infty$ would be violated, unless constant $= 0$.

A summary of the various $S, \mathcal{W}, \mathcal{D}$ combinations considered above is given in table 1.

4. Analysis of anharmonic oscillator potentials: $mx^2 + gx^{2q}$

It is clear that equation (2.3) represents a pointwise convergent formula for reconstruction; whereas, equations (3.6a, b), and its approximation through the dyadic-frame formula in equation (2.2), achieves a global representation involving all scales and translations.

Our moment formulation provides the flexibility wherein if one is given a wavelet function of the form $\mathcal{W} = \mathcal{N}\partial_x^i\mathrm{e}^{Q(x)}$ ($Q(x)$ a polynomial), and its dual, $\mathcal{D}$, then we can calculate the wavelet transform $W\Psi(a, b)$ (as detailed below) and numerically integrate equations (3.6a, b), in order to recover $\Psi(b)$.

Alternatively, if the associated $\mathcal{S}(x)$ function (equation (3.7)) is of a (similar) exponential form ($\mathcal{S}(x) = \mathcal{N}_{\mathcal{S}}\hat{P}(x)\mathrm{e}^{\hat{Q}(x)}$, both $\hat{P}$ and $\hat{Q}$ polynomials) then we can generate equations (3.6a, b) directly, through the integration of equation (2.8). That is, one can use equation (2.8), without any immediate focus on the underlying wavelet analysis. In this process, as $a_f \to 0$, $U_S[a_f, b]$ (equation (3.6a)) will define a multiscale approximation to the wavefunction. The following examples adopt this perspective.

4.1. *Mexican hat wavelet,* $\mathcal{W} = -\mathcal{N}_h\partial^2\mathrm{e}^{-\frac{x^2}{2}}$

Consider the anharmonic oscillator potential problem

$$-\partial_x^2\Psi(x) + [mx^2 + gx^{2q}]\Psi(x) = E\Psi(x) \tag{4.1}$$

for $q = 2, 3, 4$, the quartic, sextic and octic anharmonic oscillators, respectively.

Translating by 'b', one obtains

$$-\partial_x^2\Psi(x+b) + [m(x+b)^2 + g(x+b)^{2q}]\Psi(x+b) = E\Psi(x+b). \tag{4.2}$$

Let $\Phi_{\gamma,b}(x) \equiv \mathrm{e}^{-\gamma x^2}\Psi(x+b)$ ($\gamma \equiv \frac{1}{2a^2}$). Substituting $\Psi(x+b) = \mathrm{e}^{\gamma x^2}\Phi_{\gamma,b}(x)$ in equation (4.1) one obtains

$$\begin{aligned}&-[\partial_x^2 + 4\gamma x\partial_x + \{2\gamma + 4\gamma^2 x^2\}]\Phi_{\gamma,b}(x)\\ &\qquad + \left[m\{x^2 + 2bx + b^2\} + g\sum_{i=0}^{2q}\binom{2q}{i} b^{2q-i}x^i\right]\Phi_{\gamma,b}(x) = E\Phi_{\gamma,b}(x)\end{aligned} \tag{4.3}$$

where $\binom{2q}{i} = \frac{(2q)!}{(2q-i)!i!}$.

The power moments of interest are $\mu_{\gamma,b}(p) \equiv \int_{-\infty}^{\infty}\mathrm{d}x\, x^p\Phi_{\gamma,b}(x)$. Multiplying both sides of equation (4.3) by x^p and performing the necessary integration by parts, one obtains the moment equation:

$$\begin{aligned}&-p(p-1)\mu_{\gamma,b}(p-2) + [\gamma(4p+2) + mb^2 + gb^{2q} - E]\mu_{\gamma,b}(p)\\ &\qquad + [2bm + 2gqb^{2q-1}]\mu_{\gamma,b}(p+1)\\ &\qquad + [m - 4\gamma^2 + gq(2q-1)b^{2q-2}]\mu_{\gamma,b}(p+2)\\ &\qquad + g\sum_{i=3}^{2q-1}\binom{2q}{i} b^{2q-i}\mu_{\gamma,b}(p+i) + g\mu_{\gamma,b}(p+2q) = 0.\end{aligned} \tag{4.4}$$

From equation (4.4) one generates the highest-order moment $\mu_{\gamma,b}(p+2q)$ from the lower-order moments. The linear nature of the moment equation leads to the fact that given the *missing moments* $\{\mu_{\gamma,b}(l)|0 \leqslant l \leqslant m_s = 2q-1\}$, as well as the energy, E, one can generate all the other moments. This is expressed through the relation given in equation (2.5).

For the present case of the *Mexican hat wavelet*, we have

$$\partial_\gamma\mu_{\gamma,b}(p) = -\mu_{\gamma,b}(p+2). \tag{4.5}$$

For the first $1 + m_s - 2$ missing moments ($0 \leqslant l \leqslant m_s - 2$) this equation simply states that $\partial_\gamma\mu_{\gamma,b}(l) = -\mu_{\gamma,b}(l+2)$. For $l = m_s - 1$, and m_s, the linear relation in equation (2.5) comes in since the moments $\mu_{\gamma,b}(m_s+1)$ and $\mu_{\gamma,b}(m_s+2)$ depend on the missing moments. That is,

$$\partial_\gamma\mu_{\gamma,b}(l) = -\mu_{\gamma,b}(l+2) \qquad 0 \leqslant l \leqslant m_s - 2 \tag{4.6a}$$

and

$$\partial_\gamma\mu_{\gamma,b}(l) = -\left(\sum_{l'=0}^{m_s} M_{\gamma,b,E}(l+2,l')\mu_{\gamma,b}(l')\right) \tag{4.6b}$$

for $l = m_s - 1$, and m_s. Alternatively, summarizing all the above, we have

$$\frac{\partial}{\partial\gamma}\begin{pmatrix}\mu_{\gamma,b}(0)\\ .\\ \mu_{\gamma,b}(i)\\ .\\ \mu_{\gamma,b}(m_s-1)\\ \mu_{\gamma,b}(m_s)\end{pmatrix}$$

$$= -\begin{pmatrix} 0 & 0 & 1 & 0 & . & 0\\ 0 & 0 & 0 & . & . & 0\\ 0 & 0 & 0 & 0 & \delta_{i,j-2} & 0\\ 0 & 0 & 0 & 0 & . & .\\ M_{\gamma,b,E}(m_s+1,0) & . & . & . & . & M_{\gamma,b,E}(m_s+1,m_s)\\ M_{\gamma,b,E}(m_s+2,0) & . & . & . & . & M_{\gamma,b,E}(m_s+2,m_s)\end{pmatrix}$$

$$\times \begin{pmatrix} \mu_{\gamma,b}(0) \\ \cdot \\ \mu_{\gamma,b}(j) \\ \cdot \\ \mu_{\gamma,b}(m_s-1) \\ \mu_{\gamma,b}(m_s) \end{pmatrix}. \tag{4.7}$$

Since the asymptotic form of the (physical) anharmonic oscillator wavefunctions, $\Psi(x) \to \mathrm{e}^{-\frac{\sqrt{g}}{q+1}|x|^{q+1}}$, decreases much faster ($q \geqslant 2$), than the Gaussian form of the Mexican hat exponential factor, $\mathrm{e}^{-\gamma x^2}$, we know that the moments $\mu_{\gamma,b}(p)$ are analytic in γ, particularly at the origin. This means that equation (4.7), for the case $q \geqslant 2$, cannot have any singular coefficients.

From section 1, knowledge of the physical energy, E, and missing moments at infinite scale ($\gamma = \frac{1}{2a^2} = 0$), $\mu_{0,0}$ ($l \leqslant m_s$), suffice to determine all of the missing moments at arbitrary scale, $a = \frac{1}{\sqrt{2\gamma}}$, and translation, b.

Within the context of EMM quantization, only the ground state energy, E_{gr}, and corresponding missing moments, $\mu_{gr;0,0}$ ($l \leqslant m_s$), can be determined. This is because EMM quantization requires that the configuration desired be non-negative. For excited states, this is not possible. However, by working with the configuration $(\Psi(x) + c)\mathrm{e}^{-\Gamma x^2}$, for some appropriate Γ value, and some sufficiently positive, empirically determined constant, c, we can still implement the EMM quantization procedure and determine the excited energy, E_{exc}, and corresponding missing moments at $\gamma = \Gamma$, and $b = 0$: $\mu_{\mathrm{exc};\Gamma,0}$ ($l \leqslant m_s$) (Handy and Lee 1991).

This 'c-shift' approach worked very well for the quartic and sextic anharmonic potentials. For the octic case, it worked too slowly. We circumvented this difficulty by determining the energies from another EMM formulation (the EMM-$|\Psi|^2$ formulation) (Handy 1987), and used direct Runge–Kutta (RK) integration on the Schrödinger equation in order to determine the zeros of the wavefunctions, $\Psi(x_{0;i}) = 0$, for the second and fourth excited states. One can then apply EMM to the modified expression $\Omega(x) = \Pi_i(x - x_{0;i})\mathrm{e}^{-\gamma x^2}\Psi(x)$, which can be taken to be non-negative. In this manner, the moments $\mu_{\mathrm{exc.};\gamma,0}(p) = \int_{-\infty}^{\infty} \mathrm{d}x\, x^p \mathrm{e}^{-\gamma x^2}\Psi(x)$ were determined, for $\gamma = \Gamma = 1$.

As noted in section 1, once E_{gr} and $\{\mu_{\mathrm{gr};0,0}(l) | l \leqslant m_s\}$ are determined, one can generate the $\{\mu_{\mathrm{gr};0,b}(l) | l \leqslant m_s\}$ moments through equation (2.10). Afterwards, one simply integrates equation (4.7) using fourth-order RK methods. Implicit in this entire process is the adoption of the normalization prescription in equation (2.6), implemented at $\gamma = 0$ and $b = 0$.

For the excited states, since the missing moments are determined at $\gamma = \Gamma$ and $b = 0$, one cannot use equation (2.10) to generate the $\mu_{\mathrm{exc.};\Gamma,\mathrm{b}}$ ($l \leqslant m_s$). Instead, we must implement another integration, in the b-direction, in order to generate these moments. Once the $\mu_{\mathrm{exc.};\Gamma,\mathrm{b}}$ ($l \leqslant m_s$) are determined, one can integrate equation (4.7) in either direction ($\gamma \to 0$ or $\gamma \to \infty$) in order to generate the wavelet transform (if desired) or recover the corresponding excited state through equation (2.3).

The aforementioned b-integration is accomplished by noting that

$$\partial_b \mu_{\gamma,b}(p) = 2\gamma\mu_{\gamma,b}(p+1) - p\mu_{\gamma,b}(p-1) \tag{4.8}$$

for the Mexican hat case. Utilizing this equation, for all of the missing moments ($p \leqslant m_s$), yields a closed set of coupled, first-order, differential equations in the missing moments (an equation similar to equation (4.7)). One can integrate it by using the EMM generated excited state moments at $\gamma = \Gamma$. As for the ground state case, the initial moments are normalized according to equation (2.6) for $\gamma = \Gamma = 1$ and $b = 0$.

An important relation pertinent to the numerical implementation of the above is the expansion

$$\begin{aligned}\mu_{\gamma,b}(p) &= \int_{-\infty}^{\infty} \mathrm{d}x\, x^p \mathrm{e}^{-\gamma x^2}\Psi(x+b) \\ &= \frac{1}{\gamma^{\frac{1+p}{2}}}\int_{-\infty}^{\infty}\mathrm{d}y\, y^p \mathrm{e}^{-y^2}\Psi\left(\frac{y}{\sqrt{\gamma}}+b\right) \\ &= \frac{1}{\gamma^{\frac{1+p}{2}}}\sum_{n=0}\frac{\nu_2(p+n)}{n!}\gamma^{-\frac{n}{2}}\Psi^{(n)}(b)\end{aligned} \tag{4.9}$$

where $\Psi^{(n)}(b) \equiv \partial_b^n\Psi(b)$ and $\nu_2(p+n) = \int_{-\infty}^{\infty}\mathrm{d}y\, y^{(p+n)}\mathrm{e}^{-y^2}$. Clearly, $\nu_2(\text{odd}) = 0$. Accordingly, for $p =$ even, the expansion involves only inverse powers of γ (besides the $\gamma^{-\frac{1+p}{2}}$ factor).

The expansion in equation (4.9) is valid for large γ values. In practice, for the problems considered here, the RK integration iterates generated from equation (4.7) already begin to satisfy equation (4.9) at relatively small γ values, $\gamma = \mathrm{O}(10)$. What this means is that we can truncate equation (4.9) and use it as a sequence acceleration scheme for extracting $\Psi(b)$. More precisely, let $\mu_{\gamma_i,b}(p)$ denote a RK integration iterate, then we can solve for the A coefficients ($n = 2\eta$ and $p =$ even):

$$\mu_{\gamma_i,b}(p) = \frac{1}{\gamma_i^{\frac{1+p}{2}}}\sum_{\eta=0}^{N}\gamma_i^{-\eta}A_\eta^{p,b,I,N} \tag{4.10}$$

for $I \leqslant i \leqslant I+N$. The $\gamma_i^{-\eta}$ defines an $(N+1)\times(N+1)$ matrix, which can be inverted to yield the $A_\eta^{p,b,I,N}$s.

For fixed p and b, if the initial iterate $\mu_{\gamma_I,b}(p)$ is associated with a sufficiently large γ_I value (within the RK domain of numerical stability), then as N increases (as well as 'I') the $A_\eta^{p,b,I,N}$ coefficients should better approximate the expansion in equation (4.9). This is numerically verified for $0 \leqslant N \leqslant 8$, within the limits of our numerical analysis. In particular, most of the plots in figures 1–3 and figure 10 were obtained for $N \geqslant 4$. The results of the preceding analysis verified equation (2.3), for $p = 0$ and 2, through the relation $\mathrm{Lim}_{I\to\infty}\frac{A_0^{p,b,I,N}}{\nu_2(p)} = \Psi(b)$. Note that $\nu_2(0) = \sqrt{\pi}$, and $\nu_2(2) = \frac{\sqrt{\pi}}{2}$.

The numerical results for the quartic, sextic and octic anharmonic oscillators ($q = 2, 3, 4$, respectively) are depicted in figures 1–3. We show the results for the first three symmetric states. Note that once the moment normalization in equation (2.6) is adopted, equation (2.3) yields the estimate for the corresponding configuration space wavefunction at $b = 0$, $\Psi(0)$. Utilizing this as input, we calculate the 'exact' wavefunction through direct integration of the Schrödinger equation, in order to compare with the estimates for $b \neq 0$ from equation (2.3). The excellent results depicted correspond to $m = g = 1$. In table 2 we list the energies and initial moment values.

In the quartic case, $q = 2$, we computed both the pointwise estimates for the wavefunctions as well as the corresponding Mexican hat wavelet transforms:

$$\begin{aligned}W\Psi(a,b) &= \frac{\mathcal{N}_h a^2}{\sqrt{a}}\int \mathrm{d}x - \partial_x^2 \mathrm{e}^{-\frac{(x-b)^2}{2a^2}}\Psi(x) \\ &= \frac{\mathcal{N}_h a^2}{\sqrt{a}}\int \mathrm{d}x - \partial_x^2 \mathrm{e}^{-\frac{x^2}{2a^2}}\Psi(x+b)\end{aligned}$$

or

$$W\Psi(a,b) = \mathcal{N}_h(2\gamma)^{\frac{1}{4}}[\mu_{\gamma,b}(0) - 2\gamma\ \mu_{\gamma,b}(2)]. \tag{4.11}$$

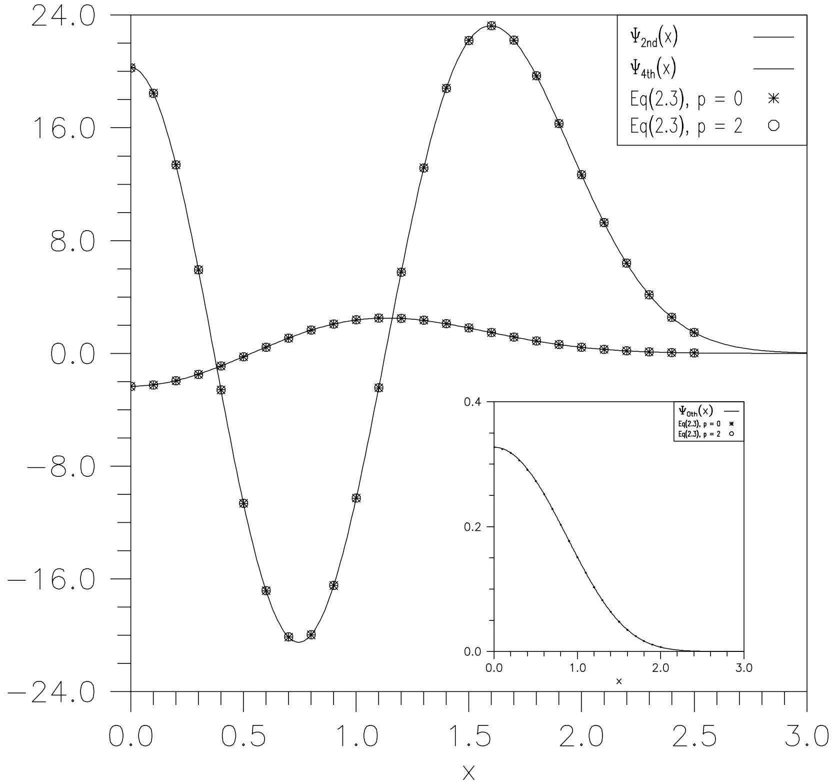

Figure 1. MQ—$\partial_x^2 e^{-\frac{x^2}{2}}$ reconstruction for $V(x) = x^2 + x^4$.

Clearly, whereas the the pointwise estimates for $\Psi(b)$ only require calculating the limits in equation (2.3), the determination of the wavelet transforms requires being able to calculate the moments for all γ values. For the quartic anharmonic oscillator ground state, we are able to generate the missing moments at $\gamma = 0$, and arbitrary 'b', and integrate equation (4.7) forwards ($\gamma \to \infty$).

This is not the case for the excited states. One must integrate backwards ($\gamma \to 0^+$) in order to determine the missing moments in the region $0 \leqslant \gamma < 1$. When we did so, using as input the previously obtained missing moments $\{\mu_{1,b}(l)\}$, we found that for $b > 1$, the generated $\mu_{0,b}(l)$ values were significantly in error. In particular, $\mu_{0,b}(0)$ did not remain constant for all 'b', as it should. This numerical instability arose despite the fact that if one integrates forward ($\gamma \to \infty$), utilizing the same starting $\mu_{1,b}(l)$ values, good pointwise estimates for $\Psi(b)$ can be obtained (to better than 1%).

In order to generate accurate $\mu_{\gamma,b}(l)$ values, particularly for $0 \leqslant \gamma < 1$, (with which to generate the wavelet transform) we took the $b = 0$ backwards integration generated values for the missing moments and used them to generate all the missing moments, $\{\mu_{0,b}(l)\}$, through equation (2.10). With these more accurate starting missing moments, we then integrated forwards and generated the missing moments within the region $[0, \mathrm{O}(10^2)] \times [-2, 2]$, leading to exceptionally accurate pointwise results for $\Psi(b)$ (i.e. the agreement between the asymptotic estimates for $p = 0, 2$ in equation (2.3) was better than six decimal places). This is the underlying numerical analysis for figure 1 and the wavelet transforms depicted in figures 4–9.

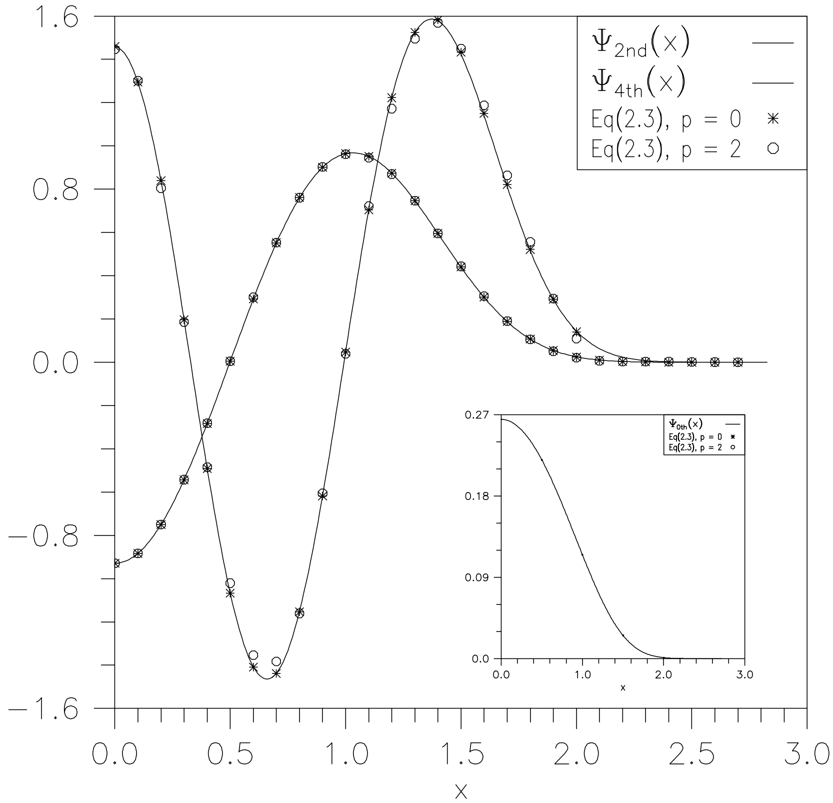

Figure 2. MQ—$\partial_x^2 e^{-\frac{x^2}{2}}$ reconstruction for $V(x) = x^2 + x^6$.

An important observation relevant to the Hamiltonians investigated in this work is that since the expansion in equation (4.9) agrees with the RK iterates (for sufficiently large γ values), within the region of numerical stability for the RK integration, we can then use it to approximate the missing moments in regions of numerical instability for the RK iterates. In this manner, the wavelet transform can also be approximated in such regions as well. These considerations were not necessary for the wavelet transform plots in figures 4–9.

4.2. *Quartic wavelet,* $\mathcal{W} = -\mathcal{N}\partial_x^2 e^{-\frac{x^4}{2}}$

The analysis for the quartic wavelet transform

$$W\Psi(a,b) = \frac{\mathcal{N}_4}{\sqrt{a}} \int \mathrm{d}x(-)\partial_{\frac{x}{a}}^2 \mathrm{e}^{-\frac{(x-b)^4}{2a^4}} \Psi(x) \tag{4.12}$$

or

$$W\Psi(a,b) = \frac{\mathcal{N}_4}{\sqrt{a}} \int \mathrm{d}x(-)\partial_{\frac{x}{a}}^2 \mathrm{e}^{-\frac{(x)^4}{2a^4}} \Psi(x+b) \tag{4.13a}$$

$$= \frac{\mathcal{N}_4}{2^{\frac{3}{8}}} \gamma^{\frac{5}{8}} [12\mu_{\gamma,b}(2) - 16\gamma\mu_{\gamma,b}(6)] \tag{4.13b}$$

where

$$\mu_{\gamma,b}(p) = \int \mathrm{d}x\, x^p \mathrm{e}^{-\gamma x^4} \Psi(x+b) \tag{4.13c}$$

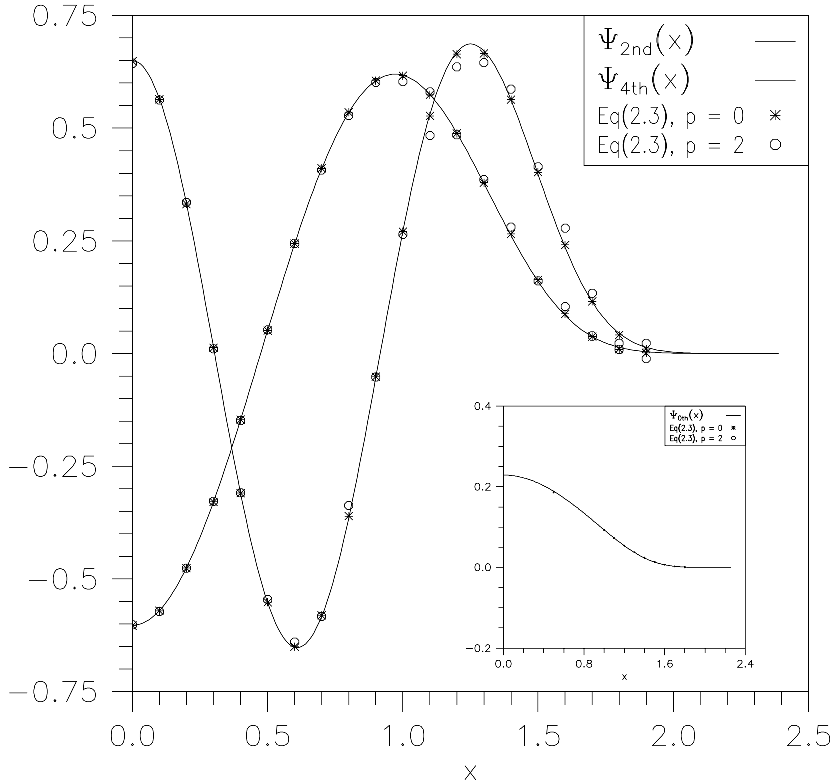

Figure 3. MQ—$\partial_x^2 e^{-\frac{x^2}{2}}$ reconstruction for $V(x) = x^2 + x^8$.

proceeds similarly to the Mexican hat case. Note that now $\gamma \equiv \frac{1}{2a^4}$. In particular, denoting $\Phi_{\gamma,b}(x) = e^{-\gamma x^4}\Psi(x+b)$, the analogous substitutions in the Schrödinger equation (as done in the context of equation (4.4)) leads to the moment equation ($\mu_{\gamma,b}(p) = \int dx\, x^p \Phi_{\gamma,b}(x)$):

$$\begin{aligned} -p(p-1)\mu_{\gamma,b}(p-2) &+ [mb^2 + gb^{2q} - E]\mu_{\gamma,b}(p) + [2bm + 2gqb^{2q-1}]\mu_{\gamma,b}(p+1) \\ &+ [m + \gamma(8p+12) + gq(2q-1)b^{2q-2}]\mu_{\gamma,b}(p+2) \\ &+ g\sum_{i=3}^{2q-1}\binom{2q}{i} b^{2q-i}\mu_{\gamma,b}(p+i) + g\mu_{\gamma,b}(p+2q) - 16\gamma^2\mu_{\gamma,b}(p+6) = 0. \end{aligned} \tag{4.14}$$

It is readily apparent that for the quartic and sextic anharmonic oscillator potentials ($q = 2$ and 3, respectively), solving for the highest-order moment ($\mu_{\gamma,b}(p+6)$ in both cases) will involve a singular coefficient. Specifically, in the quartic case one has $\mu_{\gamma,b}(p+6) = \frac{\text{moment expression}}{16\gamma^2}$; whereas for the sextic problem, the corresponding moment equation is of the form: $\mu_{\gamma,b}(p+6) = \frac{\text{moment expression}}{16\gamma^2 - g}$. These results are simple to understand.

For the quartic anharmonic problem, the moments (equation (4.13*c*)) are not analytic at the origin in the complex-γ plane. This is because the asymptotic form of the physical bound state solutions, (i.e. $e^{-\sqrt{g}\frac{|x|^3}{3}}$) is much weaker than the $e^{-\gamma x^4}$ wavelet exponential for $\gamma < 0$.

Table 2. Energy and missing moment values.

$V(x)$	$Q(x)$ (equation (1.1))	E	$\mu_{\gamma,0}(l=0,2,\ldots)$ $(\mu_{\gamma,0}(\text{odd})=0)$	γ
x^2+x^4	$-x^2$	1.392 351 641 5306[a]	0.642 670 622 325 26[a]	0
			0.357 329 377 674 74	
x^2+x^4	$-x^2$	8.655 049 957[b]	−0.286 464 852 1[b]	1
			1.286 464 852 1	
x^2+x^4	$-x^2$	18.057 557 4[b]	0.641 570 459[b]	1
			0.358 429 541	
x^2+x^6	$-x^2$	1.435 624 619 003[a]	0.493 699 995 305 89[a]	0
			0.231 502 508 700 18	
			0.274 797 495 993 93	
x^2+x^6	$-x^2$	9.966 621 999 6[b]	−0.059 348 906 8[b]	1
			0.461 920 793 71	
			0.597 428 113 09	
x^2+x^6	$-x^2$	22.910 18[b]	0.067 623 46[b]	1
			0.159 290 95	
			0.773 085 59	
x^2+x^8	$-x^2$	1.491 019 895 662[a]	0.409 046 841 743 26[a]	0
			0.170 212 946 241 30	
			0.172 497 535 939 30	
			0.248 242 676 076 15	
x^2+x^8	$-x^2$	10.993 737 34 [c]	−0.017 873 341 8[d]	1
			0.275 731 625 2	
			0.317 071 306 4	
			0.425 070 410 2	
x^2+x^8	$-x^2$	26.743 448 6[c]	0.036 202 497 2[d]	1
			0.087 695 169 7	
			0.290 586 179 5	
			0.585 516 153 6	
x^2+x^4	$-x^4$	1.392 351 641 530[c]	0.712 374 885 413 96[e]	1
			0.180 129 004 250 33	
			0.107 496 110 335 71	
x^2+x^6	$-x^4$	1.435 624 619 003	1[f]	$\frac{1}{4}$
			0.358 906 154 750 85	
			0.314 406 813 959 02	
x^2+x^8	$-x^4$	1.491 019 895 662[a]	0.409 046 841 743 26[a]	0
			0.170 212 946 241 30	
			0.172 497 535 939 30	
			0.248 242 676 076 15	

[a] Conventional EMM analysis.
[b] C-shift EMM analysis.
[c] Energy predetermined from EMM-$|\Psi|^2$ formulation.
[d] Zeros of wavefunction are predetermined through direct RK on the Schrödinger equation, together with predetermined energy, followed by generation of moments from conventional EMM analysis of $\Pi_i(x - x_{0;i})\Psi(x)$.
[e] Conventional EMM with inputed predetermined energy.
[f] The potential $V(x) = x^2 + x^6$ defines a zero missing moment problem at $\gamma = \frac{1}{4}$; hence the adopted normalization is $\mu_{\frac{1}{4},0}(0) = 1$.

The same applies for the sextic anharmonic oscillator whose bound state wavefunctions have the asymptotic form: $e^{-\sqrt{g}\frac{x^4}{4}}$. The moments are analytic at $\gamma = 0$ but not at $\gamma = -\frac{\sqrt{g}}{4}$ (or $\gamma^2 = \frac{g}{16}$).

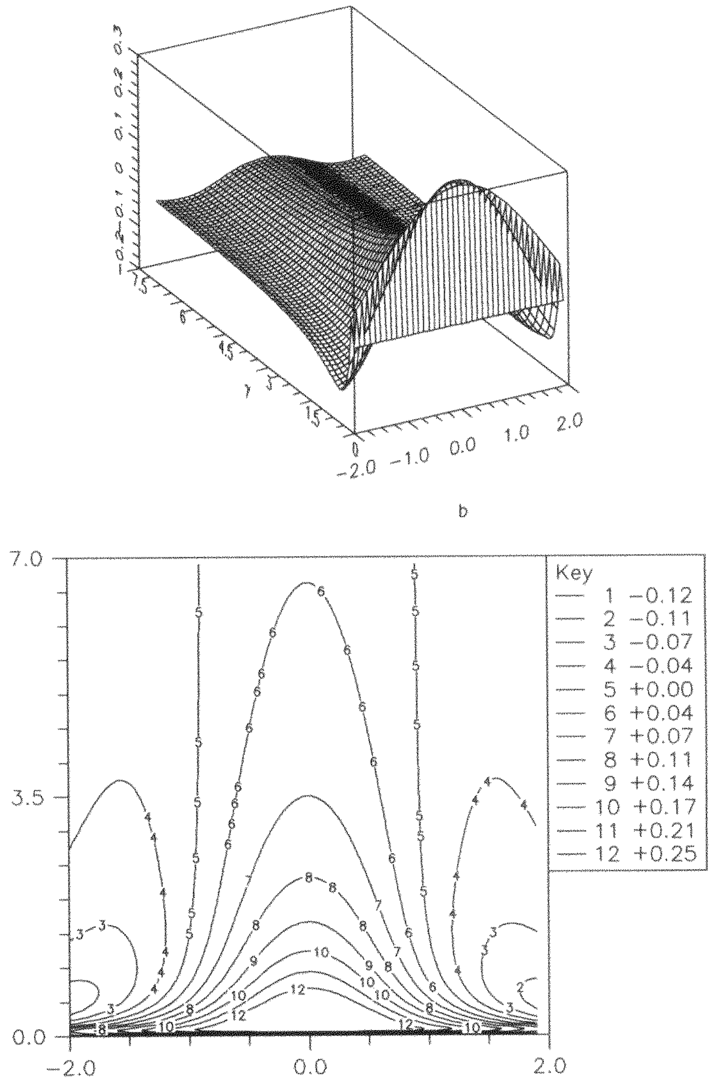

Figure 4. Mexican hat wavelet transform, $W\Psi(a, b)$, for the $V(x) = x^2 + x^4$ ground state.

The integral $\int_{-\infty}^{\infty} dx\, e^{-\gamma x^4}\Psi_{\text{unphysical}}(x)$ exists in the limit $\gamma \to \infty$. However, from the JWKB zeroth-order approximation to the unphysical wavefunction, $\Psi_{\text{unphysical}}(x) \approx e^{\frac{\sqrt{g}}{4}x^4}$, such integrals become singular at $\gamma = +\frac{\sqrt{g}}{4}$.

In general, the integral $\int_{-\infty}^{\infty} dx\, e^{Q(\frac{x}{a})}\Psi_{\text{unphysical}}(x)$ will not exist, in the $a \to 0$ limit, if the asymptotic behaviour of the unphysical wavefunction dominates the exponentially decreasing expression $e^{Q(\frac{x}{a})}$ ($Q(x)$ assumed to be a polynomial with a negative, highest-degree coefficient). The only possible way of defining such integrals is by an appropriate analytic continuation. Such is the case for the Mexican hat wavelet and anharmonic potentials considered previously, as well as the $\partial_x^2 e^{-\frac{x^4}{2}}$ wavelet analysis of the octic anharmonic potential (discussed below). For the $\partial_x^2 e^{-\frac{x^4}{2}}$ wavelet analysis of the quartic

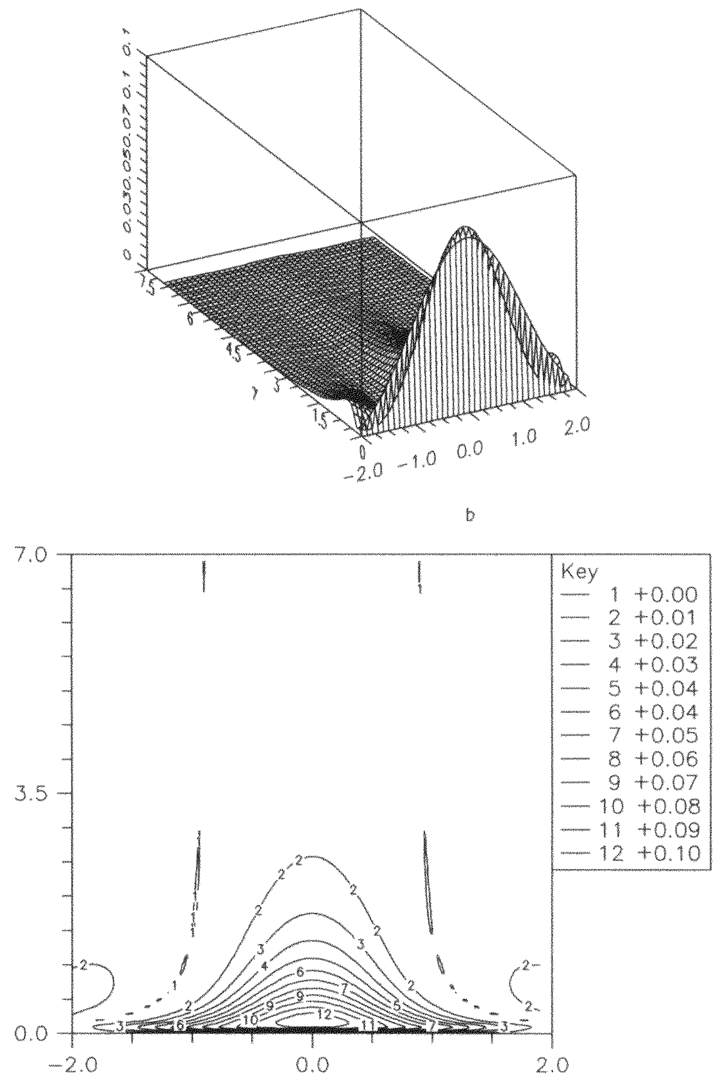

Figure 5. Square of Mexican hat wavelet transform, $W\Psi(a,b)^2$, for the $V(x) = x^2 + x^4$ ground state.

anharmonic oscillator problem, the corresponding integral exists for all non-negative values of γ.

None of the above complications holds for the octic anharmonic potential.

Before continuing with a description of the manner by which the moments, at all scales and translations, are obtained, we develop the counterparts to equations (4.7) and (4.8) for the quartic wavelet case under consideration.

In order to generate a coupled set of first-order differential equations for the moments, we simply make use of the relations

$$\partial_\gamma \mu_{\gamma,b}(l) = -\mu_{\gamma,b}(l+4) \tag{4.15}$$

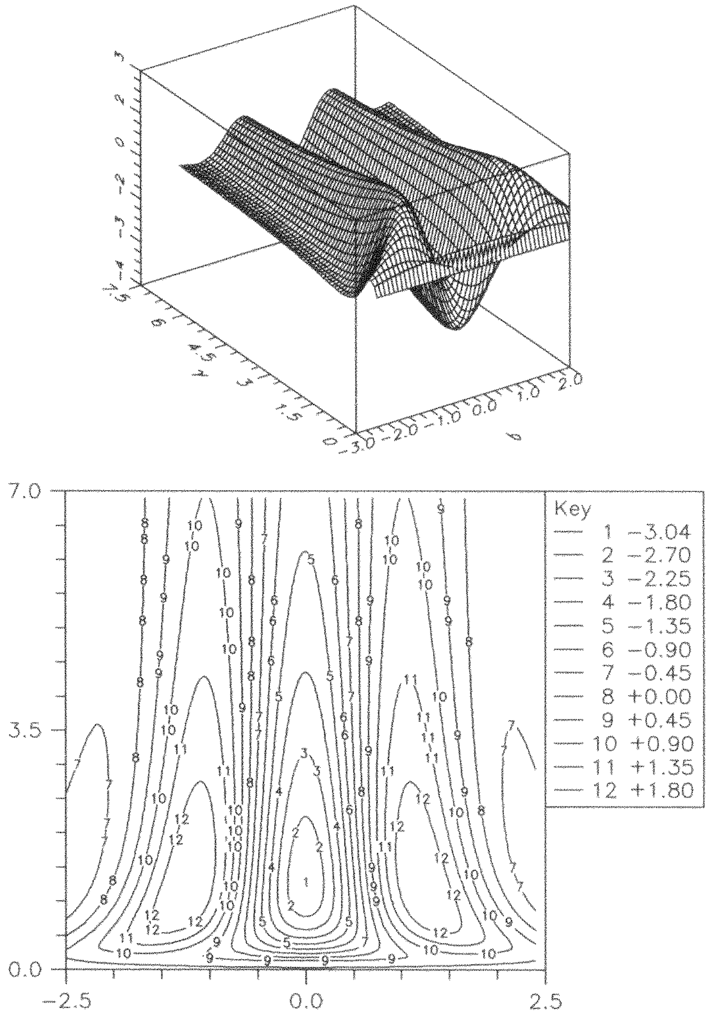

Figure 6. Mexican hat wavelet transform, $W\Psi(a,b)$, for the $V(x) = x^2 + x^4$ second excited state.

and

$$\partial_b \mu_{\gamma,b}(l) = 4\gamma\ \mu_{\gamma,b}(l+3) - l\mu_{\gamma,b}(l-1). \tag{4.16}$$

Although these equations hold for all l values, it is sufficient to restrict them to the missing moments, $0 \leqslant l \leqslant m_s$.

We symbolize the linear dependence of the moments on the missing moments by: $\mu_{\gamma,b}(p) = \sum_{l=0}^{m_s} M^{(4)}_{\gamma,b,E}(p,l)\mu_{\gamma,b}(l)$ (again, $M^{(4)}_{\gamma,b,E}(i,j) = \delta_{i,j}$). The $M^{(4)}_{\gamma,b,E}(p,l)$ coefficients are singular at $\gamma = 0$ and $\gamma = \pm\frac{\sqrt{g}}{4}$, for the quartic and sextic anharmonic oscillators, respectively. In addition, the structure of equation (4.15) leads to a significantly

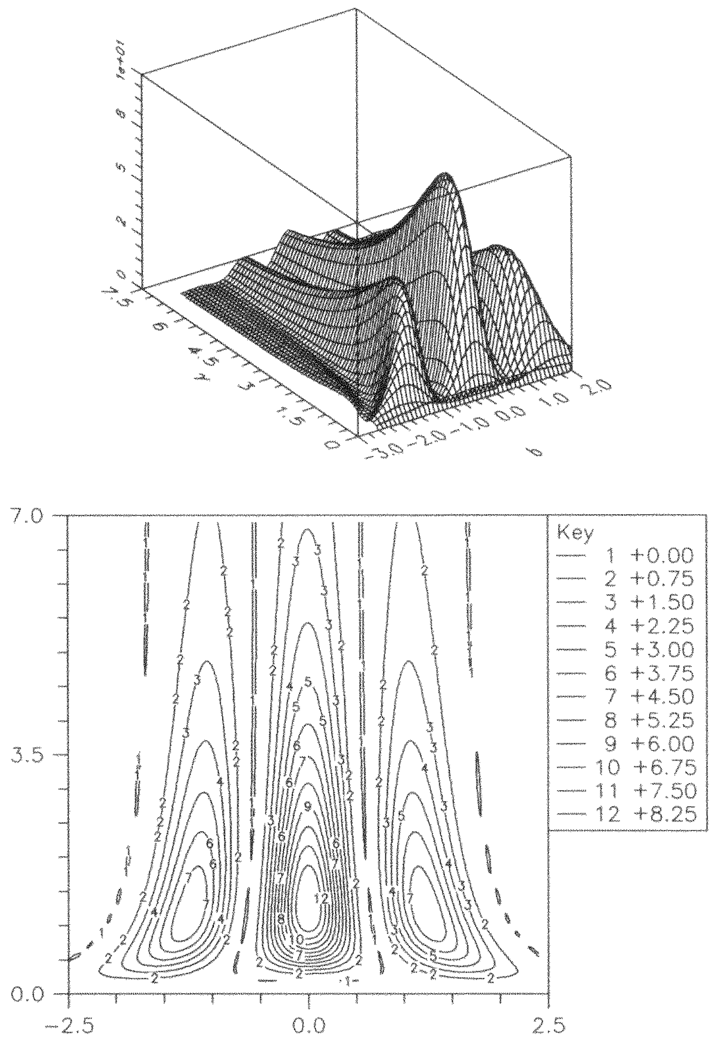

Figure 7. Square of Mexican hat wavelet transform, $W\Psi(a,b)^2$, for the $V(x) = x^2 + x^4$ second excited state.

different matrix structure to that appearing in equation (4.7)

$$
\frac{\partial}{\partial \gamma}\begin{pmatrix} \mu_{\gamma,b}(0) \\ \cdot \\ \mu_{\gamma,b}(i) \\ \cdot \\ \mu_{\gamma,b}(m_s-3) \\ \mu_{\gamma,b}(m_s-2) \\ \mu_{\gamma,b}(m_s-1) \\ \mu_{\gamma,b}(m_s) \end{pmatrix}
$$

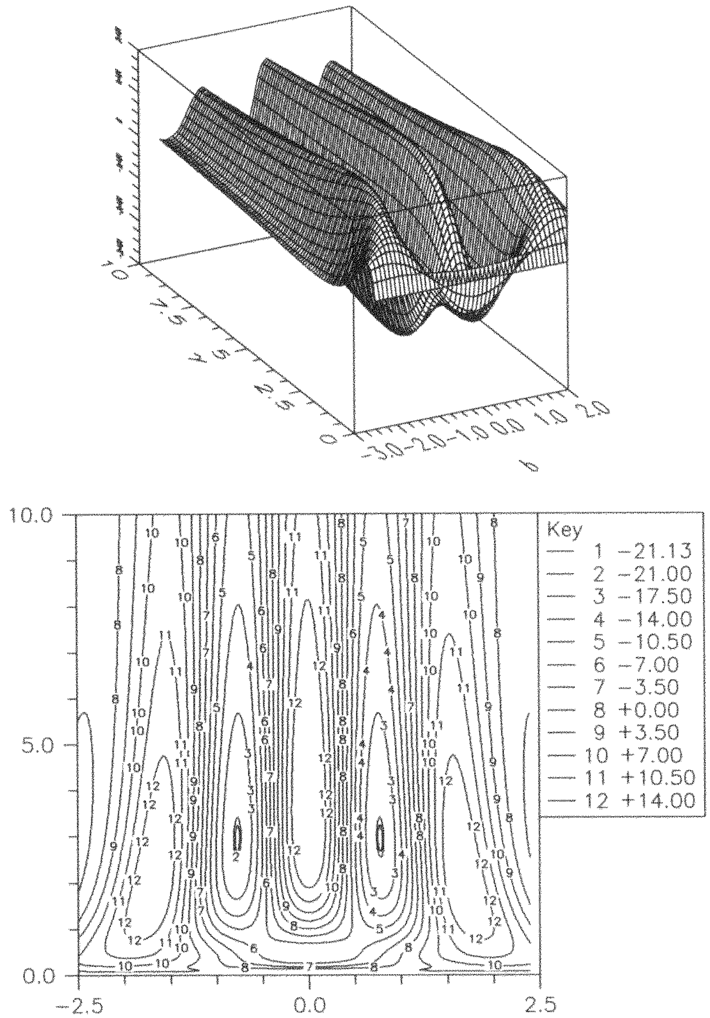

Figure 8. Mexican hat wavelet transform, $W\Psi(a,b)$, for the $V(x) = x^2 + x^4$ fourth excited state.

$$
= -\begin{pmatrix}
0 & 0 & 0 & 0 & 1 & 0 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & \ldots & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \delta_{i,j-4} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots & 1 \\
M^{(4)}_{\gamma,b,E}(m_s+1,0) & . & . & . & . & . & . & M^{(4)}_{\gamma,b,E}(m_s+1,m_s) \\
M^{(4)}_{\gamma,b,E}(m_s+2,0) & . & . & . & . & . & . & M^{(4)}_{\gamma,b,E}(m_s+2,m_s) \\
M^{(4)}_{\gamma,b,E}(m_s+3,0) & . & . & . & . & . & . & M^{(4)}_{\gamma,b,E}(m_s+3,m_s) \\
M^{(4)}_{\gamma,b,E}(m_s+4,0) & . & . & . & . & . & . & M^{(4)}_{\gamma,b,E}(m_s+4,m_s)
\end{pmatrix}
$$

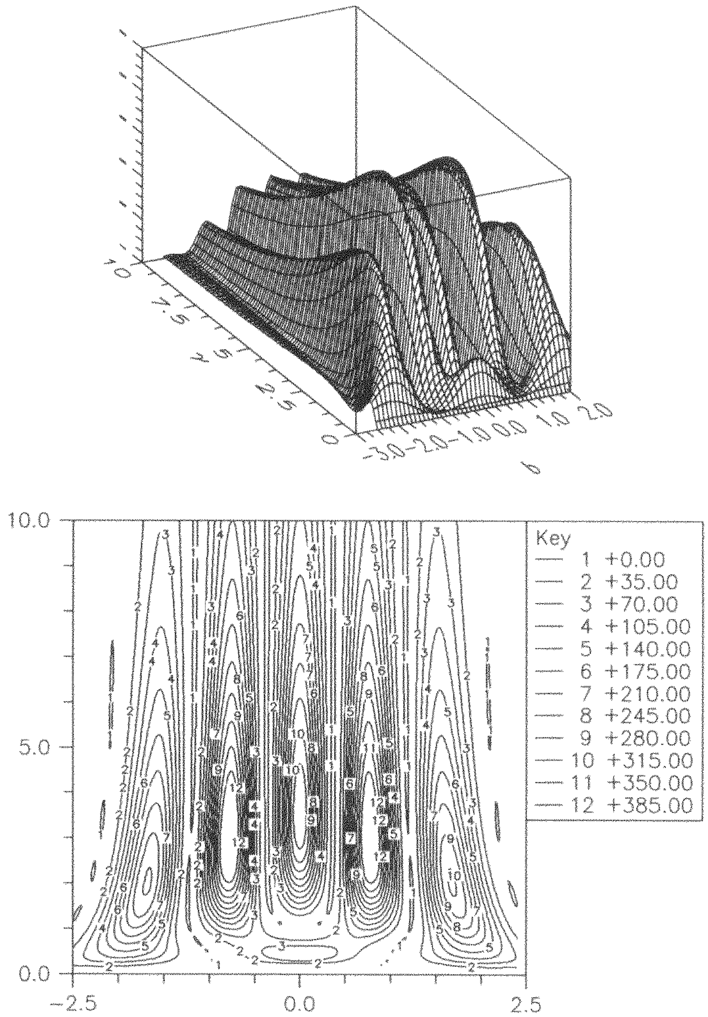

Figure 9. Square of Mexican hat wavelet transform, $W\Psi(a,b)^2$, for $V(x) = x^2 + x^4$ fourth excited state.

$$\times \begin{pmatrix} \mu_{\gamma,b}(0) \\ \cdot \\ \mu_{\gamma,b}(j) \\ \cdot \\ \mu_{\gamma,b}(m_s-3) \\ \mu_{\gamma,b}(m_s-2) \\ \mu_{\gamma,b}(m_s-1) \\ \mu_{\gamma,b}(m_s) \end{pmatrix}. \tag{4.17}$$

The singular nature of the $M^{(4)}_{\gamma,b,E}$ coefficients, for the quartic and sextic anharmonic oscillators, does not affect the fact that the physical moments are analytic for $\gamma > 0$. We can exploit this in order to facilitate the integration of equation (4.17) in the limit $\gamma \to \infty$.

4.2.1. The quartic anharmonic potential and the $-\partial_x^2 e^{-\frac{x^4}{2}}$ wavelet. As noted above, the $\mu_{\gamma,b}(p)$ moments for the quartic anharmonic oscillator will not be analytic at $\gamma = 0$, although they are finite and computable using EMM. However, because of the singular $M^{(4)}_{\gamma,b,E}$ coefficients, we cannot (numerically) integrate equation (4.17) in order to determine the moments at all scales. For this reason, it is preferable to determine the moments for some positive value of γ. We do this for $\gamma = 1$ and determine, using EMM, the $\mu_{1,0}(l)$ (missing) moments. Subsequently, we use equation (4.16) to generate their b-dependence, and then use the $\{\mu_{1,b}(l)|0 \leqslant l \leqslant m_s\}$ in the numerical integration of equation (4.17).

For completeness, we need to be more specific in how we use EMM in this case. Normally, EMM will not work on configurations of the form $\Phi(x) = \mathrm{e}^{-\gamma x^4}\Psi(x)$, where the asymptotic growth of the unphysical states ($\Psi(x) \to \mathrm{e}^{+\sqrt{g}\frac{|x|^3}{3}}$) is slower than the asymptotic decrease of the $\mathrm{e}^{-\gamma x^4}$ factor. Under such conditions, EMM cannot determine the physical energy.

However, if the energy is known *a priori*, then EMM can be used to determine the $\mu_{\gamma,0}(l)$ power moments. For this problem, we can use other EMM re-formulations (Handy 1987) (such as the EMM-$|\Psi|^2$ formulation) to generate the physical energy, and then use the conventional EMM formulation to determine the desired moments. This is the procedure adopted here.

4.2.2. The sextic anharmonic potential and the $-\partial_x^2 e^{-\frac{x^4}{2}}$ wavelet. Again, as noted in the preceding discussion, the $\mu_{\gamma,b}(p)$ moments for the sextic anharmonic oscillator are analytic at $\gamma = 0$. We can use EMM to determine the $\mu_{0,0}(l)$'s (missing moments), followed by the generation of the $\mu_{0,b}(l)$'s, and then the integration of equation (4.17), in order to determine the moments at all scales. However, the singular nature of the $M^{(4)}_{\gamma,b,E}$ coefficients (at $\gamma = \frac{\sqrt{g}}{4}$) , will complicate the numerical integration of these equations. Nevertheless, since the moments are analytic at $\gamma = \frac{\sqrt{g}}{4}$, we can develop a perturbative analysis there.

We can use EMM to determine the moments $\{\mu_{\frac{\sqrt{g}}{4},0}(p)|0 \leqslant p \leqslant 30\}$, as well as the $\{\mu_{\frac{\sqrt{g}}{4},b}(p)|0 \leqslant p \leqslant 30\}$ moments (through b-integration of equation (4.16)), and then approximate the moments for $\gamma = \frac{\sqrt{g}}{4} + \delta\gamma$ through the power series expansion:

$$
\begin{aligned}
\mu_{\frac{\sqrt{g}}{4}+\delta\gamma,b}(p) &= \int \mathrm{d}x\, x^p \exp\left(-\delta\gamma x^4 - \frac{\sqrt{g}}{4}x^4\right)\Psi(x+b) \\
&= \int \mathrm{d}x\, x^p \left(\sum_{i=0} \frac{(-\delta\gamma\ x^4)^i}{i!}\right)\exp\left(-\frac{\sqrt{g}}{4}x^4\right)\Psi(x+b) \\
&= \sum_{i=0} \frac{(-\delta\gamma)^i}{i!}\mu_{\frac{\sqrt{g}}{4},b}(p+4i).
\end{aligned}
\tag{4.18}
$$

The above expansion enables us to determine the missing moments at some $\gamma = \frac{\sqrt{g}}{4}+\delta\gamma$, sufficiently far from the singular point, from which to integrate equation (4.17) in the $\gamma \to \infty$ limit. For the case $m = g = 1$ we can take $\delta\gamma = 0.1$ (for $|b| \leqslant 2$).

4.2.3. The octic anharmonic potential and the $-\partial_x^2 e^{-\frac{x^4}{2}}$ wavelet. For the octic anharmonic oscillator, none of the above complications is present. Accordingly, we can determine the $\mu_{0,0}(l)$'s, generate the $\mu_{0,b}(l)$'s, and proceed to numerically integrate the corresponding version of equation (4.17). We implemented the various numerical approaches outlined above. The plots for the ground state wavefunction, for all three cases, are depicted in

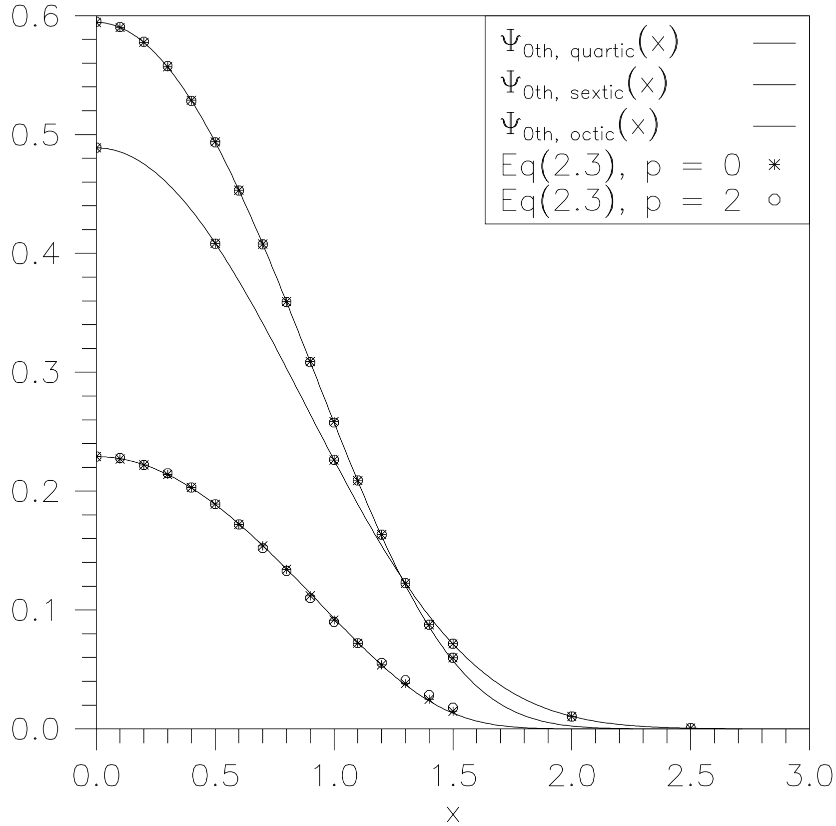

Figure 10. MQ—$\partial_x^2 e^{-\frac{x^4}{2}}$ reconstruction for $V(x) = x^2 + x^{2q}$, $q = 1, 2, 3$.

figure 10. The results are excellent. Again, we used the quartic wavelet counterpart to the asymptotic expansion in equation (4.9), or:

$$\begin{aligned}\mu_{\gamma,b}(p) &= \int_{-\infty}^{\infty} \mathrm{d}x\, x^p e^{-\gamma x^4} \Psi(x+b) \\ &= \frac{1}{\gamma^{\frac{1+p}{4}}} \int_{-\infty}^{\infty} \mathrm{d}y\, y^p e^{-y^4} \Psi\left(\frac{y}{\gamma^{\frac{1}{4}}} + b\right) \\ &= \frac{1}{\gamma^{\frac{1+p}{4}}} \sum_{n=0} \frac{\nu_4(p+n)}{n!} \gamma^{-\frac{n}{4}} \Psi^{(n)}(b)\end{aligned} \tag{4.19}$$

where $\Psi^{(n)}(b) \equiv \partial_b^n \Psi(b)$ and $\nu_4(p+n) = \int_{-\infty}^{\infty} \mathrm{d}y\, y^{(p+n)} e^{-y^4}$.

For the quartic wavelet, we have $\nu_4(0) = 1.8128$, while $\nu_4(2) = 0.612\,708$. An important distinction between the above expansion and that for the Mexican hat case (equation (4.9)) is that for $p =$ even, one is working with inverse powers of $\sqrt{\gamma}$. An analogous numerical analysis to that in equation (4.10) was implemented, leading to the excellent results depicted in figure 10.

For the quartic wavelet case, we did not investigate the excited states. These can also be studied through the methods presented for the excited states in the Mexican hat wavelet formulation.

5. Conclusion

We have established that MQ, in the context of rational fraction Schrödinger potentials, is equivalent to CWT theory. The rescaled and translated power moments, $\mu_{\alpha,b}(p)$, satisfy a simple finite set of coupled, first-order, differential equations in $\alpha \equiv \frac{1}{a}$, enabling their generation to arbitrary scale, a, as well as the generation of the desired continuous wavelet transform. Knowledge of the latter, combined with appropriate dyadic reconstruction formulae, allow us to approximate the desired solution. Prior studies by HM show that this approach can lead to poor results because only dyadic scale information ($a = 2^m$ and $b = n2^m$) can only be sampled. A better approach is to use equation (2.3) to recover the desired solution. However, this manifestly nonwavelet-based result, is in fact equivalent to a wavelet-based reconstruction analysis in which all scales and translations ($0 \leqslant \frac{1}{a} < \infty, -\infty < b < \infty$) are involved (as shown in section 3). Indeed, the important (group-theory based) signal-wavelet reconstruction formula given in equation (3.6*b*), is a straightforward result motivated by desiring a more global interpretation of equation (2.3). While the determination of the energy is, essentially, an infinite scale ($a = \infty$) result (achived through the use of such methods as the EMM), the recovery of the corresponding wavefunction ensues from a multiscale analysis proceeding from $a = \infty$ to $a = 0$, through the aforementioned reconstruction analysis.

We applied this formalism to important anharmonic potentials, including the quartic, sextic and octic anharmonic oscillators, and examined the first three symmetric states in each case. Excellent results were achieved in all cases. Also, in contrast to the previous HM formulations, we examined the consequences of the formalism with respects to various mother wavelet functions, including the *Mexican hat* wavelet, and those based on $Q(x) = -\frac{1}{2}x^4$.

Acknowledgments

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Appendix

It is a well known theorem that the bosonic ground state wavefunction, in any dimension, must be of uniform signature, and can be taken to be positive ($\Psi_{\mathrm{gr}} > 0$). Accordingly, there should be an intimate relationship between MQ of the ground state and the classic moment problem (Shohat and Tamarkin 1963, Akhiezer 1965). This is exploited in the EMM approach (Handy and Bessis 1985, Handy *et al* 1988a, b). Specifically, the bosonic ground state energy, E_{gr}, and normalized missing moments, $\{\mu_{0,0}(l) | 1 \leqslant l \leqslant m_s\}$, are determined by imposing the infinite set of constraints arising from the moment problem:

$$\int_{-\infty}^{\infty} \mathrm{d}x \left(\sum_{i=0}^{N} c_i' x^i \right)^2 \Psi_{\mathrm{gr}}(x) > 0 \qquad \text{(A.1)}$$

for $N < \infty$, and arbitrary c_i''s. Alternatively, in terms of the moments, we obtain the quadratic form inequalities

$$\sum_{i=0}^{N}\sum_{j=0}^{N} c_i'\mu_{0,0}(i+j)c_j' > 0. \tag{A.2}$$

Substituting the missing moment dependence from equation (2.5), one obtains

$$\sum_{l=0}^{m_s}\mu_{0,0}(l)\left[\sum_{i=0}^{N}\sum_{j=0}^{N} c_i' M_{0,0,E}(i+j,l)c_j'\right] > 0. \tag{A.3}$$

Imposing the normalization in equation (2.6), $\mu_{0,0}(0) = 1 - \sum_{l=1}^{m_s}\mu_{0,0}(l)$, an (uncountably) infinite set of linear inequalities are obtained constraining the missing moments and (implicitly) the energy:

$$\sum_{l=1}^{m_s}\mathcal{A}[E;c',l]\mu_{0,0}(l) < \mathcal{B}[E;c'] \qquad \text{for all } c_i's \tag{A.4}$$

where $\mathcal{A}[E;c',l] \equiv \sum_{i=0}^{N}\sum_{j=0}^{N} c_i'[M_{0,0,E}(i+j,0) - M_{0,0,E}(i+j,l)]c_j'$, and $\mathcal{B}[E;c'] \equiv \sum_{i=0}^{N}\sum_{j=0}^{N} c_i' M_{0,0,E}(i+j,0)c_j'$. We denote the polytope solution to equation (A.4) by $\mathcal{U}_N(E)$.

These infinitely many linear inequalities are equivalent to a finite number of nonlinear inequalities (in the missing moments) as defined by the corresponding set of Hankel–Hadamard determinantal inequalities (also arising from the moment problem)

$$\Delta_{0,N}[\mu_{0,0}(p)] = \Delta_{0,N}[E,\mu_{0,0}(1),\ldots,\mu_{0,0}(m_s)] > 0 \tag{A.5}$$

where

$$\Delta_{0,N}[\mu_{0,0}(p)] \equiv \mathrm{Det}\begin{pmatrix} \mu_{0,0}(0) & \mu_{0,0}(1) & \ldots & \mu_{0,0}(N) \\ \mu_{0,0}(1) & \mu_{0,0}(2) & \ldots & \mu_{0,0}(N+1) \\ . & . & \ldots & . \\ \mu_{0,0}(N) & \mu_{0,0}(N+1) & \ldots & \mu_{0,0}(2N) \end{pmatrix} \tag{A.6}$$

and $N \to \infty$.

The missing moments of the physical, bosonic, ground state wavefunction must satisfy either equation (A.4) or (equivalently) equation (A.5). In the original EMM formulation (Handy and Bessis 1985), the determinantal inequalities were used on problems of missing moment order no greater than two ($m_s \leqslant 2$). However, for problems with larger numbers of missing moments (in particular, all multidimensional Schrödinger equation problems involve an infinite hierarchy of missing moments, $m_s \to \infty$) one must adopt the linear formulation represented by equation (A.4). In this case, practical demands require the identification of an optimal, finite number of c' vectors that can quickly tell us, for a given E value, if equation (A.4) has no solution, $\mathcal{U}_N(E) = \{\emptyset\}$. This is done through the combination of linear programming (Chvatal 1983) and the deployment of a 'cutting method' developed by Handy and co-workers (Handy *et al* 1988a, b). This approach, to given order N, generates a feasibility energy interval $(E_N^{(L)}, E_N^{(U)})$ which contains the true ground state energy, $E_N^{(L)} \leqslant E_{\mathrm{gr}} \leqslant E_N^{(U)}$. As $N \to \infty$, the lower and upper bounds converge (geometrically) to the physical solution: $\mathrm{Lim}_{N\to\infty}E_N^{(L)} = E_{\mathrm{gr}} = \mathrm{Lim}_{N\to\infty}E_N^{(U)}$. Also, the size of the corresponding feasible polytope, $\mathcal{U}_N(E)$, for $E \in [E_N^{(L)}, E_N^{(U)}]$, reduces as well, as $N \to \infty$. Only for the correct physical energy, E_{gr}, will $\mathrm{Lim}_{N\to\infty}\mathcal{U}_N(E_{\mathrm{gr}}) = \{\mu_{\mathrm{gr}}(1),\ldots,\mu_{\mathrm{gr}}(m_s)\}$.

Numerous examples have been published since the linear programming-based EMM formalism was developed in 1988, establishing the power of the method. This approach was used to yield the first converging, eigenenergy bounding, analysis for the famous, and highly singular, three-dimensional problem: the *quadratic Zeeman effect for superstrong magnetic fields* (Handy *et al* 1988a, b).

Although the preceding discussion focused on the bosonic ground state, one can extend the same formalism to excited states provided one works with the representation $(\Psi(x)+c)R(x)$, where c is a sufficiently positive constant ensuring that $\Psi_{\rm excited}(x)+c \geqslant 0$ (empirically determined), and the reference function, $R(x)$, is appropriately chosen in accordance with the zeroth-order asymptotic form of the physical solution. This is explained in the work by Handy and Lee (1991).

Of special importance to the philosophy presented at the outset is the fact that the above inequality constraints automatically take into account all necessary scale and translation parameter variations. That is, the polynomial $P_{N;\tilde{c}}(x) \equiv \sum_{i=0}^{N} c_i x^i$, under an arbitrary affine transformation $P_{N;\tilde{c}}(\frac{x-b}{a})$, will become another Nth-degree polynomial with different c-coefficient values, $P_{N;\tilde{c}}(\frac{x-b}{a}) = \sum_{i=0}^{N} c_i' x^i$. However, these are automatically sampled in the variational implementation of equation (A.1). The same holds for more general sums, $\sum_\eta P_{N;\tilde{c}_\eta}(\frac{x-b_\eta}{a_\eta})$. Accordingly, equation (A.1) is equivalent to working with

$$\int_{-\infty}^{\infty} \mathrm{d}x \left(\sum_\eta P_{N;\tilde{c}_\eta}\left(\frac{x-b_\eta}{a_\eta}\right)\right)^2 \Psi_{\rm gr}(x) > 0 \qquad \text{(A.7)}$$

for arbitrary c, a, b variational parameters. Of course, equation (A.1) is a better formulation since the nonlinear appearance of the a, b parameters in equation (A.7) is assimilated through the linear contribution of the c''s.

This should be contrasted with an alternate variational prescription, such as the traditional Rayleigh–Ritz approach, wherein explicit translation and scale variables, $\{a_\eta, b_\eta\}$, should be introduced within the basis set, $\mathcal{B}_i(x)$ (i.e. Gaussians, etc), in addition to the usual variational coefficients:

$$E_{\rm gr} < \mathrm{Min}_{c,a,b} \frac{\langle \sum_{\eta,i} c_{\eta,i}\mathcal{B}_i(\frac{x-b_\eta}{a_\eta})|H|\sum_{\eta,j} c_{\eta,j}\mathcal{B}_j(\frac{x-b_\eta}{a_\eta})\rangle}{\langle \sum_{\eta,i} c_{\eta,i}\mathcal{B}_i(\frac{x-b_\eta}{a_\eta})|\sum_{\eta,j} c_{\eta,j}\mathcal{B}_j(\frac{x-b_\eta}{a_\eta})\rangle}. \qquad \text{(A.8)}$$

The contribution of the linear c variables remains distinct from that of the nonlinearly contributing a_η, b_η variational parameters.

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