Wavelets in curvilinear coordinate quantum calculations: $\text{H}_2^+$ electronic states

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Abstract

Multiscale wavelets are used to solve the quantum eigenvalue equations for the hydrogen molecular ion $\text{H}_2^+$ in the Born-Oppenheimer approximation. Normally restricted to Cartesian systems, "wavelets on the interval" (a normal wavelet family augmented by special edge functions) have recently been applied to such boundary value problems as the hydrogen atom in spherical polar coordinates [J. Mackey, et al., J. Comp. Phys. 168, 356 (2001)]. These methods are extended here to ground and excited electronic states of the simplest molecule, for which the electronic Hamiltonian is separable in confocal elliptic coordinates. The set of curvilinear coordinate quantum systems for which wavelet bases have been applied is thus enlarged.
I. Introduction

There is strong interest in the adaptation of wavelet methods to the solution of differential equations. Wavelet basis functions are indexed by both location and scale and can be chosen to provide different levels of resolution in different places. This advantage has great appeal for problems exhibiting large dynamic ranges. A number of papers have investigated wavelet use in quantum mechanical problems,\textsuperscript{1-18} though this technology is only in the early stages of development. In the case of orthogonal compact support wavelets, for instance, it is only very recently that it has been shown possible to solve the standard hydrogen atom problem to more than a few decimal places.\textsuperscript{18} This relied upon an extension of wavelets from the usual Cartesian variables\textsuperscript{19} to spherical polar coordinates in terms of which the hydrogenic Hamiltonian is separable. The simplest molecular example, the hydrogen molecular ion H\textsubscript{2}\textsuperscript{+} with fixed nuclei, is examined in the present paper. The electronic Hamiltonian in the Born-Oppenheimer approximation is well-known to separate in confocal elliptic (or spheroidal) coordinates,\textsuperscript{20} a consequence of the existence of an extra constant of the motion for the two-center Kepler problem.\textsuperscript{21,22} We will demonstrate that systematic accuracy can be obtained for this problem using wavelets expressed in these coordinates, and thereby provide another benchmark for wavelet-based quantum calculations.

There are many different wavelet families, the best choice to use in any given problem remaining an open question. We focus here on those wavelets possessing orthogonality as well as compact support, i.e., rigorous restriction of each basis function to a specific interval. The prototypical examples are those determined by Daubechies.\textsuperscript{19} All basis functions are generated by different translations and dilations of just two independent functions, the scaling function and the wavelet. Despite the fact that the scaling function and wavelet do not have simple analytic
forms, methods have been developed by which they can be used in numerical applications.\textsuperscript{23,24} It is also possible to extend such methods to multiwavelets, a recent wavelet variant containing more than one scaling function and one wavelet,\textsuperscript{25-32} which can have certain advantages (e.g., symmetry of basis functions, greater localization). In the present paper, as in our recent work,\textsuperscript{18} we choose the multiwavelet family on the interval $[0, 3]$ derived by Chui and Lian\textsuperscript{27} as our primitive basis for calculations. The basis consists of symmetric and antisymmetric pairs of functions, a fact which is useful in avoiding any left-versus-right bias in calculations. This family has better function approximation properties than either the Chui-Lian or Geronimo, et al.,\textsuperscript{25,26} families on the interval $[0, 2]$. Still better capabilities can be obtained by using even longer multiwavelets. The current choice represents a compromise between better function approximation and shorter length (tighter localization). The choice is not critical, however, and it is anticipated that a variety of different single- and multi-wavelet families will eventually be used and compared in Hamiltonian calculations.

A key issue for the solution of boundary conditions on wave functions expressed in curvilinear coordinates is that the calculations proceed on finite or semi-infinite intervals. For Daubechies wavelet families, adaptation to fixed intervals was enabled several years ago by defining special scaling functions and wavelets to be used near the interval edges.\textsuperscript{33-38} Such an approach also generalizes to multiwavelets,\textsuperscript{18,39} and was used in the case of the hydrogen atom to accommodate the cusp conditions that must be satisfied by the hydrogenic wave functions.\textsuperscript{40} We use the same interval version of the Chui-Lian multiwavelets for the current investigation of $\text{H}_2^+$. Given the basis development made before, the calculations proceed relatively straightforwardly for $\Sigma$ states. For states with higher orbital angular momenta, the electronic Hamiltonian exhibits singularities at the edges of the elliptic coordinate ranges, the boundary conditions there
requiring special handling. Despite the complicating presence of the singularities, all of the required integrals are finite and can be evaluated by an adaptive wavelet quadrature similar to one discussed before for orthogonal wavelets on a Cartesian axis. An assessment of this direct multiscale method of calculation versus one in which the singularities are first removed is made here.

The development of wavelet technology for differential equations is of broader value than these simple eigenvalue calculations (which can be performed more efficiently through other specific algorithms). Localized treatment of spatial resolution can be of just as much value for nuclear coordinates, for time-dependent linear or nonlinear Schrödinger equations, for density matrices, and for a great number of applications outside of quantum mechanics. It is a reasonable hope that wavelet-based solvers for differential equations may be produced that are highly adaptive and highly automated. The potential robustness of such codes is reflected in part in the variety of different problems to which wavelet methods can be successfully applied.

II. \( \text{H}_2^+ \) Electronic Hamiltonian

The Schrödinger equation for electronic motion in the hydrogen molecular ion \( \text{H}_2^+ \) under the Born-Oppenheimer approximation takes the form

\[
\left[ -\frac{\hbar^2}{2\mu_r} \nabla_r^2 + V(R,r) - E(R) \right] \Psi_{el}(r;R) = 0,
\]

where \( \mathbf{R} \) is the internuclear vector and \( \mathbf{r} \) is the Jacobi vector from the nuclear center of mass to the electron. The reduced mass \( \mu_r \) is that of the electron and the combined system of two protons. \( V \) is the potential due to the electron-proton attractions, and the electronic wave function \( \Psi_{el}(r;R) \) depends only parametrically upon the bond length \( R \). Letting \( r_1 \) and \( r_2 \) be the distances
between the electron and the two protons, one may transform to an angle \( \varphi \) about the bond and confocal elliptic coordinates\(^{20}\)

\[
\mu = \frac{r_2 - r_1}{R}, \quad -1 \leq \mu \leq 1, \quad (2)
\]

\[
\nu = \frac{r_1 + r_2}{R}, \quad 1 \leq \nu < \infty. \quad (3)
\]

The angular portion of the wave function may be separated immediately by setting

\[
\Psi_{el}(r; R) = X_m(\nu, \mu; R) \frac{1}{\sqrt{2\pi}} e^{i m \varphi}, \quad (4)
\]

which brings Eq. (1) to the form

\[
\left\{ -\frac{2\hbar^2}{\mu R^2 (\nu^2 - \mu^2)} \left[ \frac{\partial}{\partial \nu} \left( \nu^2 - 1 \right) \frac{\partial}{\partial \nu} + \frac{\partial}{\partial \mu} \left( 1 - \mu^2 \right) \frac{\partial}{\partial \mu} - \frac{m^2}{\nu^2 - 1} - \frac{m^2}{1 - \mu^2} \right] \right.
\]

\[
- \frac{4e^2 \nu}{R (\nu^2 - \mu^2)} - E(R) \right\} X_m(\lambda, \mu; R) = 0, \quad (5)
\]

with \( X_m \) normalized according to

\[
\int_1^\infty d\nu \int_1^{-1} d\mu \left( \nu^2 - \mu^2 \right) |X_m(\nu, \mu; R)|^2 = 1. \quad (6)
\]

Multiplying Eq. (5) by the Jacobian factor \( (\nu^2 - \mu^2) \), Eq. (5) can be written as

\[
\left( H_\mu + H_\nu \right) X_m(\nu, \mu; R) = 0., \quad (7)
\]

with the 1D Hamiltonian-like operators

\[
H_\mu = -\frac{\partial}{\partial \mu} \left( 1 - \mu^2 \right) \frac{\partial}{\partial \mu} + \frac{m^2}{1 - \mu^2} + \frac{\mu R^2 E(R)}{2\hbar^2} \mu^2, \quad (8)
\]

\[
H_\nu = -\frac{\partial}{\partial \nu} \left( \nu^2 - 1 \right) \frac{\partial}{\partial \nu} + \frac{m^2}{\nu^2 - 1} + \frac{2\mu e^2 R}{\hbar^2} \nu - \frac{\mu R^2 E(R)}{2\hbar^2} \nu^2. \quad (9)
\]
Equation (7) is an eigenvalue problem with eigenvalue zero. The operator $H_{\nu} - H_{\mu}$, which clearly commutes with $H_{\mu} + H_{\nu}$, may be simultaneously diagonalized and is related to the constant of the motion discussed by Erikson and Hill$^{21}$ and Coulson and Joseph$^{22}$. If the eigenvalue of $H_{\nu} - H_{\mu}$ is denoted $2A$, and the wave function $X_m$ is written in the separable form

$$X_m(\nu, \mu; R) = Y_m(\mu; R) Z_m(\nu; R),$$

then $A$ plays the role of a separation constant for the two elliptic coordinates,

$$\left( H_{\mu} + A \right) Y_m(\mu; R) = 0,$$
$$\left( H_{\nu} - A \right) Z_m(\nu; R) = 0.$$

Many investigations$^{20,41-45,49}$ over the years have dealt with the semianalytical and numerical solution of the combined set of Eqs. (11) and (12) for both the ground $^1\Sigma_g^+$ $(m = 0)$ and excited states. Eigensolutions require simultaneous quantization of $A$ and $E$ or, equivalently, $A$ and $p$ where

$$p^2 = -\frac{\mu R^2 E(R)}{2\hbar^2}. \tag{13}$$

One may first choose a value for $p$ (i.e., the combination $R^2E$) and solve Eq. (11) for $A$. The same value of $p$ may then be used in Eq. (12) and the value of $R$ found which produces the same value of $A$. In the following, atomic units for which $\mu_r = e = \hbar = 1$ are used.

III. Multiwavelets on the Interval

The Chui-Lian multiwavelet family used here is constructed from two scaling functions and two wavelet functions which are conveniently arranged as column vectors

$$\phi(x) = \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \end{pmatrix}, \quad \psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}. \tag{14}$$

7
All four components are unit-normalized and vanish outside the interval $0 \leq x \leq 3$. Those with subscript 1 are symmetric and those with subscript 2 are antisymmetric around the midpoint $x = 3/2$. The scaling functions may be expressed as linear combinations of copies of themselves squeezed to half their original widths and shifted by multiples of 1/2,

$$\phi(x) = \sum_{k=0}^{3} c_k \cdot \phi(2x - k),$$

(15)

where $c_k$ is a 2 by 2 constant matrix. The wavelets may similarly be expressed as linear combinations of the same shifted and squeezed scaling functions

$$\psi(x) = \sum_{k=0}^{3} d_k \cdot \phi(2x - k).$$

(16)

These relations between functions on neighboring octaves are simply matrix versions of those appearing for standard "scalar" or "single" cases such as Daubechies wavelets, corresponding to lowpass and highpass filtering operations respectively.

Unit normalized functions at different scales and locations are defined by

$$\phi_{j\alpha}(x) = 2^{j/2} \phi_\alpha \left(2^j x - k\right), \quad \psi_{j\alpha}(x) = 2^{j/2} \psi_\alpha \left(2^j x - k\right), \quad \alpha = 1,2.$$  

(17)

On each scale $j$, all of these functions are orthogonal. Let us assume that, for a sufficiently fine scale $j = J$, a function $f(x)$ may be approximately expanded in terms of scaling functions

$$f(x) = \sum_{k=-\infty}^{\infty} \sum_{\alpha=1}^{2} \left< \phi_{J\alpha}, f \right> \phi_{J\alpha}(x)$$

(18)

with an error depending on the level of resolution. The sequences of scaling functions shown in the center of Fig. 1 provide an example of such a basis for $J = 0$. For higher $J$, the density of basis functions is increased and the error in the function approximation is strongly reduced. The fineness of resolution required is determined by the specific structure of $f(x)$ and may be
decided, for instance, by setting a threshold of maximum error to be met by the series approximation.

One may repeatedly trade scaling functions at one scale for a combination of scaling functions and wavelets at the next coarsest scale [cf., Eqs. (15) and (16)]. The new scaling functions represent an averaging (lowpass filtering) of the old, whereas the wavelets represent detail lost (highpass filtering) in the averaging. The orthogonal wavelet subspace is exactly complementary to the coarser scaling function subspace in the sense that their direct sum is equal to the original (finer) scaling function subspace. That is to say, the wavelet transform between different scales is orthogonal and invertible. If this process is iterated to a coarsest level \( j = j_0 \), the resulting basis contains scaling functions at \( j = j_0 \) and wavelets at all \( j \) between \( j_0 \) and \( J - 1 \),

\[
f(x) \approx \sum_{k=-\infty}^{\infty} \sum_{\alpha=1}^{2} \langle \phi_{j_0 k \alpha} \mid f \rangle \phi_{j_0 k \alpha}(x) + \sum_{j=j_0}^{J-1} \sum_{k=-\infty}^{\infty} \sum_{\alpha=1}^{2} \langle \psi_{j k \alpha} \mid f \rangle \psi_{j k \alpha}(x).
\]  

The wavelet contributions allow one to keep track of the differences in detail between adjacent levels of resolution of the scaling functions. Such a multiresolution expansion is exactly equivalent to the single resolution expansion if all values of \( k \) are retained, but gains a great advantage when \( k \) is restricted to specific regions. It then becomes possible to throw out the high levels of detail (wavelets) in regions where \( f(x) \) is relatively smoothly varying while keeping them where it is not. In practical calculations, this is accomplished very simply by discarding all the (orthogonal and linearly independent) wavelet basis functions for which the magnitudes of the expansion coefficients \( \langle \psi_{j k \alpha} \mid f \rangle \) fall below a preset threshold. One thus obtains a compressed representation, and the degree of compression can become very significant when \( f(x) \) has a large dynamic range. (The coarsest scale \( j_0 \) can be chosen to be that for which further steps of the wavelet transform provide no further compression, i.e., all or most of the \( \langle \psi_{j_0 k \alpha} \mid f \rangle \)
have magnitudes greater than the threshold.) This character of wavelet bases is widely exploited in signal and image processing and holds promise for application to the solution of differential equations.

The regions on which neighboring basis functions are nonzero are staggered. It is awkward to use such wavelet bases confined an interval with a definite edge or edges. One generally needs all functions approaching and straddling an edge in order to retain the full function approximation power of the wavelet basis throughout the interval. The presence of tails of basis functions outside the interval, however, is a severe complication and especially at the coarsest scales where the outside tails are widest. One answer appropriate to approximation of functions with periodic boundary conditions is to use periodized wavelet bases which wrap around the boundary. In the general case, however, this is not appropriate since periodization compromises part of the localized behavior for which wavelets were initially developed. Instead, functions \( \Phi_{jn}^L, \Phi_{jn}^R, \Psi_{jn}^L, \Psi_{jn}^R \) covering the regions near the left (\( L \)) and right (\( R \)) edges are defined which are merged with a set of inner functions made up of the standard Chui-Lian multiscaling functions and multiwavelets. The edge functions for level \( j \) are scaled and renormalized copies of those for level 0,

\[
\Phi_{jn}^L(x) = 2^{j/2} \Phi_{0n}^L(2^j x) = 2^{j/2} \Phi_n^L(2^j x),
\]

etc. The left-hand edge functions satisfy modified recursion relations

\[
\Phi_n^L(x) = \sum_{n'=n}^2 A_{nn'} \Phi_{n'}^L(2x) + \sum_{k=1}^3 \sum_{\alpha=1}^2 B_{nk\alpha} \phi_{\alpha} (2x-k),
\]

\[
\Psi_n^L(x) = \sum_{n'=n}^2 F_{nn'} \Phi_{n'}^L(2x) + \sum_{k=1}^3 \sum_{\alpha=1}^2 G_{nk\alpha} \phi_{\alpha} (2x-k),
\]

where \( n = 0, 1, 2, A \) and \( F \) are upper-triangular matrices, \(^{18}\) and the collected coefficient matrices satisfy \( I_3 \) is the 3D identity matrix)
\[ \mathbf{A} \cdot \mathbf{A}^T + \mathbf{B} \cdot \mathbf{B}^T = 2 \mathbf{I}_3, \]  
(23)

\[ \mathbf{F} \cdot \mathbf{F}^T + \mathbf{G} \cdot \mathbf{G}^T = 2 \mathbf{I}_3, \]  
(24)

\[ \mathbf{F} \cdot \mathbf{A}^T + \mathbf{G} \cdot \mathbf{B}^T = 0. \]  
(25)

The edge functions are unit-normalized as well as orthogonal to each other and to all inner functions on the same scale. They are designed so that \( \Phi_n^L \) and \( \Psi_n^L \) behave as \( x^n \) as \( x \to 0 \), a property which proves useful in satisfying boundary conditions (see below). The edge functions on the right are just reflections of those on the left, as shown for scale 0 in Figs. 1 and 2.

The single-scale expansion of a function within the interval now takes the form,

\[
f(x) = \sum_{n=0}^{2} \langle \Phi_j^L | f \rangle \Phi_j^L(x) + \sum_k \sum_{\alpha=1}^{2} \langle \phi_{jka} | f \rangle \phi_{jka}(x) + \sum_{n=0}^{2} \langle \Phi_j^R | f \rangle \Phi_j^R(x),
\]
(26)

whereas the multi-resolution approximation is given by (take \( j_0 = 0 \) for simplicity)

\[
f(x) = \sum_{n=0}^{2} \langle \Phi_0^L | f \rangle \Phi_0^L(x) + \sum_k \sum_{\alpha=1}^{2} \langle \phi_{0ka} | f \rangle \phi_{0ka}(x) + \sum_{n=0}^{2} \langle \Phi_0^R | f \rangle \Phi_0^R(x)
+ \sum_{j=0}^{J-1} \sum_{n=0}^{2} \langle \Psi_j^L | f \rangle \Psi_j^L(x) + \sum_{j=0}^{J-1} \sum_{k=1}^{2} \sum_{\alpha=1}^{2} \langle \psi_{jka} | f \rangle \psi_{jka}(x) + \sum_{j=0}^{J-1} \sum_{n=0}^{2} \langle \Psi_j^R | f \rangle \Psi_j^R(x).
\]
(27)

The sums over \( k \) run over those values for which the inner functions do not touch the edges. The incorporation of the edge functions allows the contributions from each scale to be restricted to the interval. Both the inner and edge wavelets are designed to be orthogonal to quadratic or lower-order polynomials. In the special case that \( f(x) \) is a quadratic polynomial, then, all wavelet expansion coefficients \( \langle \Psi_{jn}^L | f \rangle, \langle \psi_{jka} | f \rangle, \langle \Psi_{jn}^R | f \rangle \) in Eq. (27) vanish and only the scaling function contributions in the first line survive. Quadratic polynomials are thus exactly represented throughout the interval by scaling functions alone.
IV. Σ States (m = 0)

For states with $m = 0$, e.g., the ground $1s\sigma_g$ state, the matrices for $H_\mu$ and $H_\nu$ within level-$j$ scaling function bases may be constructed straightforwardly using the results of Mackey, et al.\textsuperscript{18} In that work, matrix elements of differential operators and simple powers of $x$ are evaluated for the full interval basis. (Modifications to the kinetic energy matrix discussed there are not made in the present work.)

Using atomic units, the ground state at $R = 2$ has energy $E = -0.6026342144949$ and separation constant $A = 0.8117295846248$.\textsuperscript{45,46} From Eq. (13), this yields $p = 1.4850146224835$. We first consider calculations for $H_\mu$ using only a set of scaling functions on a single scale. If the $k$-index runs from 1 to $k_{\text{max}}$, there are $2k_{\text{max}}$ inner functions and 6 edge functions. The total interval of length 2 is thus broken into $k_{\text{max}} + 4$ subintervals, yielding a basis spacing of $2/(k_{\text{max}} + 4)$. Table 1 shows the error in the calculation of the separation constant $A$ for a series of consecutive decreases-by-two in the spacing. It is seen that the error diminishes by factors of 16-21 over this range for each decrease in spacing (fourth order error in the spacing). Thus the multiscaling functions on the interval provide a systematically improvable basis for eigenvalue calculations here, as demonstrated before\textsuperscript{18} in the case of the Legendre equation (the $p = 0$ limit of the eigenvalue equation for $\mu$).

Turning to the equation for $\nu$, the matrix elements for $H_\nu$ with $m = 0$ are also immediately obtainable from the previous work. The primary difference is that the interval is semi-infinite, ranging from $\nu = 1$ to $\nu = \infty$. In practice, a finite interval is used which extends to sufficiently large $\nu$ that the eigenvalue is insensitive to the location of the right-hand edge, at which point the wave function is very small. Table 2 shows (for three different values of basis function spacings) the convergence of the eigenvalues with increasing upper cutoff $\nu_{\text{max}}$. For
each consecutive value of \( \nu_{\text{max}} \), the only change is that new inner functions are added between the previous set and the right-hand (outer) edge functions. It is seen that \( \nu_{\text{max}} = 15 \) is uniformly adequate for the precision to which the exact separation constant is specified. Convergence with respect to increase in resolution (decrease in spacing) is then examined in Table 3 for \( \nu_{\text{max}} \) fixed at this value. While more basis functions are required than for the \( H_\mu \) equation, exponential convergence close to the fourth power of the spacing is again found.

Multiresolution bases were then investigated using Eqs. (15), (16), (21) and (22). At each scale used, the wavelet coefficients in the \( H_\mu \) eigenvector were found to be significantly smaller than the scaling function coefficients. Some of the wavelet coefficients were smaller than others, but not dramatically so. This meant that compression advantages were relatively minor, at least using high eigenvalue accuracy as a requirement. This was anticipated since the multiresolution capabilities of wavelet bases will only be important for problems with more significant variations in scale.

Nevertheless, the multiscale calculations revealed an issue that has not been discussed before. The number of edge functions constructed earlier\(^{18}\) was chosen to preserve throughout the interval the approximation order three, i.e., the ability of the scaling functions to exactly represent the three monomial power \( x^i, i = 0, 1, 2 \). This paralleled the choices made for single wavelet families.\(^{34-38}\) Therefore only three additional scaling functions (as well as three associated wavelets) were needed at each edge. While this is clearly adequate for single-scale calculations, the count of functions is less than optimal for use of a multiscale representation. Taking into account that the inner scaling function recursions for scale \( j \) do not use the first and last sets of inner functions on scale \( j+1 \), the total number of values of \( k \) on the two scales turn out to be related by \( k_{\text{max}, j+1} = 2k_{\text{max}, j} + 4 \). Including edges, there are \( 4k_{\text{max}, j} + 14 \) scaling functions
at level $j+1$, while there are $2k_{\text{max},j} + 6$ scaling functions and an equal number of wavelets at level $j$, that is, $4k_{\text{max},j} + 12$ total. Thus, there are two more basis functions required on the finer scale than on the coarser. A use of the highpass and lowpass filters contracts the basis and prevents direct invertibility of the transformation. The numerical consequences are shown in Table 4, where the finest basis in Table 1 is used as the starting point and each consecutive row corresponds to filtering the basis to consecutively coarser scaling functions and wavelets, retaining all wavelets generated as we go. The two approximate expansions in Eqs. (26) and (27) thus have small but finite differences using the edge functions constructed before.

As Chui and Lian point out, the inner functions could have had approximation order four except that the ability to exactly span up to cubic polynomials was given up in order to obtain functions that were symmetric and antisymmetric. If we had four edge functions of each type, the level $j+1$ scaling functions would be $4k_{\text{max},j} + 16$ in number, the level $j$ scaling functions and wavelets would each be $2k_{\text{max},j} + 8$ in number, and the transformation between scales would preserve the number of basis functions. Thus, it will be a matter of future investigation to find sets of four edge functions of each type which are suitable for merging with the symmetrized Chui-Lian inner basis functions, yet which preserve the ability of the current set to easily satisfy typical quantum boundary conditions. For the present purposes, the current construction will still have application for multiscale calculations, as shown in the next section.

V. Non-$\Sigma$ States ($m \neq 0$)

When $m \neq 0$, the additional terms in $H_\mu$ and $H_\nu$ [Eqs. (8) and (9)] become singular at the domain boundaries $\mu = \pm 1$ and $\nu = +1$, respectively. These special points physically correspond to the electron being at the position of one or the other of the nuclei. Regularity of the
eigenfunctions and their derivatives at these points may be regarded as cusp conditions in elliptic coordinates. For the "inner" $\mu$ equation, analysis of the specific behavior near the edges proceeds as in the related case of the associated Legendre functions, leading to the form

$$Y_m(\mu;R) = (1 - \mu^2)^{|n|/2} \tilde{Y}_m(\mu;R).$$

(28)

Similar analysis for the "outer" $\nu$ equation may take into account the singularity at $\nu = -1$ even though this is slightly outside of the domain of $\nu$, leading to

$$Z_m(\nu;R) = (\nu^2 - 1)^{|n|/2} \tilde{Z}_m(\nu;R).$$

(29)

The extraction of the leading local behaviors was used long ago in the development of the semi-analytic solutions for the wave functions.$^{20,41,42,49}$ The prefactors represent a complication for use of wavelet bases since the latter are naturally adapted to functions that can be locally expanded on some scale as polynomials. For odd values of $m$, the prefactors are distinctly non-polynomial at the domain edges.

A. Direct Calculations Including Boundary Singularities

It is nevertheless possible to investigate the direct expansion of $Y_m$ and $Z_m$ in wavelet bases. The singular terms in $H_\mu$ and $H_\nu$ require special treatment. This is most simply discussed in a scaling function basis on a single scale $J$ as used before.$^{18}$ The boundary condition that each wave function vanishes at the edges is satisfied by deleting from the basis those particular functions which do not vanish there, viz., the edge functions $\Phi^L_{J,0}$ and $\Phi^R_{J,0}$. All matrix elements of $(1 - \mu^2)^{-1}$ and $(\nu^2 - 1)^{-1}$ between the remaining basis functions are finite, although a bit demanding to calculate numerically. The first step requires an adaptive quadrature for matrix elements$^{16}$ of $1/x$ between inner scaling functions to the right of, but not touching, $x =
0. The matrix elements of $1/x$ between edge functions and between edge and neighboring inner functions are then obtained easily from those results, as detailed previously. Finally, the collected matrix elements of $1/x$ form the basis of a new adaptive wavelet quadrature similar to that described before but modified to matrix elements of functions $f(x)$ which may contain a leading $1/x$ behavior at the origin. The first two steps only need to be performed once. All matrix elements used are converged to an accuracy of better than one part in $10^{10}$, although tests using one part in $10^{14}$ have also been carried out to make sure that the results are insensitive to the change.

At $R = 2.0$, the parameters for the lowest $\Pi$ state ($2p\sigma_u$) are $E = 0.07122818010413$, $A = -1.8250515276$, and $p = 0.9260365218455$. Using these parameters for $m = 1$, diagonalization of $H_\mu$ was carried out for a series of truncated bases (no $n = 0$ edge scaling functions) with progressively finer resolution. The errors shown in Table 5, unlike those for the $m = 0$ case examined earlier, only decrease linearly with basis spacing. This is directly attributable to the singularities at $\mu = \pm 1$ and the inability of the edge functions to precisely capture the leading behavior $(1 - \mu^2)^{1/2}$ at the edges, cf. Eq. (28). In an analogous and familiar case, the inability of Gaussian functions to satisfy Coulomb potential cusp conditions similarly places limits on the level of accuracy that may be obtained with their use. While one may systematically reduce the error in the present wavelet example by increasing basis size, the slow convergence would lead to unacceptably high numbers of basis functions, e.g., over $10^5$ functions would be required just to reduce the error to $< 10^{-5}$.

The multiresolution capabilities of wavelet bases offers a unique way to address the problem caused by the edge singularities. One may hope to reduce that part of the error without accumulating large numbers of basis functions by including fine-scale wavelets just near the
edges. At each level $j$, it is necessary to eliminate the edge functions $\Phi_{j,0}^L$ and $\Phi_{j,0}^R$. It is also necessary to reconsider the edge wavelets $\Psi_{j,0}^L$ and $\Psi_{j,0}^R$ which take nonzero values at their respective edges. Initial numerical experiments in which these functions were simply deleted gave poor results. As formally pointed out by Monasse and Perrier$^{38}$ in the single wavelet case, it is required that these wavelets be modified instead of deleted. This is a complication arising from imposition of boundary conditions (distinct from the truncation issue raised in the last section). In our particular case, that part of each $n = 0$ edge wavelet that fails to vanish at an edge must be subtracted. Inspection of the two-scale Eq. (22) for the left-hand edge shows that this can be accomplished trivially by setting $F_{0,0}$, the coefficient of $\Phi_0^L(2x)$, to zero. All other $F_{n,0}$ are already zero since $F$ is upper triangular, so this does not affect the inner products of any of the other rows with the first. Of course, the modified wavelet is no longer normalized to unity, but this is fixed by a simple renormalization. The first rows of the $F$ and $G$ matrices are multiplied by a common factor such that the sum of the inner products of these rows with themselves is again two, cf., Eq. (24). Except for the renormalization, the shape of the wavelet remains the same in the right-half of the interval, i.e., beyond the region where $\Phi_0^L(2x)$ is nonzero. The new orthogonal wavelet set shown in Fig. 3 contains the modified $\Psi_0^L$ and the original $\Psi_1^L$ and $\Psi_2^L$. The wavelet $\Psi_0^R$ undergoes the corresponding changes.

To quantitatively examine compressibility in a multiresolution basis, the scaling function basis with spacing 1/32 was assigned as $j = J = 3$ and convolved with the scaling function and wavelet filters three times, resulting in a full interval multiresolution basis consisting of 12 $j = 0$ scaling functions and 14 $j = 0$, 30 $j = 1$ and 62 $j = 2$ wavelets. Figure 4 shows the magnitude of the coefficients in the corresponding $H_\mu$ eigenvector for the $2p\sigma_u$ state with dashed lines.
separating the four blocks of multiscale functions. It is seen that each successively finer wavelet block gives eigenvector coefficients in the middle of the interval that are significantly smaller, much the same situation as is obtained for the singularity-free ground state. (There are also systematic variations between the contributions of the symmetric and antisymmetric functions in the middle of the interval -- for regions and scales where a wave function is relatively smooth, the symmetric inner wavelets have greater contribution than the antisymmetric ones.) Near the edges, however, one obtains monotonic but slow decrease in the magnitudes of the coefficients, quantitatively indicating the need for inclusion of edge functions on increasingly fine scales.

The number of small wavelet coefficients observed in Fig. 4 suggests that the multiscale basis may be strongly compressed with only modest loss of accuracy. One may delete those functions for which the magnitudes of the coefficients fall below a particular threshold. For example, using a cutoff value of $10^{-4}$ eliminates all but 30 of the original 118 basis functions, only nominally increasing the eigenvalue error from 0.0152998 to 0.0154382. For larger-basis and larger-dimension problems, one would of course prefer guidelines for which basis functions can be deleted \textit{a priori}, i.e., without requiring preliminary calculations using an uncompressed basis. This is too complicated to pursue fully here since there are three sources of error to consider: (i) the dominant error from edge effects, which behaves approximately linearly with the decrease in basis function spacing, (ii) the smaller general error in the interior region apart from the singularity effects, which in the ground state example behaved quartically with spacing, and (iii) the truncation error discussed in Section IV resulting from transforming to a multiscale basis using the current family of multiwavelets on the interval. Regarding (iii), the $j = 0, 1, 2$ multiscale basis with 118 elements and an eigenvalue error of 0.0152998 is only a bit worse than
the single scale $J = 3$ basis of 124 functions with error 0.0152368, i.e., truncation effects add an error of only a few parts in $10^5$ in the present example.

If we restrict attention to (i), then we do have the general *a priori* guideline that addition of a few basis functions near the edges on several finer scales should significantly reduce the overall error. A series of calculations with selected wavelets of increasingly higher $j$ was undertaken, the $j = 0$ level corresponding to the spacing 1/16. At this level there were 60 scaling functions and, on each side, the three edge wavelets and the neighboring three pairs of inner wavelets. For $j > 0$, the edge wavelets and just one inner pair of wavelets were included for each side. The results in Table 6 demonstrate that one only needs to add a few side wavelets at each successive level $j$ in order to reduce the error almost by a factor of 1/2, the behavior found from Table 5 for the single scale bases at different resolutions. Deviation from this behavior is found for the finest scales as the error is reduced to be comparable to that from sources other than the edge effects. The finest scale wavelets used here have a spacing of 1/16,384, and would thus represent an extremely large basis if all functions were included. In contrast, selective use of the wavelet basis keeps the total number of basis functions quite modest while reducing the error by nearly three orders of magnitude. Similarly, the $H_\nu$ eigenvalue equation will benefit from selective inclusion of wavelets near $\nu = 1$. Further reduction of the error over that in Table 6 could be pursued, but the relatively slow convergence rate and the need for systematic study of the other sources of error push us to look elsewhere for a solution method.

B. Conversion to Generalized Symmetric Eigenvalue Problem
A different approach is to consider wavelet expansion of $\tilde{Y}_m$ rather than $Y_m$, cf. Eq. (28). The function $\tilde{Y}_m$ obeys an equation which may be derived from Eqs. (8) and (11) for $Y_m$. This may be expressed in the convenient form

$$
\left(\tilde{H}_\mu + A \tilde{W}_\mu\right)\tilde{Y}_m(\mu; R) = 0,
$$

(30)

where

$$
\tilde{H}_\mu = -\frac{\partial}{\partial \mu} (1 - \mu^2)^{|m|+1} \frac{\partial}{\partial \mu} + (m^2 + |m| - p^2 \mu^2)(1 - \mu^2)^{|m|},
$$

(31)

$$
\tilde{W}_\mu = (1 - \mu^2)^{|m|},
$$

(32)

are explicitly Hermitian with respect to the volume element $d\mu$. If a wavelet basis is used to expand the function $\tilde{Y}_m$ and the vector of expansion coefficients is denoted by $\tilde{Y}$, the resulting matrix equation

$$
\tilde{H}_\mu \tilde{Y} = -A \tilde{W}_\mu \tilde{Y}
$$

(33)

contains only symmetric matrices and forms a generalized symmetric eigenproblem. As opposed to the direct method of the previous subsection, there are no terms here that are badly behaved at $\mu = \pm 1$. The price that we pay is that the matrix of the function $\tilde{W}_\mu$ rather than the identity matrix appears on the right-hand side. An equivalent statement is that we are expanding the full wave function in basis functions of the form $(1 - \mu^2)^{1/2} \phi_{k\alpha}(\mu)$, etc., which are nonorthogonal with overlap matrix $\tilde{W}_\mu$.

The generalized eigenvalue problem may be converted into a standard eigenvalue problem by orthogonalizing the wavelet basis with respect to the measure $\tilde{W}_\mu d\mu$. Sweldens has investigated the explicit construction of "weighted wavelets," in which different wavelet families are constructed for different weight functions. We are more generally interested in
determining how versatile a single wavelet basis can be made since this will affect the design of wavelet-based adaptive differential equation solvers. With that in mind, we adopt a simpler strategy using the intervalized Chui-Lian basis for all calculations. The matrix elements involved in $\tilde{W}_\mu$ and $\tilde{H}_\mu$ need only integrals that can be calculated by methods described before. By Cholesky decomposition of $\tilde{W}_\mu$ into the product of a lower triangle matrix and its transpose,

$$\tilde{W}_\mu = L \cdot L^T,$$

the generalized eigenvalue problem is converted into a standard eigenvalue problem for the symmetric matrix $L^{-1} \cdot \tilde{H}_\mu \cdot (L^T)^{-1}$.

The value of $A$ was determined in a series of calculations shown in Table 7. These are identical in size to those carried out for the ground state in Table 1, and also converge as the fourth power of the basis function spacing. The numbers in fact turn out to be slightly more accurate in the excited state for the same size basis. The largest basis has reached the precision of the molecular parameters used (one part in $10^{13}$). Thus, it becomes firmly established that wavelet bases are capable of obtaining high accuracy for $A$ even for $|m| = 1$ states of $H_2^+$. In similar fashion, with the calculation of more integrals, eigensolutions for higher $|m|$, as well as for the other coordinate $\nu$, can be calculated. From both the standpoints of accuracy and simplicity, conversion to the generalized eigenproblem is clearly preferred over the direct approach.

**VI. Discussion**
The use of an interval wavelet basis extended to confocal elliptic coordinates has been shown to allow accurate solution of the eigenvalue equations for ground and excited electronic states of the hydrogen molecular ion. For states with angular momentum component \( m = 0 \), the orthonormal wavelet basis requires nothing more than solution of a standard eigenvalue problem. For states with angular momentum component \( m \neq 0 \), essential singularities in the Hamiltonian complicate the situation. With well-chosen basis functions at the edges, it has been shown possible to use the customizable resolution of a multiscale basis to significantly reduce the error due to the singularities. However, this requires a significant amount of work and convergence is slow. Quick convergence is instead achieved by extracting the exact local behavior of the solutions near the singularities before expansion in the wavelet basis. This leads to a generalized symmetric eigenvalue problem which is straightforwardly solved using Cholesky decomposition. Given the current primitive developmental stage of wavelet methods for solution of differential equations, it is important to establish that high accuracy can be achieved in different types of quantum systems. It is also important to emphasize that the general findings here should not depend on the specific wavelet family used to construct the interval basis.

For most standard quantum problems, as mentioned earlier, individualized methods are likely to be more efficient. Nevertheless, in a situation similar to use of finite elements for solution of the Schrödinger equation,\(^{52,53}\) the combination of flexibility and systematic improvability of wavelet bases holds the possibility of developing adaptive computer codes in which one can dial the accuracy according to desire and computational resources. Wavelet bases have certain advantages such as explicit multiscale character and, in many cases, orthogonality (significant with respect to avoiding linear dependence in large bases). Furthermore, as is now clear, they may be adapted for a number of curvilinear coordinate problems in addition to the
original Cartesian coordinate formulations. From the standpoint of chemical physics, this is of interest because of the large number of curvilinear coordinate systems (e.g., valence bond, Jacobi, Radau, hyperspherical, etc., and even confocal elliptic\textsuperscript{54}) that may be used in describing large amplitude nuclear motion, whether stationary or time-dependent Schrödinger equations are of interest.

One particularly important challenge that will need to be addressed is the judicious selection of detail wavelets to be included in or deleted from calculations. In time evolution problems, one may dynamically monitor the magnitudes of the coefficients in different regions and on different scales in order to make such decisions. If protracted ranges of basis functions have small coefficients, they are candidates for deletion. Conversely, if coefficients near the edge of a region grow, basis functions just outside the edge are candidates for inclusion. Solution of the stationary Schrödinger equation for large bases is another issue, however. As mentioned earlier, one would like to have guidelines for how to most effectively increase a given size basis with detail wavelets. Vastly enlarging the basis and then examining coefficient magnitudes would not generally be an efficient method. Similarly, frequently repeated calculations with small additions to the basis would be inefficient. One possible avenue is to be guided by direct calculation of couplings between new candidate functions and selected eigenfunctions from prior (modest size) calculations. Such issues will need to be investigated thoroughly in order to take full advantage of the wave function compression offered by wavelet bases.

It is to be expected that, as it has in the signal processing field, wavelet technology in quantum mechanics will undergo a subsequent phase of testing and development of better wavelets as well as better algorithms. To foster this goal, a set of software utilities for basic
operations with general compact support wavelet families is being collected in a C++ program, MultiWavePack.\textsuperscript{55} The current focus, for example, is on addition of the ability to automatically construct edge functions for compact support wavelet families. It is intended that continuing development of the capabilities will occur as the general wavelet technology improves.

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References


Table 1. Error in determination of the separation constant $A$ from diagonalization of $H_\mu$ for the ground state in single-scale bases of multiscaling functions on the interval.

| $k_{\text{max}}$ | # Scaling Functions | Spacing | $|\text{Error}(A)|$ |
|------------------|---------------------|---------|------------------|
| 4                | 14                  | 1/4     | 5.7e-6           |
| 12               | 30                  | 1/8     | 2.7e-7           |
| 28               | 62                  | 1/16    | 1.5e-8           |
| 60               | 126                 | 1/32    | 8.9e-10          |
| 124              | 254                 | 1/64    | 5.5e-11          |
Table 2. Convergence with cutoff $\nu_{\text{max}}$ of separation constant $A$ calculated by diagonalization of $H_\nu$ at $R = 2$ a.u. for the ground state in single-scale bases of multiscaling functions. Three different spacings are used.

| $\nu_{\text{max}}$ | $k_{\text{max}}$ | |Error($A$)| | $\nu_{\text{max}}$ | $k_{\text{max}}$ | |Error($A$)| | $\nu_{\text{max}}$ | $k_{\text{max}}$ | |Error($A$)| |
|---------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|------------------|
| spacing = 1        |                  |                  |                  |                  | spacing = 1/2    |                  |                  |                  | spacing = 1/4    |
| 10                 | 5                | 0.0421665827450  |                  | 14               | 0.0025651071066  |                  | 32               | 0.0001339590808 |                  |
| 11                 | 6                | 0.0421665859366  |                  | 16               | 0.0025651135816  |                  | 36               | 0.0001339654943 |                  |
| 12                 | 7                | 0.0421665861383  |                  | 18               | 0.0025651140078  |                  | 40               | 0.0001339659158 |                  |
| 13                 | 8                | 0.0421665861508  |                  | 20               | 0.0025651140352  |                  | 44               | 0.0001339659429 |                  |
| 14                 | 9                | 0.0421665861516  |                  | 22               | 0.0025651140370  |                  | 48               | 0.0001339659446 |                  |
| 15                 | 10               | 0.0421665861517  |                  | 24               | 0.0025651140371  |                  | 52               | 0.0001339659447 |                  |
Table 3. Error in determination of the separation constant $A$ from diagonalization of $H_{\nu}$ for the ground state in single-scale bases of multiscaling functions on the interval using cutoff $\nu_{\text{max}} = 15$.

| $k_{\text{max}}$ | # Scaling Functions | Spacing | $|\text{Error}(A)|$  |
|------------------|---------------------|---------|----------------------|
| 10               | 26                  | 1       | 4.2e-2               |
| 24               | 54                  | 1/2     | 2.6e-3               |
| 52               | 110                 | 1/4     | 1.3e-4               |
| 108              | 222                 | 1/8     | 7.5e-6               |
| 220              | 446                 | 1/16    | 4.5e-7               |
| 444              | 892                 | 1/32    | 2.8e-8               |
Table 4. Error in the separation constant $A$ for the ground state (using $H_{\mu}$) resulting from recursive transformations of scaling functions to scaling functions and wavelets on coarser scales with concomitant reduction of total basis size.

| # Wavelet Scales | # Basis Functions | $|\text{Error}(A)|$ |
|------------------|-------------------|-------------------|
| 0                | 254               | 5.5e-11           |
| 1                | 252               | 6.1e-11           |
| 2                | 250               | 3.2e-10           |
| 3                | 248               | 1.0e-8            |
| 4                | 246               | 2.5e-7            |
Table 5. Error in determination of the separation constant $A$ from diagonalization of $H_\mu$ for the $2p\sigma_u$ state in single-scale bases on the interval with $n = 0$ edge functions removed.

| $k_{\text{max}}$ | # Scaling Functions | Spacing | $|\text{Error}(A)|$ |
|------------------|---------------------|---------|-----------------|
| 4                | 12                  | 1/4     | 1.2e-1          |
| 12               | 28                  | 1/8     | 6.0e-2          |
| 28               | 60                  | 1/16    | 3.0e-2          |
| 60               | 124                 | 1/32    | 1.5e-2          |
| 124              | 252                 | 1/64    | 7.6e-3          |
| 252              | 508                 | 1/128   | 3.8e-3          |
Table 6. Error in the separation constant $A$ for the $2p\sigma_u$ state resulting from inclusion of selected wavelets near the edges to the last scaling function basis in Table 4.

| # Wavelet Scales | # Basis Functions | $|\text{Error}(A)|$  |
|------------------|-------------------|-------------------|
| 1                | 78                | 1.5e-2            |
| 2                | 88                | 7.7e-3            |
| 3                | 98                | 3.9e-3            |
| 4                | 108               | 1.9e-3            |
| 5                | 118               | 9.8e-4            |
| 6                | 128               | 5.0e-4            |
| 7                | 138               | 2.6e-4            |
| 8                | 148               | 1.4e-4            |
| 9                | 158               | 8.1e-5            |
| 10               | 168               | 5.1e-5            |
Table 7. Error in determination of the separation constant $A$ for the $2p\sigma_u$ state from solution of the symmetric generalized eigenvalue problem for $\tilde{H}_\mu$ in single-scale bases of multiscaling functions on the interval.

| $k_{\text{max}}$ | # Scaling Functions | Spacing | $|\text{Error}(A)|$ |
|------------------|---------------------|---------|------------------|
| 4                | 14                  | 1/4     | 1.3e-8           |
| 12               | 30                  | 1/8     | 7.2e-10          |
| 28               | 62                  | 1/16    | 4.3e-11          |
| 60               | 126                 | 1/32    | 2.4e-12          |
| 124              | 254                 | 1/64    | 1.7e-13          |
Figure 1. Scaling function basis for a finite interval. The two central inner series of scaling functions are from the Chui-Lian multiwavelet family. The top series consists of translated copies $\phi_1(x - k)$ of the symmetric scaling function $\phi_1(x)$, while the bottom series consists of copies $\phi_2(x - k)$ of the antisymmetric function $\phi_2(x)$. In this particular example we have $1 \leq k \leq 5$, though the range of $k$ may be much larger in practice. The detailed shapes of $\phi_1(x)$ and $\phi_2(x)$ are dictated by requirements including symmetry, orthonormality, length and approximation order. For example, they must be oscillatory since lobes of different signs are
required for orthogonality of neighboring copies. The three additional functions on the left (vertically offset for clarity) and their mirror images on the right are edge scaling functions constructed by Mackey, et al. In conjunction with the inner functions, they provide an expansion basis supporting multiresolution analysis which is exact for quadratic polynomials throughout the interval $0 \leq x \leq 9$. The left edge functions have been designed to behave as simple powers of $x$ near $x = 0$ to facilitate the satisfaction of typical boundary conditions for quantum problems. All functions shown here form an orthonormal set.
Figure 2. Wavelet basis for a finite interval. The functions shown are the wavelets corresponding to the scaling functions of Fig. 1. The inner functions shown top center are copies $\psi_1(x - k)$, $1 \leq k \leq 5$ of the symmetric Chui-Lian wavelet $\psi_1(x)$ and those shown bottom center are copies $\psi_2(x - k)$ of the antisymmetric wavelet $\psi_2(x)$. The three edge wavelets on the left behave as simple powers of $x$ near $x = 0$, in correspondence with the edge scaling functions of Fig. 1, and the three right edge wavelets are mirror images. The wavelets generally have slightly more structure or oscillation than scaling functions since they are orthogonal to smooth low order polynomials and must span the difference in detail between adjacent resolution levels of scaling functions. All wavelets shown here are orthogonal to each other and to all scaling functions in Fig. 1. In addition, one may construct similar wavelet bases with all wavelets squeezed by a power of two and the numbers of inner functions increased to maintain the same interval length; by construction, these finer-scale wavelets are also orthogonal to all wavelets here and scaling functions in Fig. 1.
Figure 3. Modified set of left-edge wavelets for use when boundary conditions force vanishing of the wave function at $x = 0$. Such a condition requires deletion of $\Phi_0^L$ from the scaling function basis since it does not vanish at $x = 0$. The functions $\Phi_1^L$ and $\Phi_2^L$ are left intact since they vanish there by construction. Similarly, $\Psi_1^L$ and $\Psi_2^L$ are unchanged. The function $\Psi_0^L$, however, only needs modification instead of deletion. Referring to Eq. (22), the component proportional to $\Phi_0^L(2x)$, which fails to vanish at $x = 0$, has been removed and the residual function renormalized. The resulting $\Psi_0^L(x)$ now vanishes at $x = 0$ while, except for the renormalization, its shape is unchanged in the interval $3/2 \leq x \leq 3$. Orthogonality with respect to
all other included basis functions is also maintained. Right-hand edge wavelets edge are reflections of those shown here when the wave function must also vanish at that edge.

Figure 4. Magnitudes of components for the $2p_{0u}$ eigenvector of $H_{\mu}$ in a multiscale basis of $j = 0$ scaling functions with spacing $\Delta \mu = 1/4$ (far left) and $j = 0, 1, 2$ wavelets. The dashed lines separate the different groups of coefficients. Within each group, the leftmost and rightmost coefficients represent the contributions of the respective edge functions and the middle coefficients are those of the inner functions with indices $(k, \alpha)$ ordered $(1, 1), (1, 2), (2, 1), (2, 2), \ldots$. The inner wavelet coefficients shrink much more quickly with finer resolution than the edge
wavelet coefficients, giving a quantitative measure of the effects of the singularities at the
domain edges.