Solving the One-dimensional Schrödinger equation using a set of Daubechies wavelet scaling functions

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Abstract. In this contribution basis sets derived from Daubechies wavelets scaling functions[1] are used to solve the one-dimensional Schrödinger equation on the interval $[-x_{\max} : x_{\max}]$. We present the results for the harmonic oscillator as function of the number N of intervals. Double logarithmic fits of the energy error against N are also shown. Fast convergence is found.
Finally further applications to the three-dimensional Schrödinger equation also with a view to density functional calculations are discussed.

1 Introduction

In solving the Kohn-Sham equations for the orbitals, the choice of a basis set decides strongly the accuracy of a code [1, 3]. Daubechies wavelet scaling functions have most of the properties that are desired of a basis set to be used for the simulation of isolated or inhomogeneous [1] systems such as molecules and materials. They are compactly supported, being non-zero only within a [1, 2]finite interval. Making it well-suited for approximating data with sharp discontinuities. Their orthogonality ensures that the basis set is well-behaved and stable, [2]leading to accurate results in DFT calculations. Also they have the ability to accurately represent polynomial functions, and their regularity or smoothness make them a powerful and efficient basis set for DFT [3] calculations, enabling accurate and computationally feasible simulations of electronic structure.

1.1 Definition of Daubechies wavelet scaling functions

The provision of a systematic and localized basis set by wavelet scaling functions makes it crucial for achieving both high accuracy [2] and computational efficiency, [1, 3] reducing computational cost. When the best wavelet scaling function adapted to data is chosen, the data is sparsely represented. This sparse coding makes wavelet scaling functions an excellent tool in the field of [4] data compression. Wavelet scaling could be used in other applied fields of science such as in astronomy, acoustics, nuclear engineering, sub-band coding, signal and image processing, neurophysiology, magnetic resonance imaging, [1, 4] speech discrimination, and optics. They can also be used in fractals, turbulence, earthquake-prediction, radar, human vision, and pure mathematics [3] applications such as solving partial differential equations. Scientists had wanted more appropriate functions than the sines and cosines which comprise the bases of Fourier analysis, to approximate fluctuating, intermittent signals [4] and sharp spikes. Because some of these other functions are non-local and they are stretched to infinity. They lack merits in approximating data with sharp discontinuities. Data sparsely represented needs an excellent tool for its compression, and wavelet scaling are adapted to such data.

Using maximally symmetric Daubechies wavelet scaling function ϕ of order $16(8)$, as per figure below: This function vanishes outside of [-7,8]. The Daubechies scaling basis function is defined as:[2, 3]

$$f_i^h(x) = \frac{1}{\sqrt{h}}\phi\left(\frac{x}{h} + \frac{x_{max}}{h} - i\right) \tag{1}$$

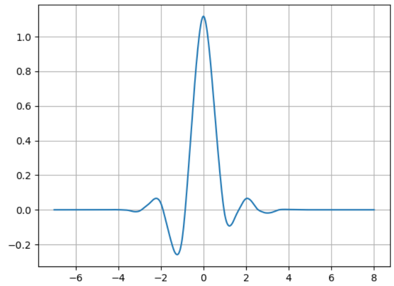

Figure 1: Daubechies wavelet scaling function

In the equation 1 above, h is the distance between the scaling functions.
Calculations were done using Python, Numpy and PyWavelets. For us to use such functions on a finite interval we need to modify some of the basis functions, such that they become periodic on $-x_{max}$ to x_{max}.
The overlap matrix

$$u_{ij} = \int_{-x_{max}}^{x_{max}} g_i(x) g_j(x) dx \tag{2}$$

is mostly sparse. Evaluating the u_{ij} we use the trapezoidal rule with $n_i = 15000$ intervals for each interval h after using cubic spline interpolation on the Daubechies scaling functions. The n_i is the number of integration intervals.
The potential energy matrix

$$v_{ij} = \int_{-x_{max}}^{x_{max}} g_i(x) x^2 g_j(x) dx \tag{3}$$

is evaluated in a similar way.
The kinetic energy matrix

$$k_{ij} = \int_{-x_{max}}^{x_{max}} \acute{g}_i(x) \acute{g}_j(x) dx \tag{4}$$

is evaluated by first calculating the derivative of the respective basis functions. Thus we obtain the Hamiltonian matrix as

$$h_{ij} = k_{ij} + v_{ij}. \tag{5}$$

1.2 Harmonic Oscillator

The Schrödinger equation of one-dimensional harmonic oscillator is given by;

$$-\frac{d^2\psi_n(x)}{dx^2} + x^2\psi_n(x) = E\psi_n(x) \tag{6}$$

Energy eigenvalues of the quantum harmonic oscillator are

$$E_v = 2v + 1 \tag{7}$$

We are interested in the ground state energy which is 1. Here we use the $x_{max} = 6$.

2 Results of Calculations of the Harmonic Oscillator

The ground state energy errors for the harmonic oscillator are given in the table 1 below. N stands for the number of intervals between zero and x_{max}, we have a total $2N$ intervals. The δE simply stands for the error of the ground state energy i.e.$E - 1$ The full calculation takes place on $[-x_{max}, x_{max}]$.

N	δE
6	0.00415612
12	$6.54564790 \times 10^{-6}$
18	$4.90738339 \times 10^{-8}$
24	$1.15641696 \times 10^{-9}$
30	$6.16224849 \times 10^{-11}$
36	$9.40092448 \times 10^{-12}$

Table 1: Ground State Energy for Harmonic Oscillator

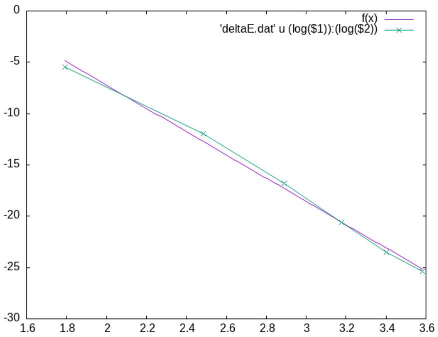

Figure 2: Least square fit

2.1 Discussion and conclusion

We can see that as the number of intervals increased so δE decreased, converging towards 1, the correct value for the ground state energy for harmonic oscillator. This shows that Daubechies wavelet scaling as basis functions converge quickly. We see δE decreasing consistently with increasing N. In the figure 2 above, log δE is plotted versus log N. The straight line is the least square fit.

We intend to study small molecules less than or equal 10 in the periodic table. The Nodes are to be derived from molecular information in .xyz files. Schrödinger-like equations are solved based on Density Functional approach, and the code is under development.

3 Acknowledgements

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