# Calculation of the Ground State Energy of the hydrogen molecular ion using scaling wavelets as basis set

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## Definition of the Basis

## Merits of Sym8 Wavelets

## Hamilitonian and Cusp Trick

## Evalulation of Matrixelements

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## Acknowledgment



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- Using three dimensional basis functions based on shifted and scaled scaling sym8 wavelet function

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

- Here $h = x_{\max}/N$, $h$ is also the distance between the scaling functions, and $N$ is the number of intervals from the origin to $x_{\max}$.
- We however modify the functions by giving it periodic boundary conditions via

$$g_i(x) = \sum_{k=-K_{max},}^{K_{max}-1} f_i(x + kL) \tag{2}$$

with $L = 2x_{\max}$, $K_{max} = 1$.

- The three dimensional basis functions are given by

$$F_{ijk}(x, y, z) = g_i(x)g_j(y)g_k(z) \tag{3}$$

- Symlet8 or sym8 wavelets are specialized wavelets within wavelet theory valued for their near-symmetry, smoothness, and high-order vanishing moments.
- Used frequently to balance accuracy and smoothness in denoising and decomposition.
- Used in detecting slow-changing trends and feature extraction applications, such as seen in EEG, ECG, and seismic data analysis.
- The sym8 wavelet is applied within the Discrete Wavelet Transform (DWT) to split signals into detailed and approximation components.
- The improved symmetry of sym8 is preferred over db8 in image processing, edge detection, and analysis where signal phase information is important.

- Hamiltonian for $H_2^+$ is

$$H = -\nabla^2 - \frac{2}{|\mathbf{r} - \mathbf{R_1}|} - \frac{2}{|\mathbf{r} - \mathbf{R_2}|}, \tag{4}$$

with $\mathbf{R_1} = (-1, 0, 0)$ and $\mathbf{R_2} = (1, 0, 0)$, the positions of the two protons.

- In order to mitigate the Coulomb cusps of the wave function at the positions of the nuclei we use the method described in
*M. Braun, K.O. Obodo, Finite element density functional calculations for light molecules using a cusp factor to mitigate the Coulomb potential, Eur. Phys. J. (230) (2019) 100310-6*.

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- Let $t_{ijk}$ the index function that maps the three 1D indices to a single index enumerating the 3D array with the original dimensions.
- Wherever you see three indices like *ijk* they actually stand for a single index. Inserting the index function everywhere would make the notation totally cumbersome.
- We define the generalized overlap matrix,

$$u_{ijk,lmn} = \int F_{ijk} WF_{lmn} d\mathcal{V} \tag{5}$$

- the generalized potential matrix

$$v_{ijk,lmn} = \int F_{ijk} V_{\text{eff}} WF_{lmn} d\mathcal{V} \tag{6}$$

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- and the generalized kinetic energy matrix,

$$q_{ijk,lmn} = \int d\mathcal{V} \left( \frac{\partial}{\partial x} F_{ijk} W \frac{\partial}{\partial x} F_{lmn} + \frac{\partial}{\partial y} F_{ijk} W \frac{\partial}{\partial y} F_{lmn} + \frac{\partial}{\partial z} F_{ijk} W \frac{\partial}{\partial z} F_{lmn} \right) \tag{7}$$

- With $d\mathcal{V} = dxdydz$
- The weight function for this molecule is $W = G^2$ with

$$G = 1 + c \exp(-2|\mathbf{r} - \mathbf{R_1}|) + c \exp(-2|\mathbf{r} - \mathbf{R_2}|) \tag{8}$$

with $c = 1.01865736....$ resulting from the cusp condition for the ansatz in the paper.

- The effective potential is

$$V_{\text{eff}} = -\frac{2}{r_1} - \frac{2}{r_2} - \frac{\nabla^2 G}{G} \tag{9}$$

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- The generalized eigenvalue problem then is

$$H\mathbf{v} = EU\mathbf{v} \tag{10}$$

and

$$H = Q + V.$$

- Here $W$ is the weight function matrix , $Q$ is the kinetic energy matrix and $V$ the effective potential matrix.

- We evaluate matrix elements using repeated Gauss Legendre Integration on the grid, and evaluate $W$ and $V_{\text{eff}}$ on a three-dimensional GL grid based on the 1D GL grid $y_i, i = 1 \cdots N_{\text{GL}}$ with weights $\omega_i$.
- Denote these values by

$$w_{ijk} = W((y_i, y_j, y_k)) \tag{11}$$

$$v_{ijk} = V_{\text{eff}}((y_i, y_j, y_k))W((y_i, y_j, y_k)) \tag{12}$$

- Using orthonormality of basis functions obtain expansion of $W$ and $WV_{\text{eff}}$ in terms of $F_{ijk}$
- Since the 3D basis functions are products of 1D ones, we must calculate the integrals of triple products of basis functions as well as those mixed with derivatives.

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- We define $h_{ij}$ by the values of the basis functions at the 1D GL points,i.e.

$$h_{ij} = g_i(y_j). \tag{13}$$

- We define $r_{ij}$ by the derivatives of the basis functions at the 1D GL points, i.e.

$$r_{ij} = g_i'(y_j). \tag{14}$$

- Summation of basis function products and their weights give integrals over the product of three basis functions

$$p_{ijk} = \sum_l h_{il} h_{jl} h_{kl} \omega_l. \tag{15}$$

- Summation as above except first and third basis functions replaced by derivative

$$s_{ijk} = \sum_l r_{il} h_{jl} r_{kl} \omega_l. \tag{16}$$

The expansion coefficients of $W$ and $WV_{\text{eff}}$ are evaluated via three dimensional Gauss Legendre integration:

$$W_{abc} = \sum_i \sum_j \sum_k \omega_i \omega_j \omega_k w_{ijk} h_{ai} h_{bj} h_{bk} \tag{17}$$

Substituting these corresponding expansions into the expressions for the matrix elements we obtain.

$$u_{ijk,lmn} = \sum_a \sum_b \sum_c W_{abc} \int F_{ijk} F_{abc} F_{lmn} d\mathcal{V} \,. \tag{18}$$

For the generalized potential this becomes

$$V_{abc} = \sum_i \sum_j \sum_k \omega_i \omega_j \omega_k v_{ijk} h_{ai} h_{bj} h_{bk} \,. \tag{19}$$

and

$$v_{ijk,lmn} = \sum_a \sum_b \sum_c V_{abc} \int F_{ijk} F_{abc} F_{lmn} d\mathcal{V} \,. \tag{20}$$

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and finally the generalized kinetic energy is obtained via

$$q_{ijk,lmn} = \int d\mathcal{V} \Big[ \frac{\partial}{\partial x} F_{ijk} W \frac{\partial}{\partial x} F_{lmn} + \tag{21}$$

$$\frac{\partial}{\partial y} F_{ijk} W \frac{\partial}{\partial y} F_{lmn} + \tag{22}$$

$$\frac{\partial}{\partial z} F_{ijk} W \frac{\partial}{\partial z} F_{lmn} \Big] \tag{23}$$

After inserting the expansions for $W$ this yields

$$q_{ijk,lmn} = \sum_a \sum_b \sum_c W_{abc} \int d\mathcal{V} \frac{\partial}{\partial x} F_{ijk} F_{abc} \frac{\partial}{\partial x} F_{lmn} +$$

$$\sum_a \sum_b \sum_c W_{abc} \int d\mathcal{V} \frac{\partial}{\partial y} F_{ijk} F_{abc} \frac{\partial}{\partial y} F_{lmn} +$$

$$\sum_a \sum_b \sum_c W_{abc} \int d\mathcal{V} \frac{\partial}{\partial z} F_{ijk} F_{abc} \frac{\partial}{\partial z} F_{lmn} . \tag{24}$$


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Substituting the form of the global basis functions we obtain

$$u_{ijk,lmn} = \sum_a \sum_b \sum_c W_{abc} p_{ial} p_{jbm} p_{kcn} \tag{25}$$

$$v_{ijk,lmn} = \sum_a \sum_b \sum_c V_{abc} p_{ial} p_{jbm} p_{kcn} \tag{26}$$

$$q_{ijk,lmn} = \sum_{a,b.c} W_{abc} s_{ial} p_{jbm} p_{kcn} + \sum_{a,b,c} W_{abc} p_{ial} s_{jbm} p_{kcn} +$$

$$\sum_{a,b,c} W_{abc} p_{ial} p_{jbm} s_{kcn} \tag{27}$$


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- Results for Ground state energy

| $x_{\max}$ | $N$ | $h$ | $N_{gl}$ | $E_{gs}$ | $\Delta E$ |
|---|---|---|---|---|---|
| 6 | 6 | 1.0 | 12 | -2.19939455 | $5.87 \times 10^{-3}$ |
| 6 | 8 | 0.75 | 12 | -2.20347204 | $1.80 \times 10^{-3}$ |
| 6 | 10 | 0.60 | 12 | -2.20461436 | $6.54 \times 10^{-4}$ |

Literature value = -2.20526843 to 9 digits

- where $N_{gl}$ is the order of Gauss-Legendre integration.

- Code is written in Python
- Numpy, scipy, pywt and numba for speedup were used in this code.
- primme eigensolver used.



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- Ground state energy can be calculated to reasonable accuracy with wavelets scaling functions basis set.

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Thank You!!!