Wavelets in Scattering Calculations

Brian M. Kessler, Fatih Bulut, Gerald L. Payne, W.P.

polyzou@uiowa.edu

The University of Iowa

What are Wavelets ?

- Fractal functions used in data compression and signal processing.
- This talk: Daubechies $K = 2, 3$ (DK) wavelets.

Properties of DK Wavelets ?

- Orthonormal basis functions.
- Compact support.
- Local pointwise representation of low-degree polynomials.
- Generated from a single function by translations and scale transforms.

Why are Wavelets Interesting ?

- Efficient representation of information.
- Used in the FBI’s fingerprint archive.
- Used in the JPEG2000 image compression algorithm.
- Fast reconstruction of information.
- Natural basis for functions with smooth structures on multiple scales.

Physics Motivation

- Sensitivity to sub-nucleon degrees of freedom requires scattering with large energy/momentum transfers.

$$\Downarrow$$

- Scattering with large energy/momentum transfers requires a relativistic quantum treatment.

$$\Downarrow$$

- Relativistic quantum models are naturally formulated in momentum space (Fourier transforms).

Physics Motivation

$\Downarrow$

- Momentum-space few-body equations for realistic systems have large dense matrices ($\sim 10^7 \times 10^7$).

$\Downarrow$

- Wavelet bases lead to equivalent linear equations with sparse matrices.

Useful Numerical Properties

- Basis functions have compact support.
- Basis functions are orthonormal.
- Basis functions never have to be computed.
- The wavelet transform automatically eliminates unimportant basis functions.
- Basis functions can locally pointwise represent polynomials.
- Wavelets lead to effi cient treatment of scattering singularities.
- There is an effi cient one-point quadrature rule.

Interesting Properties

- Wavelets are fractals.
- Basis functions are generated from a single "Mother" function by translations and dyadic scale changes.
- "Mother" function constructed from solution ("Father" function $=$ scaling function) of a linear renormalization-group equation.

Elements of Wavelet Numerical Analysis

- Dyadic scale changes:

$$\boxed{D\xi(x) := \frac{1}{\sqrt{2}}\xi(\frac{x}{2})}$$

- Integer translations:

$$\boxed{T\xi(x) := \xi(x-1)}$$

- D and T are unitary.

The Scaling Equation

$$\boxed{D\phi(x) = \sum_l h_l T^l \phi(x)} \qquad \int \phi(x)dx = 1$$

- $\phi(x)$ = scaling function = “Father” function.
- h_l are numerical coefficients that determine the type of wavelet.

Scaling Bases

- Resolution m scaling function basis:

$$\phi_{mn}(x) := D^m T^n \phi(x) \qquad (\phi_{mn}, \phi_{mn'}) = \delta_{nn'}$$

- Resolution m approximation space, $\mathcal{V}_m$:

$$\mathcal{V}_m := \{f(x) = \sum_n f_n \phi_{mn}(x); \qquad \sum_n |f_n|^2 < \infty\}$$

Approximation Space

$$\int \phi_{-mn}(x)dx = 2^{-m/2}$$

$$\phi_{-mn}(x) = 0 \qquad \text{unless} \qquad x \in [\frac{n}{2^m}, \frac{n+2K-1}{2^m}]$$

- $2K =$ number of non zero h_ls.

Approximation Space

- For large m and smooth $f(x)$

$$f(x) \approx \sum_n f_n \phi_{-mn}(x)$$

$$f_n = \int \phi_{-mn}(x) f(x) dx \approx 2^{-m/2} f(\frac{n}{2^m})$$

- Expansion coefficients proportional to function values on support of ϕ_{-mn}.

Multiresolution Analysis

- The scaling equation

$$\phi_{m+1,n} = D\phi_{mn} = \sum_l h_l \phi_{m,2n+l}$$

$$\Downarrow$$

$$\mathcal{V}_m \supset \mathcal{V}_{m+1}$$

- Wavelet spaces $\mathcal{W}_m$ are defined by

$$\mathcal{V}_{m-1} = \mathcal{V}_m \oplus \mathcal{W}_m$$

Multiresolution Analysis

- Repeated application of $\mathcal{V}_m \supset \mathcal{V}_{m+1}$

$$\Downarrow$$

$$L^2(R) \supset \cdots \supset \mathcal{V}_{m-1} \supset \mathcal{V}_m \supset \mathcal{V}_{m+1} \supset \cdots \supset \{\emptyset\}$$

- Repeated application of $\mathcal{V}_m = \mathcal{V}_{m-1} \oplus \mathcal{W}_{m-1}$

$$\Downarrow$$

$$\mathcal{V}_m = \mathcal{V}_{m+k} \oplus \mathcal{W}_{m+k} \oplus \mathcal{W}_{m+k-1} \cdots \oplus \mathcal{W}_{m+1}$$

The "Mother" Wavelet $\psi(x)$

- The Mother wavelet $\psi(x) \in \mathcal{W}_0 \subset \mathcal{V}_{-1}$:

$$\boxed{D\psi = \sum_l g_l T^l \phi; \quad g_l := (-)^l h_{k-l} \quad k \text{ odd} .}$$

- Wavelet basis functions ψ_{mn} span $\mathcal{W}_m$:

$$\psi_{mn}(x) := D^m T^n \psi(x)$$

$$(\psi_{mn}, \psi_{m'n'}) = \delta_{mm'}\delta_{nn'} \qquad (\psi_{mn}, \phi_{mn'}) = 0$$

The Scaling Coefficients

- The Daubechies' scaling coefficients, h_l are constrained by:

$$\int \psi(x) x^l = 0; \quad l = 0, 1, \cdots, K-1$$

It follows that:

$$\int \psi_{mn}(x) x^l = 0; \quad l = 0, 1, \cdots, K-1$$

The Scaling Coefficients

- The h_l are the solution of:

$$\sum_{l=0}^{2K-1} h_l = \sqrt{2} \qquad \sum_{l=0}^{2K-1} h_l h_{l-2n} = \delta_{n0}$$

$$\sum_{l=0}^{2K-1} l^m (-)^l h_{k-l} = 0 \qquad m = 0, \cdots, K-1$$

- The solutions for $K = 1, 2, 3$ are:

Daubechies Scaling Coefficients

h_l	K=1	K=2	K=3
h_0	$1/\sqrt{2}$	$(1+\sqrt{3})/4\sqrt{2}$	$(1+\sqrt{10}+\sqrt{5+2\sqrt{10}})/16\sqrt{2}$
h_1	$1/\sqrt{2}$	$(3+\sqrt{3})/4\sqrt{2}$	$(5+\sqrt{10}+3\sqrt{5+2\sqrt{10}})/16\sqrt{2}$
h_2	0	$(3-\sqrt{3})/4\sqrt{2}$	$(10-2\sqrt{10}+2\sqrt{5+2\sqrt{10}})/16\sqrt{2}$
h_3	0	$(1-\sqrt{3})/4\sqrt{2}$	$(10-2\sqrt{10}-2\sqrt{5+2\sqrt{10}})/16\sqrt{2}$
h_4	0	0	$(5+\sqrt{10}-3\sqrt{5+2\sqrt{10}})/16\sqrt{2}$
h_5	0	0	$(1+\sqrt{10}-\sqrt{5+2\sqrt{10}})/16\sqrt{2}$

Computation of $\phi(x)$ and $\psi(x)$

- $\phi(x)$ at integer points can be obtained by solving:

$$\phi(n) = \sum_{l=0}^{2K-1} \sqrt{2} h_l \phi(2n-l) \qquad \sum_n \phi(n) = 1$$

- The support of $\phi(x) \in [0, 2K-1]$.

$$\Downarrow$$

$$\phi(n) = 0 \qquad n \le 0 \quad \text{or} \quad n \ge 2K-1$$

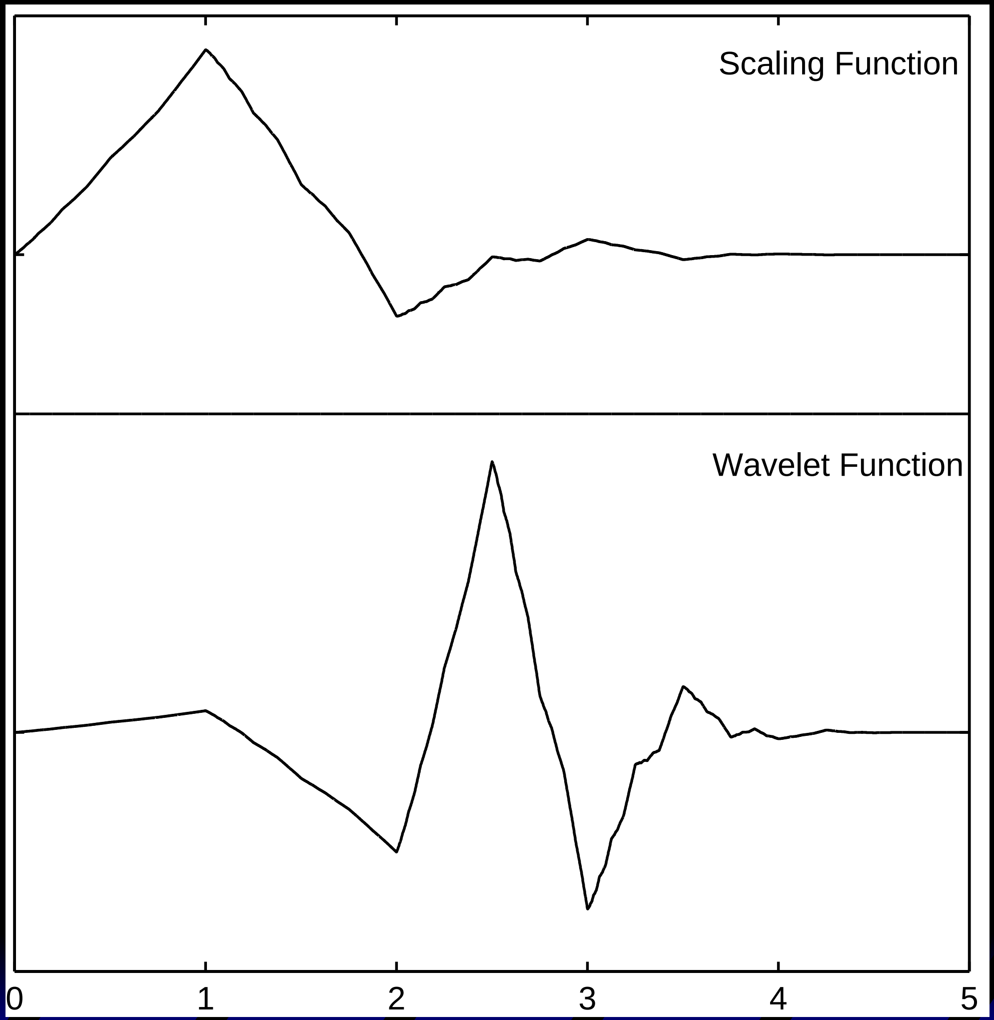
Computation of $\phi(x)$ and $\psi(x)$

- The scaling equation generates ψ and ϕ recursively at all dyadic rationals:

$$\phi(\frac{n}{2^k}) = \sum_{l=0}^{2K-1} \sqrt{2} h_l \phi(\frac{n}{2^{k-1}} - l)$$

$$\psi(\frac{n}{2^k}) = \sum_{l=0}^{2K-1} \sqrt{2} g_l \phi(\frac{n}{2^{k-1}} - l)$$

$K = 3$ Wavelet and Scaling Function



Approximation Spaces

- There are two approximation spaces related by a fast orthogonal transformation $(o(N))$.

$$\mathcal{V}_m \Leftrightarrow \mathcal{W}_{m+1} \oplus \mathcal{W}_{m+2} \oplus \cdots \oplus \mathcal{W}_{m+k} \oplus \mathcal{V}_{m+k}$$

with orthonormal bases

$$\{\phi_{mn}(x)\}_{n=-\infty}^{\infty}$$

$$\Updownarrow$$

$$\{\phi_{m+k\,n}(x)\}_{n=-\infty}^{\infty} \cup \{\psi_{ln}(x)\}_{n=-\infty,l=m+1}^{\infty,m+k}$$

Local Polynomials

$$L^2(R) = \cdots \oplus \mathcal{W}_{m-2} \oplus \mathcal{W}_{m-1} \cdots \oplus \mathcal{W}_m \oplus \mathcal{V}_m$$

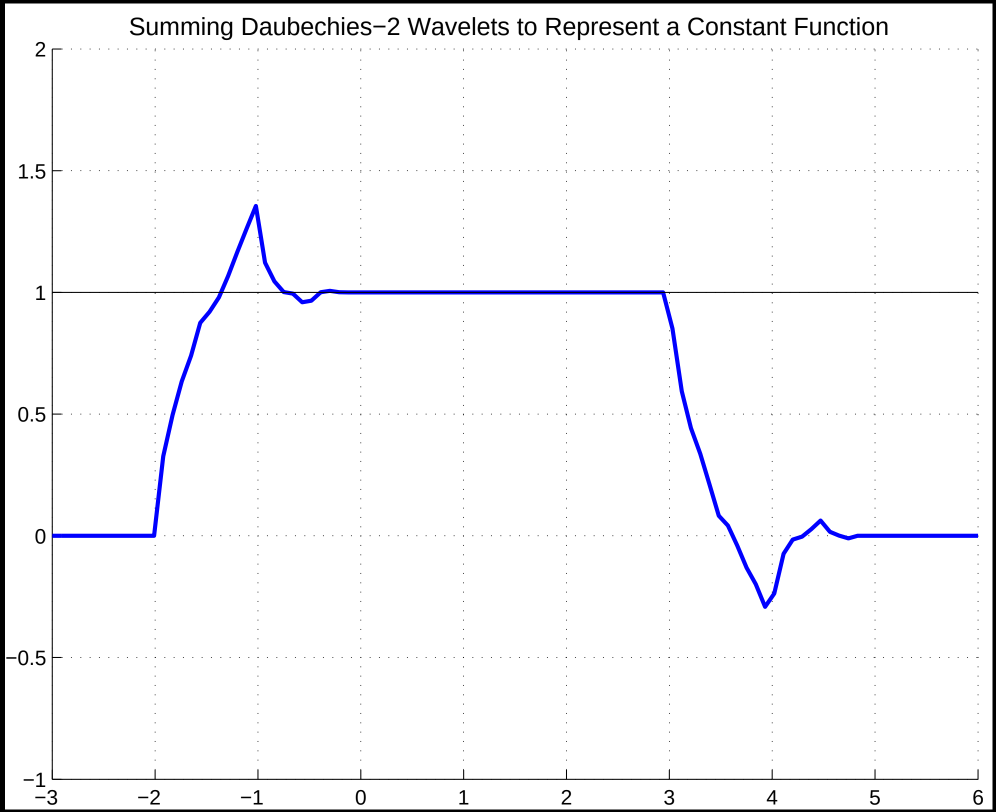
$$\int \psi_{mn} x^l = 0 \qquad \forall m, n; \quad l = 0, 1, \cdots, K-1$$

$$\Downarrow$$

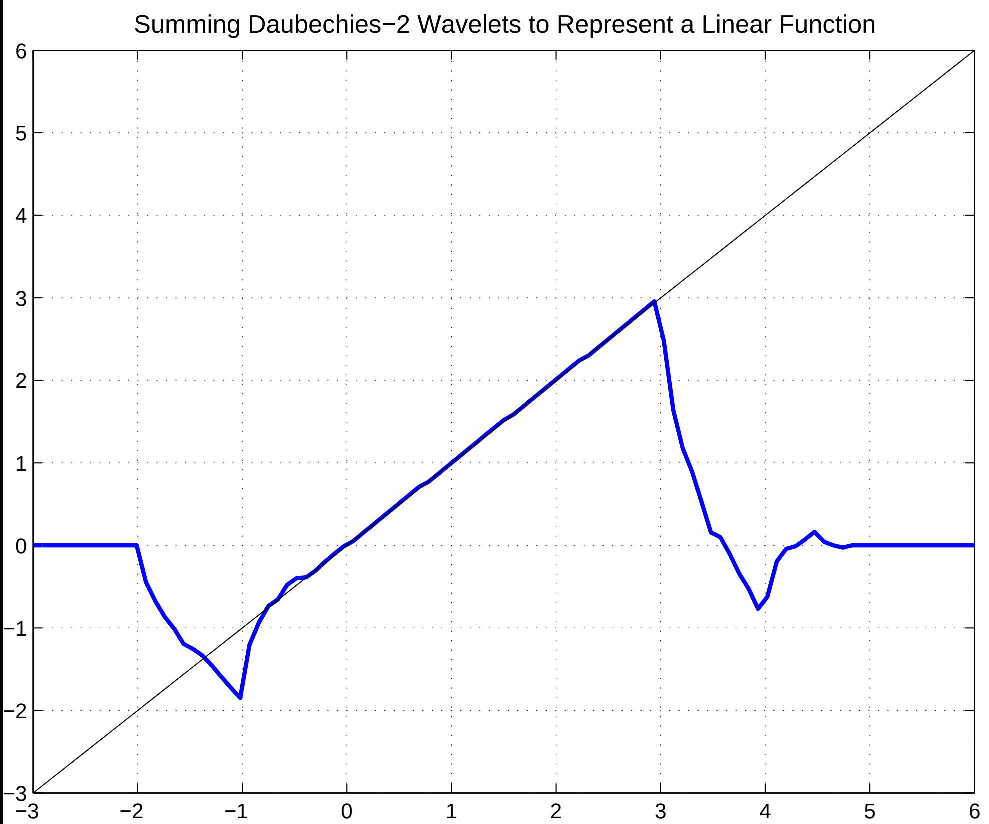
$$\boxed{\therefore \qquad x^l = \sum_n c_n \phi_{mn}(x) \qquad \text{pointwise}}$$

Unit Translates

Constant Function



Linear Function



Wavelet Numerical Analysis

- The fractal nature of wavelets makes standard numerical techniques ineffi cient.
- The scaling equation replaces all numerical methods.
- The key elements of “wavelet numerical analysis” are the compactness of the basis functions and the ability to exactly compute moments:

$$\langle x^m \rangle_\phi := (x^m, \phi) = \int x^m \phi(x) dx$$

Moments and Scaling

- The normalization condition gives:

$$\langle x^0 \rangle_\phi = 1$$

- The scaling equation gives:

$$\langle x^k \rangle_\phi = (x^k, \phi) = (Dx^k, D\phi) = \frac{1}{2^{k+1/2}} \sum_{l=0}^{2K-1} h_l (x^k, T^l \phi) =$$

$$\sum_{l=0}^{2K-1} \sum_{n=0}^{k} \binom{k}{n} h_l l^{k-n} \langle x^k \rangle_\phi$$

- These equations recursively determine all moments.

Moments and Scaling

- Similar methods can be used to get exact values for

$$(x^l, \phi_{mn}), \quad (x^l, \psi_{mn})$$

$$(\frac{d^l \phi_{mn}}{dx^l}, \phi_{m'n'}), \quad (\frac{d^l \phi_{mn}}{dx^l}, \psi_{m'n'}), \quad (\frac{d^l \psi_{mn}}{dx^l}, \phi_{m'n'}), \quad (\frac{d^l \psi_{mn}}{dx^l}, \psi_{m'n'})$$

$$(\phi_{mn}, \phi_{m'l'} \phi_{m''l''}) \cdots$$

$$\{x_k, w_k\}_{k=1}^N; \quad \int \phi(x) P_{2N-1}(x) dx = \sum_{l=1}^N P_{2N-1}(x_l) w_l$$

One-Point Quadrature

- For the Daubechies wavelets $\langle x^1 \rangle_\phi^2 = \langle x^2 \rangle_\phi$
- This means that

$$\int P(x)\phi(x)dx = P(\langle x^1 \rangle_\phi)$$

is exact for $P(x) = a + bx + cx^2$.

- The Daubechies $K = 3$ wavelets provide local pointwise representations of these polynomials.

Scattering Singularities

$$I_n := \left(\frac{1}{x \pm i0^+}, T^n \phi\right)$$

$$I_n := \left(D\frac{1}{x \pm i0^+}, DT^n \phi\right)$$

$$= \left(D\frac{1}{x \pm 0^+}, T^{2n} D\phi\right) = \sqrt{2}\sum_{l=0}^{2K-1} h_l I_{2n+l}$$

$$\mp i\pi = \int_{-a}^{a} \frac{1}{x \pm i0^+} = \sum I_n + \text{endpoint terms}$$

$$I_n = \frac{1}{n}\sum_{m=0}^{\infty} \frac{(-1)^m}{n^m}(x^m, \phi) \approx \frac{1}{n}\sum_{m=0}^{m_{max}} \frac{(-1)^m}{n^m}\langle x^m\rangle \quad \text{n large}$$

Scattering Singularities

- These linear equations can be solved for I_n;
- The partial moments needed to treat endpoint integrals can be determined exactly.
- The method can also be applied to integrate the logarithmic singularities, and moving singularities.

Integrals over the Singularity

- Example of calculated singular I_n's for the Daubechies $K = 3$ scaling function:

K=3 $I_k^{\pm}$		
$I_{-1}^{\pm}$	-0.1717835441734	$\mp i$ 4.041140804162
$I_{-2}^{\pm}$	-1.7516314066967	$\pm i$ 1.212142562305
$I_{-3}^{\pm}$	-0.3025942645356	$\mp i$ 0.299291822651
$I_{-4}^{\pm}$	-0.3076858066180	$\mp i$ 0.013302589081

Wavelet Transform

- The Wavelet transform is the real orthogonal transformation that relates the "scaling function" basis on $\mathcal{V}_m$ to the "wavelet basis" on $\mathcal{W}_{m+1} \oplus \mathcal{W}_{m+2} \oplus \cdots \oplus \mathcal{W}_{m+k} \oplus \mathcal{V}_{m+k}$
- The matrix representation of a smooth kernel in the "wavelet basis" is the sum of a sparse matrix and a matrix with small norm:

$$K_{mn} = \int \phi_n(x) K(x,y) \phi_m(y) dx dy = S_{mn} + \Delta_{mn} \qquad \|\Delta\| < \epsilon$$

- The "wavelet approximation" is to ignore Δ_{mn}.

Wavelet Transform

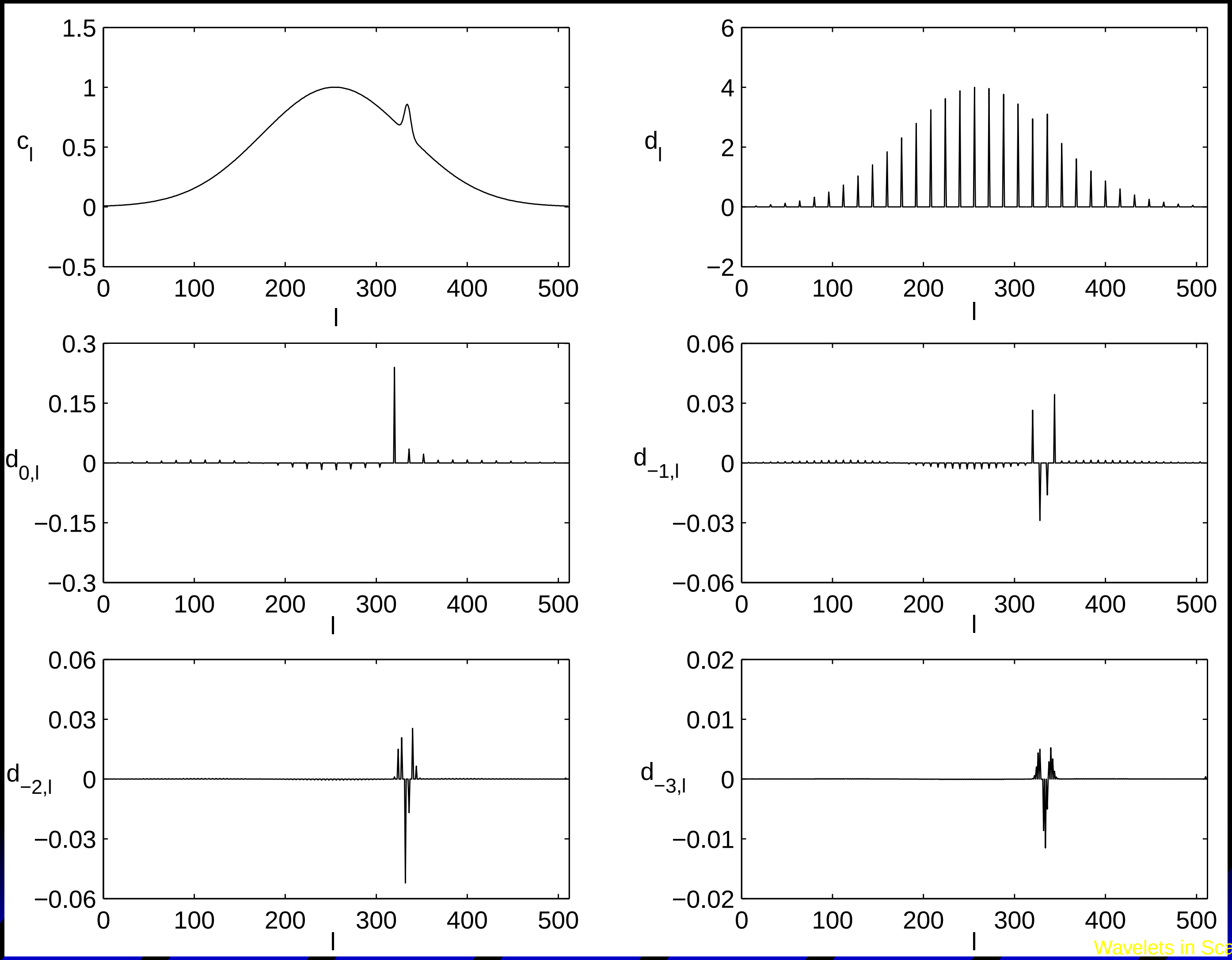
- There is an algorithm for implementing the wavelet transform that treats the coefficients h_l and g_l as coefficients of a filter.
- The wavelet transform is $o(N)$, which is faster than a fast Fourier transform.

Wavelet Transform

$$f(x) = \sum_n c_{m_f n} \phi_{m_f n}(x) = \sum_n c_{m_c n} \phi_{m_c n}(x) + \sum_{mn} d_{mn} \psi_{mn}(x)$$

$$\begin{pmatrix} c_{-3,1} \\ c_{-3,2} \\ c_{-3,3} \\ c_{-3,4} \\ c_{-3,5} \\ c_{-3,6} \\ c_{-3,7} \\ c_{-3,8} \end{pmatrix} \to \begin{pmatrix} c_{-2,1} \\ c_{-2,2} \\ c_{-2,3} \\ c_{-2,4} \\ d_{-2,1} \\ d_{-2,2} \\ d_{-2,3} \\ d_{-2,4} \end{pmatrix} \to \begin{pmatrix} c_{-1,1} \\ c_{-1,2} \\ d_{-1,1} \\ d_{-1,2} \\ d_{-2,1} \\ d_{-2,2} \\ d_{-2,3} \\ d_{-2,4} \end{pmatrix} \to \begin{pmatrix} c_{-0,1} \\ d_{-0,1} \\ d_{-1,1} \\ d_{-1,2} \\ d_{-2,1} \\ d_{-2,2} \\ d_{-2,3} \\ d_{-2,4} \end{pmatrix}$$

Wavelet Transform



Solving the L-S Equation

- Choose a fi nest resolution $\Delta = 1/2^j \Rightarrow \mathcal{V}_j$ (we use $K = 3$).
- Transform $[0, \infty]$ to a fi nite interval with the singularity at zero.
- Expand the solution in the scaling basis on $\mathcal{V}_j$.
- Use the one point quadrature for the regular integrals and the I_n for the singular integrals.
- Use the fast-wavelet transform to transform to the equivalent wavelet basis.
- Discard terms with small matrix elements.
- Solve the resulting sparse-matrix linear equation.
- Invert the solution using the fast wavelet transform.
- Insert the solution vector back in the integral equation using the one-point quadrature rule and the I_n .
- The resulting solution does NOT require the computation of the basis functions.

Model - Malfliet-Tjon V

$$H = \frac{p^2}{2m} + V$$

$$V(r) = \lambda_1 \frac{e^{-\mu_1 r}}{r} + \lambda_2 \frac{e^{-\mu_2 r}}{r}$$

$1/2m$	λ_1	μ_1	λ_2	μ_2
41.47 MeV fm^2	-570.316 MeV fm	1.55 fm^{-1}	1438.4812 MeV fm	3.11 fm^{-1}

- example: s-wave half on-shell K-matrix

Structure of equation:

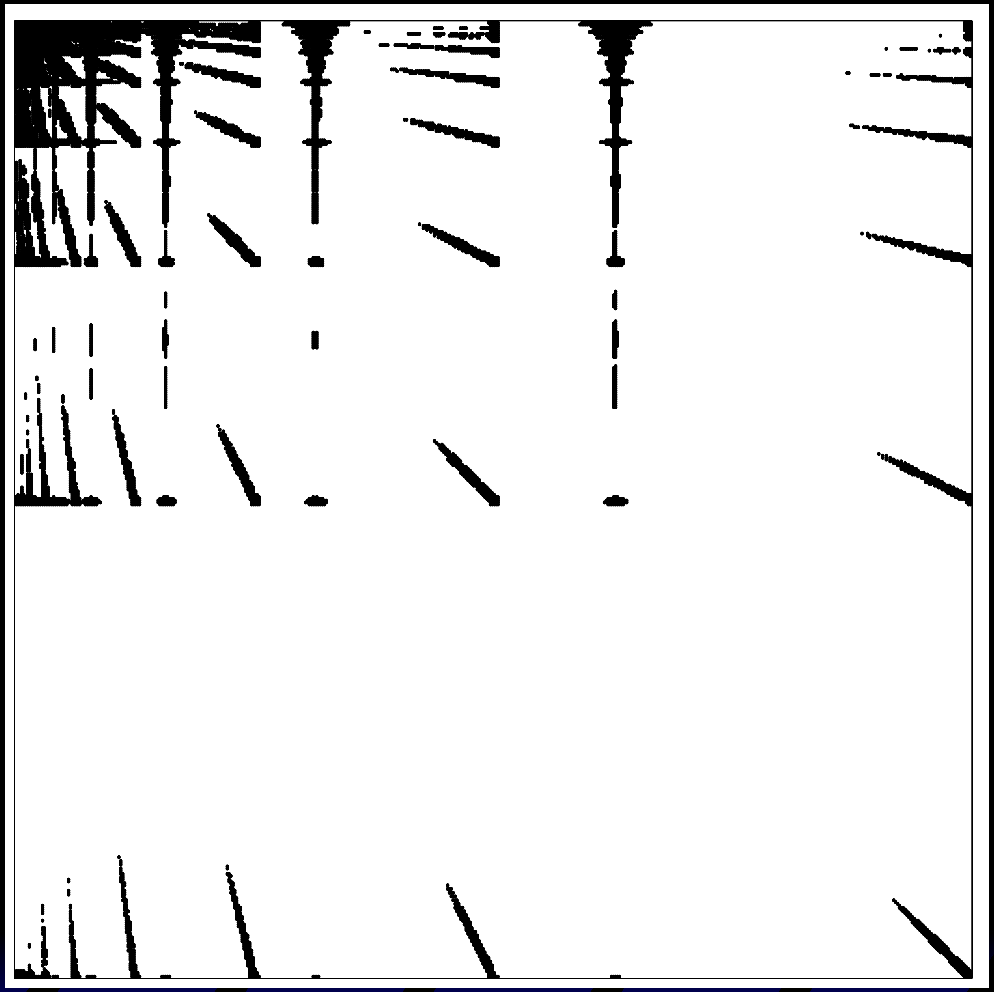
$$f(x) = g(x) + \int \frac{K(x,y)}{y} f(y)dy$$

$$f = \sum f_n \phi_n(x) \qquad x_n = \langle x^1 \rangle_{\phi_n}$$

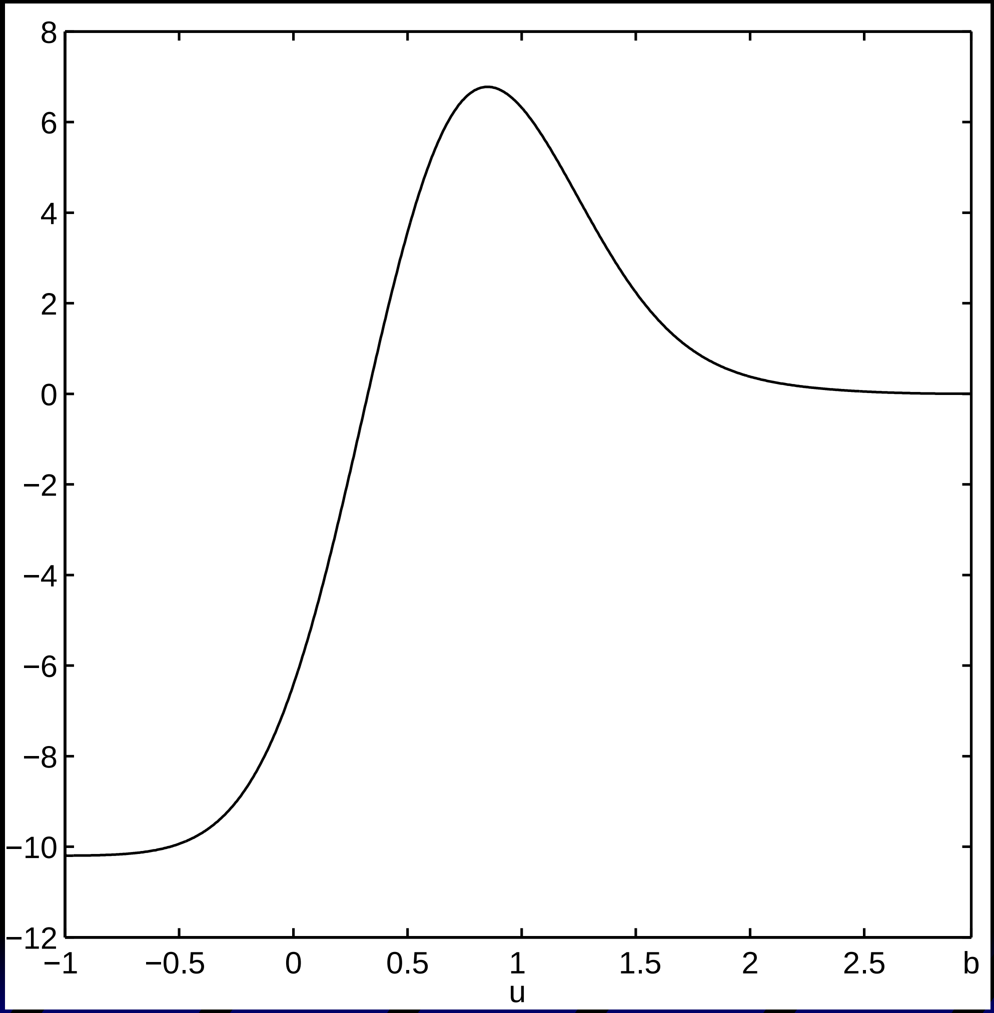
$$f_m = g(x_m) + \sum_n \left(\frac{K(x_m, y_n) - K(x_m, 0)}{y_n} + K(x_m, 0) I_n \right) f_n$$

$$f(x) = g(x) + \sum_n \left(\frac{K(x, y_n) - K(x, 0)}{y_n} + K(x, 0) I_n \right) f_n$$

Transformed Kernel



Transformed K-matrix



Why does it work?

- Consider the expansion of $f(x)$ in the wavelet basis

$$f(x) = \sum_{n=-\infty}^{\infty} d_n \phi_{mn}(x) + \sum_{n=-\infty}^{\infty} \sum_{l=m-k}^{m} c_{ln} \psi_{ln}(x);$$

$$c_{ln} = \int_{2^l n}^{2^l(n+2K-1)} \psi_{ln}(x) f(x) dx$$

- c_{ln} vanishes if $f(x)$ can be represented by a polynomial of degree K on $[2^l n, 2^l(n+2K-1)]$.

$K = 3, E = 10$ MeV

-J	N	series on-shell	interpolated on-shell
3	32	-125.051451	-125.034060
4	64	-125.007967	-125.006049
5	128	-125.005171	-125.004948
6	256	-125.004847	-125.004820
7	512	-125.004806	-125.004803

$$K = 3,\ E = 80 MeV$$

-J	N	series on-shell	interpolated on shell
3	32	-6.44161445	-6.43154124
4	64	-6.42926712	-6.42868443
5	128	-6.42842366	-6.42840177
6	256	-6.42837147	-6.42837210
7	512	-6.42836848	-6.42836877

Sparse Matrix Convergence

K=3, E=10 MeV, J=-7

ϵ	percent	on-shell value	on-shell error	mean-square error
0	100	-125.00480	0	0
10^{-9}	17.78	-125.00480	1.05×10^{-8}	2.56×10^{-8}
10^{-8}	11.38	-125.00480	5.14×10^{-8}	2.44×10^{-7}
10^{-7}	6.6	-125.00475	4.49×10^{-7}	1.88×10^{-6}
10^{-6}	3.76	-125.00269	1.69×10^{-5}	2.08×10^{-5}
10^{-5}	2.14	-124.99030	.000116	.000228
10^{-4}	1.24	-124.85112	.00123	.00217
10^{-3}	.72	-123.82508	.00944	.0117
10^{-2}	.38	-125.25766	.00202	.128

Sparse Matrix Convergence

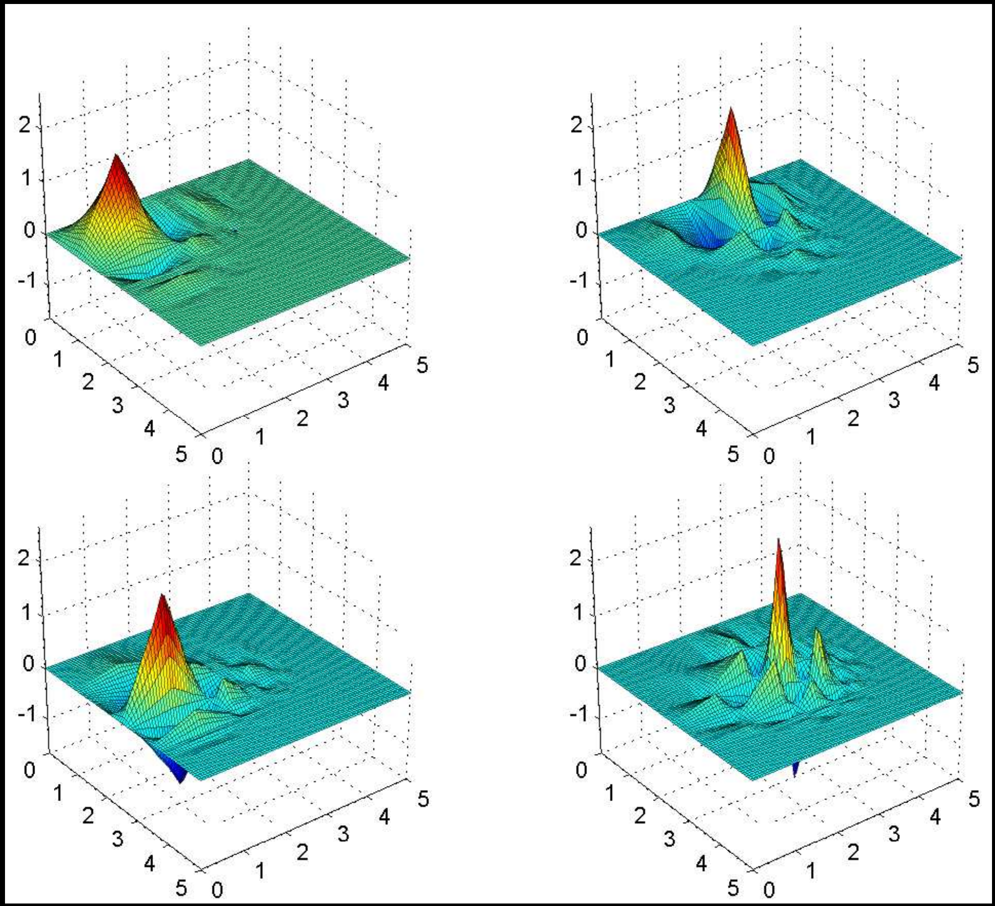
K=3, E=80, MeV J=-7

ϵ	percent	on-shell value	on-shell error	mean-square error
0	100	-6.4283688	0	0
10^{-9}	19.99	-6.4283688	1.52×10^{-10}	1.20×10^{-8}
10^{-8}	12.94	-6.4283690	3.44×10^{-8}	2.06×10^{-7}
10^{-7}	7.42	-6.4283703	2.33×10^{-7}	1.87×10^{-6}
10^{-6}	4.08	-6.4283333	5.51×10^{-6}	4.38×10^{-5}
10^{-5}	2.22	-6.4278663	7.82×10^{-5}	.000994
10^{-4}	1.21	-6.4244211	.000614	.00845
10^{-3}	.67	-6.4154328	.00201	.0229
10^{-2}	.34	-6.2935398	.021	.102

Conclusions

- Wavelet bases can be used to accurately solve the equations of scattering theory in momentum space.
- A new type of numerical analysis, called “wavelet numerical analysis”, which is based on scaling and support properties of the basis functions, is used for accurate numerical calculations.
- Wavelet “numerical analysis” leads to an accurate treatment of the scattering singularities.
- The wavelet transform leads to a sparse-matrix representation of the kernel. It automatically identifi es “irrelevant” basis functions.
- Our calculations show that a 96% reduction in the size of the matrix results in mean square error of about 1 part in 10^5 .
- We have successfully extended the method for two-body scattering without partial waves.
- We are currently applying the method to three-body problems with moving singularities.

2 D Basis Functions



2 D Sparse Matrix