# WAVELET ANALYSIS OF EXAFS DATA – RESOLUTION PROPERTIES OF THE MORLET WAVELET

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*The Morlet wavelet (MW) is a mother wavelet very suited for the analysis of Extended X-Ray Absorption Fine Structure (EXAFS) data. We determined some relevant resolution properties of the MW.*

The choice of the mother wavelet is the first crucial point for any application of wavelets. This difficulty (and at the same time the richness of the method) arises, because wavelets are built from a wide and flexible class (the function class $l^2$) of window functions $\psi(k)$ with zero mean: $\int \psi(k)dk = 0$.

For EXAFS data analysis we have chosen the complex MW /1/, see figure 1. The selection of the MW has two reasons. First, its structure is similar to an EXAFS signal, since the wavelet consists of a slowly varying amplitude term and a rapidly oscillating phase term. Second, the formal mathematical description of the wavelet analysis can be treated in analogy to the Fourier analysis.

The MW is obtained by taking a complex sine wave (like in the Fourier transform (FT)), and by confining it with a Gaussian (bell-shaped) envelope.

$$\psi(k) = e^{i\eta k} \cdot \frac{e^{-k^2/2\sigma^2}}{\sqrt{2\pi\sigma}}. \qquad (1)$$

The parameter η is the frequency of the sine and cosine functions, determining how many oscillations of the sine wave are covered by a Gaussian envelope with the half width σ=1.

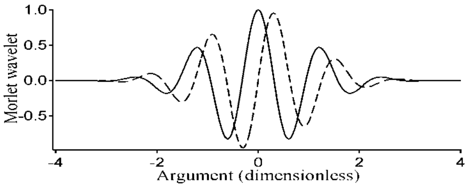

Figure 1: Real (full line) and imaginary (dashed line) part of the MW for η=5 and σ=1.

Similar to a Gaussian normal distribution, where the information uncertainty is described by the half-width σ², the WT distributes the information of the signal over some r-k cells, often called Heisenberg box /2,3/. The width of this cells is defined by the 2nd moments of the wavelet, par example in reference to k:

$$\Delta_\psi^2 = \frac{1}{\|\psi\|^2}\int_{-\infty}^{+\infty} k^2 \, |\psi(k)|^2 \, dk, \; with$$
$$\|\psi\|^2 = \int_{-\infty}^{+\infty} |\psi(k)|^2 \, dk \qquad (2)$$

Both widths (r and k) of the cells depend on the chosen wavelet. The resolution properties of the WT are determined by the size of the corresponding uncertainty cell.
For the MW (1) the Heisenberg box has the form:

$$\left[k - \frac{\eta\sigma}{\sqrt{2r}}, k + \frac{\eta\sigma}{\sqrt{2r}}\right] \times \left[r - \frac{r}{\sqrt{2\eta\sigma}}, r + \frac{r}{\sqrt{2\eta\sigma}}\right] \qquad (3)$$

From relation (3) follows that the $k - r$ window is narrowed in the *k* space for large values of *r* and is expanded for small *r*. The resolution in the *r* space decreases with increasing *r*. The Heisenberg uncertainty condition $\Delta_k \Delta_r \geq 1/2$ (see formula 3.2.17 /2/) is fulfilled by $\Delta_k \Delta_r = 1/2$. Therefore, the Morlet parameters $\eta$ and $\sigma$ determine the resolution in *k* and *r*. Figure 2 shows two typical uncertainty cells with the centers (*k*=2.5, *r*=4) and (*k*=8, *r*=1.3). The surface of both cells is equal.

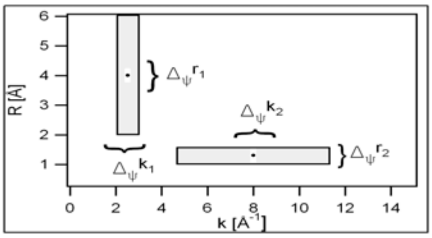

Figure 2: Two typical uncertainty cells (schematic).

To demonstrate qualitatively the effect of the described resolution properties to WT plots, the corresponding model function and their WT are plotted in figure 3. The MW parameters are η=7.5 and σ=0.5.

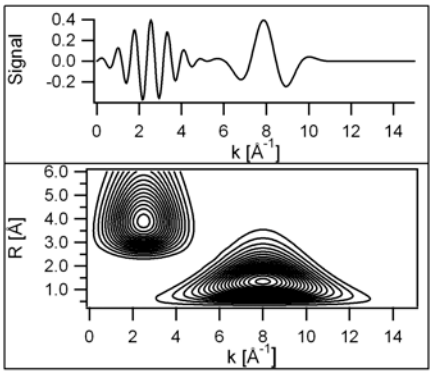

Figure 3: Model function with distances $r_1$=4.0 and $r_2$=1.3 centered at *k*=2.5 and *k*=8.0 and the WT.

The qualitative knowledge about the behavior of the uncertainty boxes is indispensable for a deeper understanding of the WT.

## References

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/3/ A. K. Louis, P. Maas and A. Rieder, *Wavelets: Theory and Applications* (Wiley, New York, 1997).