Wavelets for everything

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References

Wavelets

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Applications in Electronic Structure calculaiton

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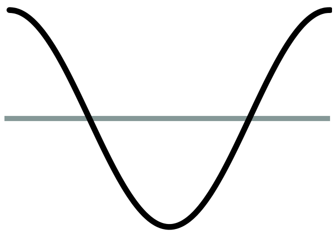
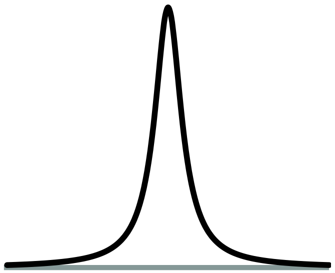
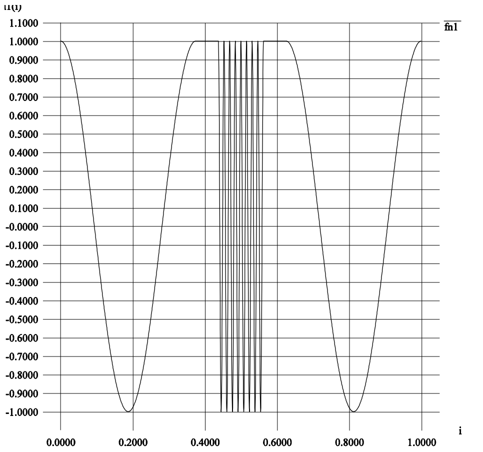
Information and efficiency





vs.



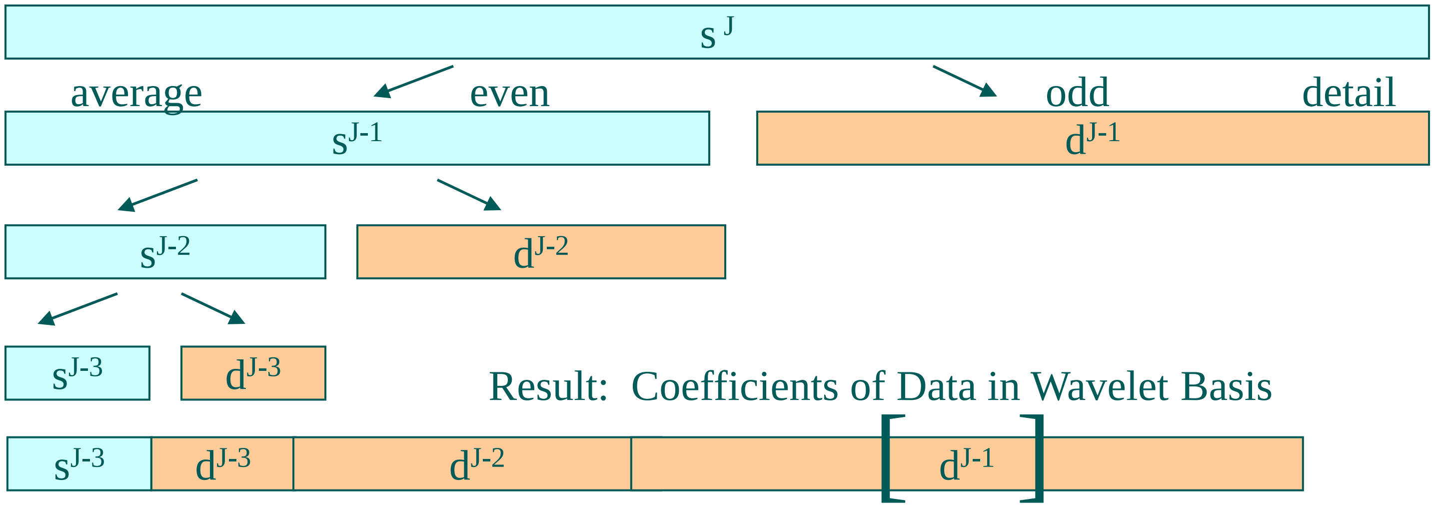
- In the absence of prior knowledge of the structure of the information, an efficient representation needs to be self-adaptive:

→ capturing the smooth average feature and the sharp detail simultaneously.

$$f(x) = \sum_i c_i b_i(x)$$

→ $b_i(x)$ should be compact in both real space and Fourier space

Wavelet transform



$$V_J = V_{j-1} \oplus W_{j-1} = V_0 \oplus W_0 \oplus \ldots \oplus W_{j-1}$$

- compact support → computational efficiency: O(N) faster than FFT O(N log(N))
- position independent transform → same basis function everywhere
- built-in multi-resolution characteristic → same basis function of different width
- s: averaged information, small amount of dense data

  ←→ basis function named "scaling function" $\phi(x)$ spanning V
- d: detailed information, sparse data only near sharp feature

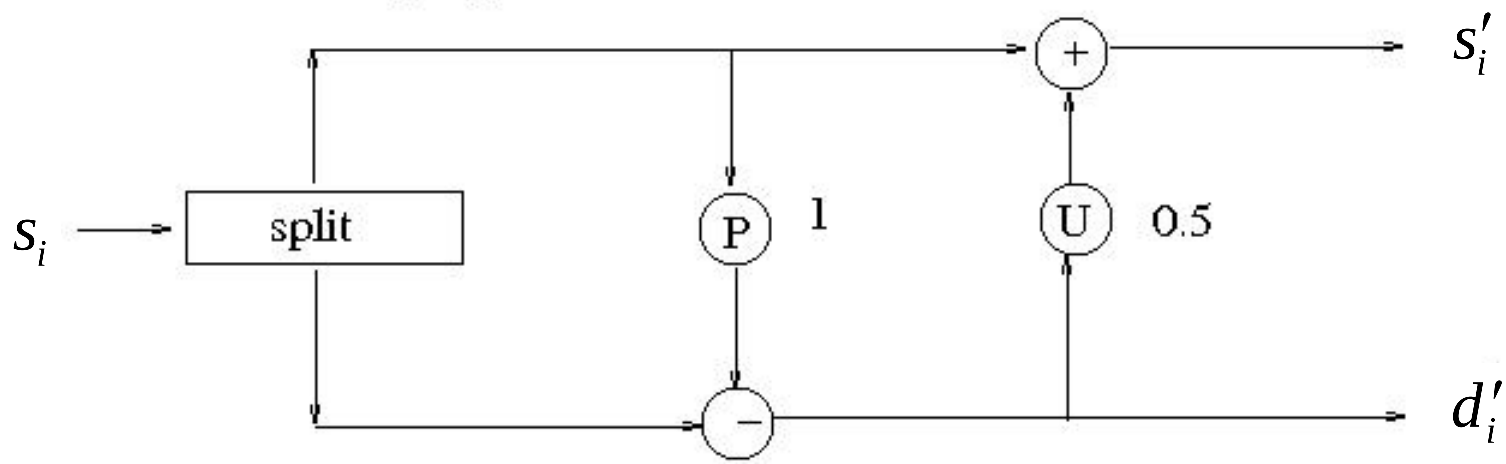
  ←→ basis function named "wavelet" $\psi(x)$ spanning W

Lifting algorithm as an example

- 1-step in CDF(2,2) wavelet transform
  Cohen, Daubechies, and Feauveau

$$s_i' = s_{2i}$$

$$s_i' = s_i' + \left(d_{i-1}' + d_i'\right)/2$$
$$= \left(-s_{2i-2} + 2s_{2i-1} + 6s_{2i} + 2s_{2i+1} - s_{2i+2}\right)/8$$



$$d_i' = s_{2i+1}$$

$$d_i' = d_i' - \left(s_i' + s_{i+1}'\right)/2$$
$$= \left(-s_{2i} + 2s_{2i+1} - s_{2i+2}\right)/2$$

- inverse transform → reverse the operation

Wavelet transform

Repeat the two-scale relation until the coarsest level is reached

FWD $$s_k^j = \sum_m \tilde{h}_{m-2k}\, s_m^{j+1}$$

$$d_k^j = \sum_m \tilde{g}_{m-2k}\, s_m^{j+1}$$

INV $$s_m^{j+1} = \sum_k \left(h_{m-2k}\, s_k^j + g_{m-2k}\, d_k^j \right)$$

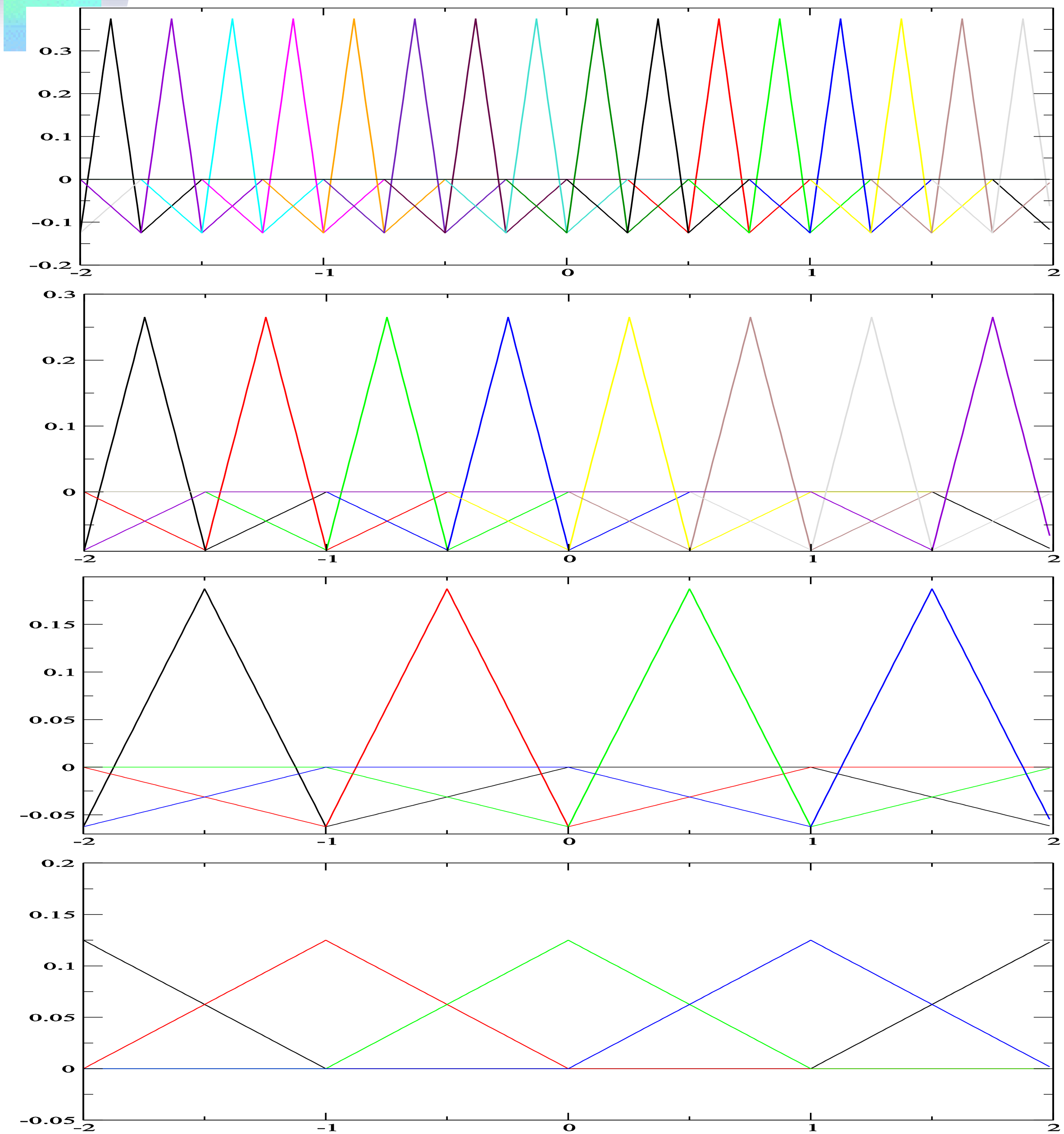
where

$$s_k^j = \left\langle \tilde{\varphi}_{j,k} \middle| f \right\rangle \qquad d_k^j = \left\langle \tilde{\psi}_{j,k} \middle| f \right\rangle$$

$$\tilde{h}_m = \left\langle \tilde{\varphi}_{j,k} \middle| \varphi_{j+1,m+2k} \right\rangle \quad \tilde{g}_m = \left\langle \tilde{\psi}_{j,k} \middle| \varphi_{j+1,m+2k} \right\rangle$$

$$h_m = \left\langle \tilde{\varphi}_{j+1,m+2k} \middle| \varphi_{j,k} \right\rangle \quad g_m = \left\langle \tilde{\varphi}_{j+1,m+2k} \middle| \psi_{j,k} \right\rangle$$

CDF(2,2) wavelets



W_2 fine

$\oplus$ $\downarrow$

W_1 wavelets

$\oplus$ $\downarrow$

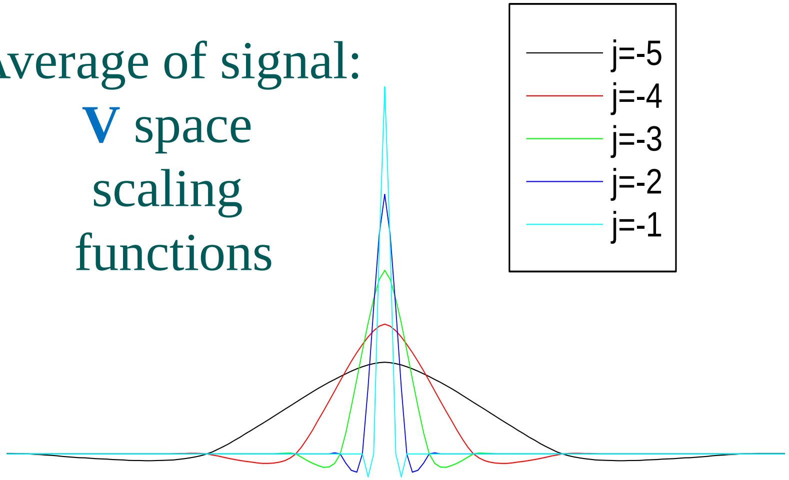
W_0

$\oplus$ $\downarrow$

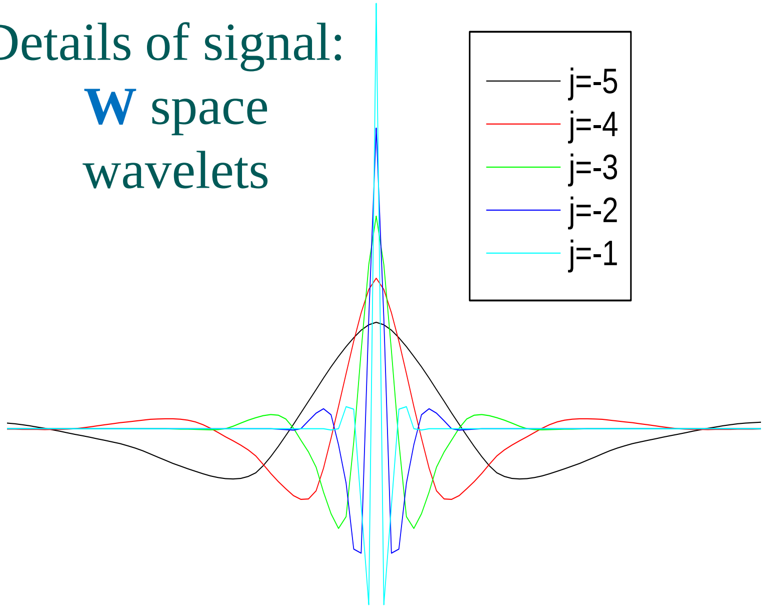
V_0 coarse scaling functions

CDF(4,4) wavelets

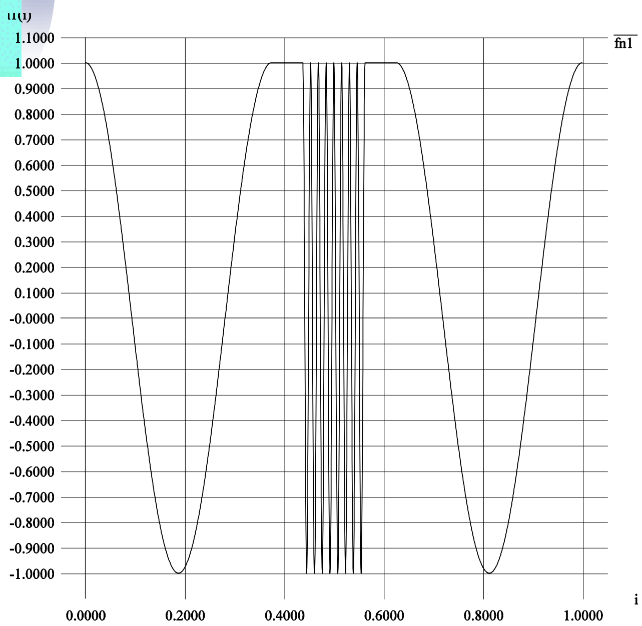
Average of signal:
V space
scaling
functions



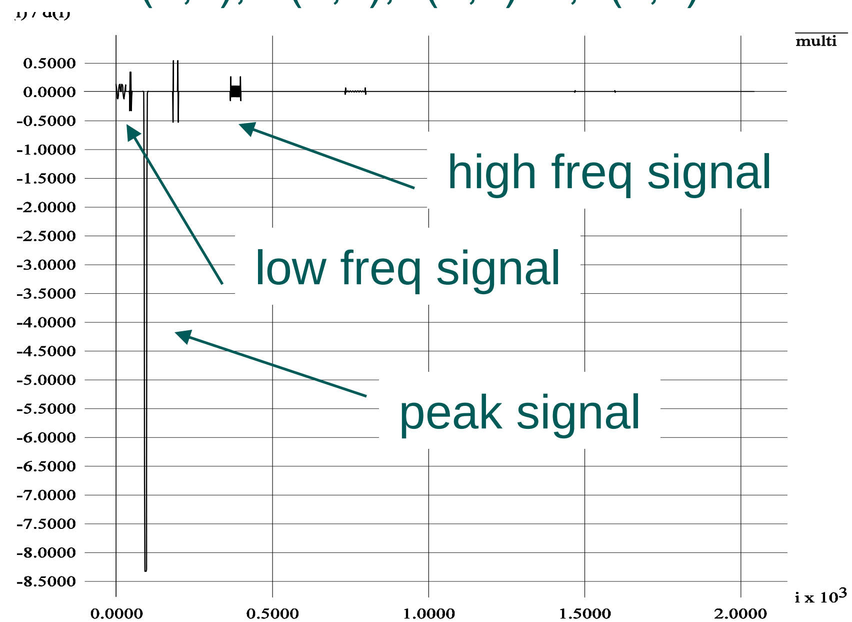
Details of signal:
W space
wavelets



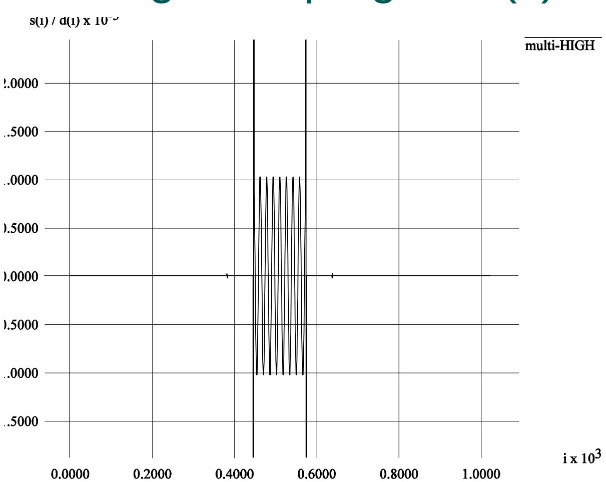
Sampled Function



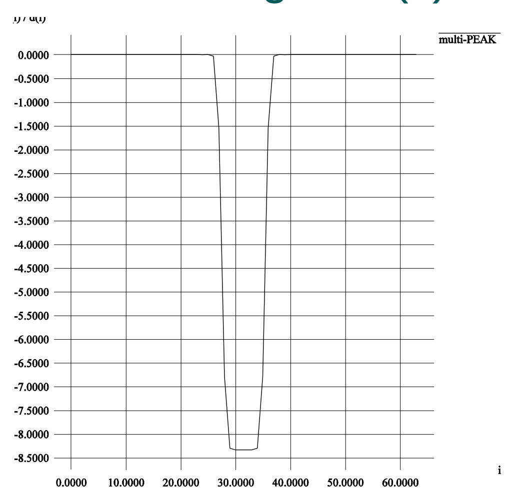
Transformed data s(0,k), d(0,k),d(1,k)…,d(J,k)



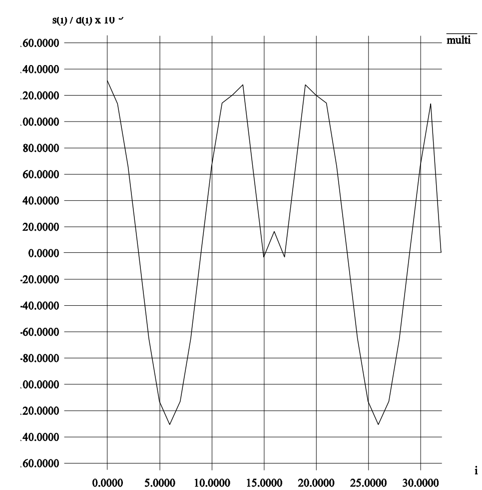
High Freq Signal d(k)



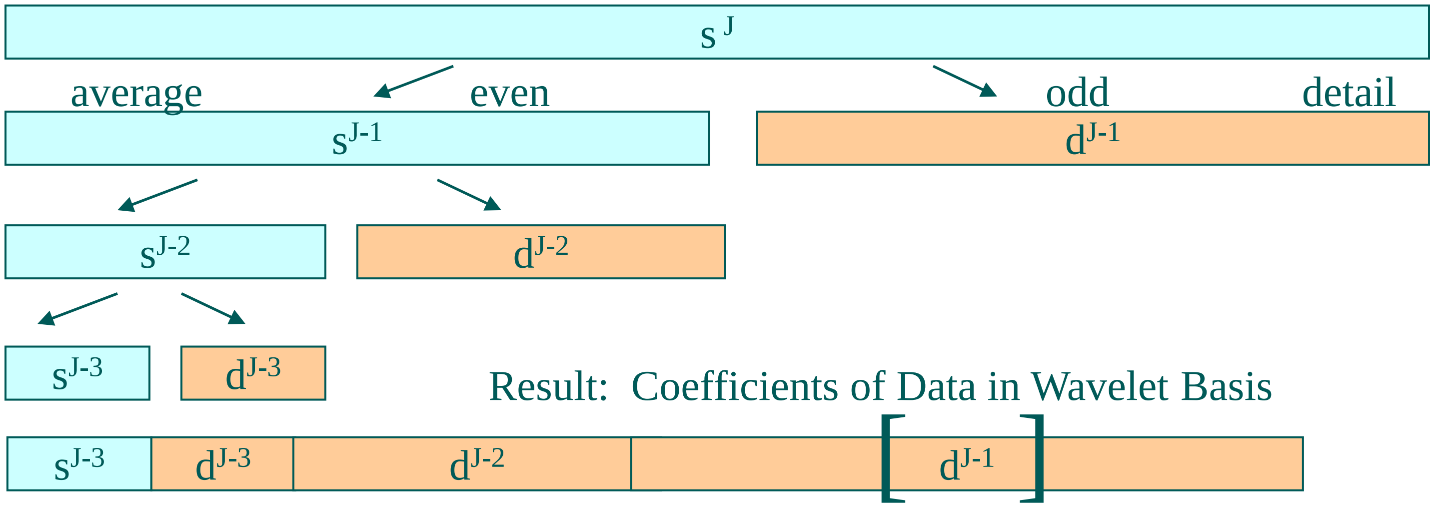
Peak Signal d(k)



Low Freq Signal s(k)



Wavelet transform



$$V_J = V_{j-1} \oplus W_{j-1} = V_0 \oplus W_0 \oplus \ldots \oplus W_{j-1}$$

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  ←→ basis function named "scaling function" $\varphi(x)$ spanning V
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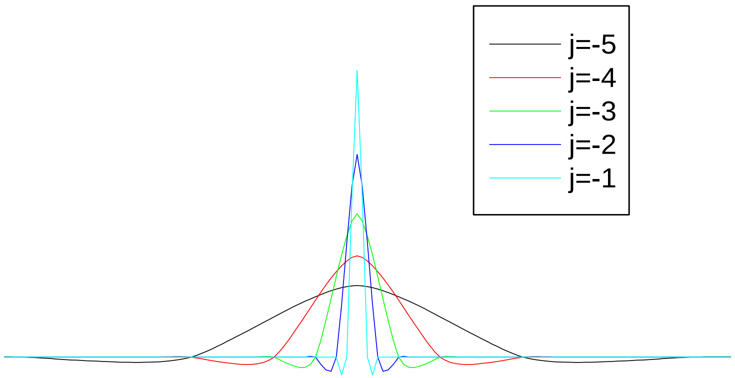
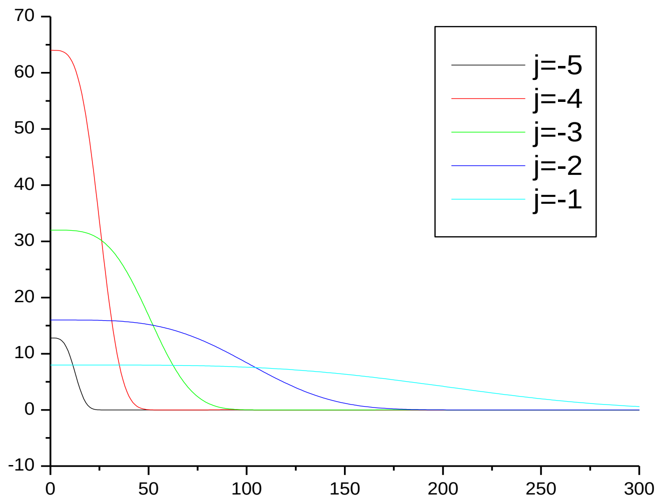
Properties of wavelets

- Strict compactness in real space



- Compactness in Fourier space

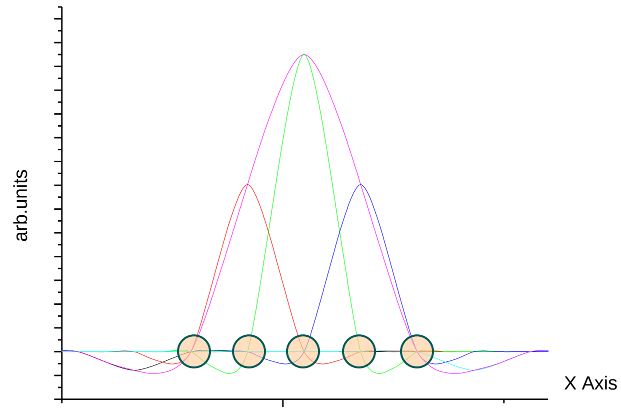


- Bi-orthogonal: duals also wavelets

  → overlap matrix unnecessary

- CDF (4,4) wavelets: Interpolating

  $f(x_i) = c_i$ for φ_i centered at x_i



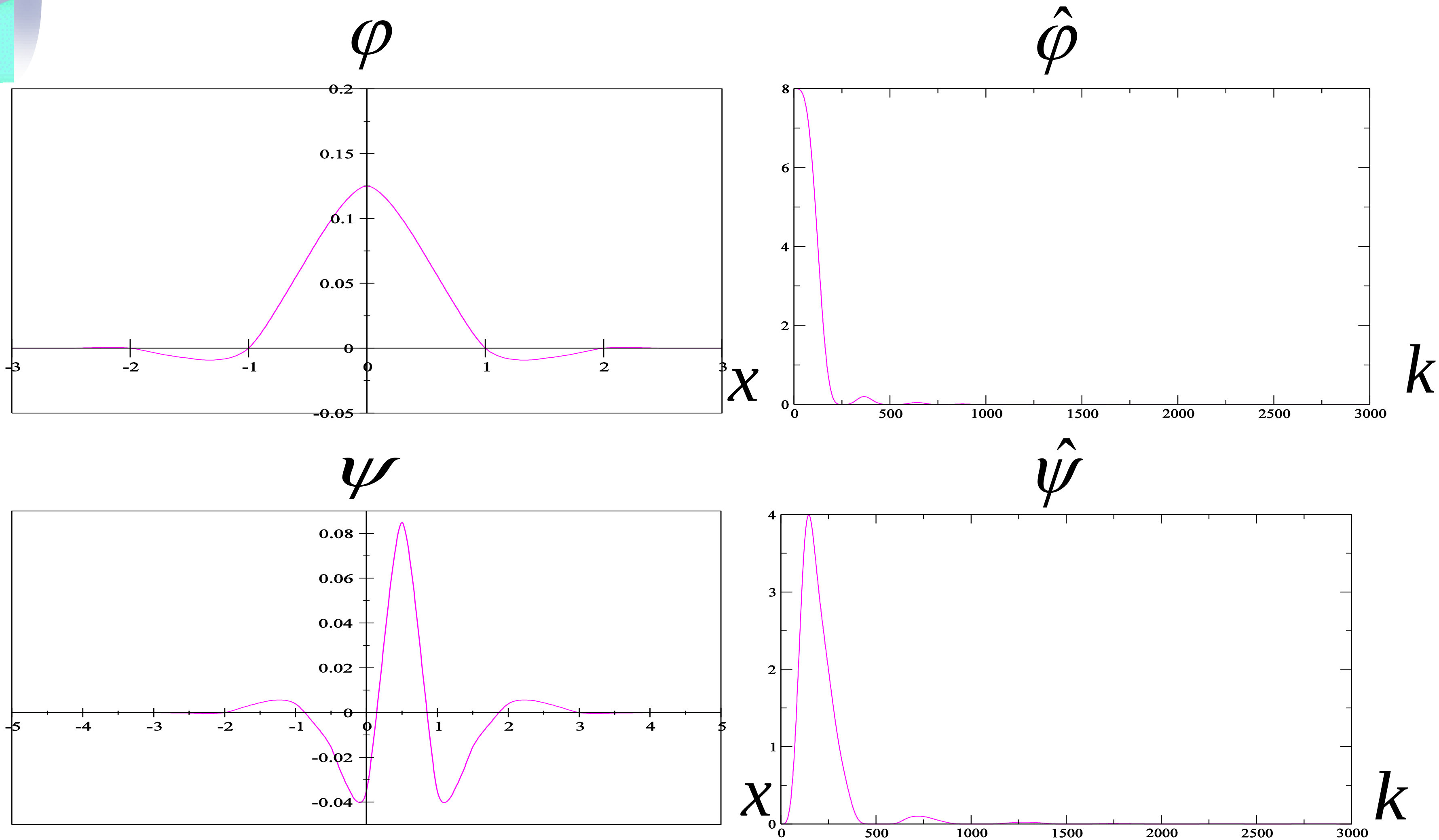
- vanishing low-order moments

$$\int \varphi(x)\,dx = 1; \quad \int x^n \varphi(x)\,dx = 0; \quad n = 1 \ldots N-1$$

$$\int x^n \psi(x)\,dx = 0; \quad n = 0 \ldots N-1$$

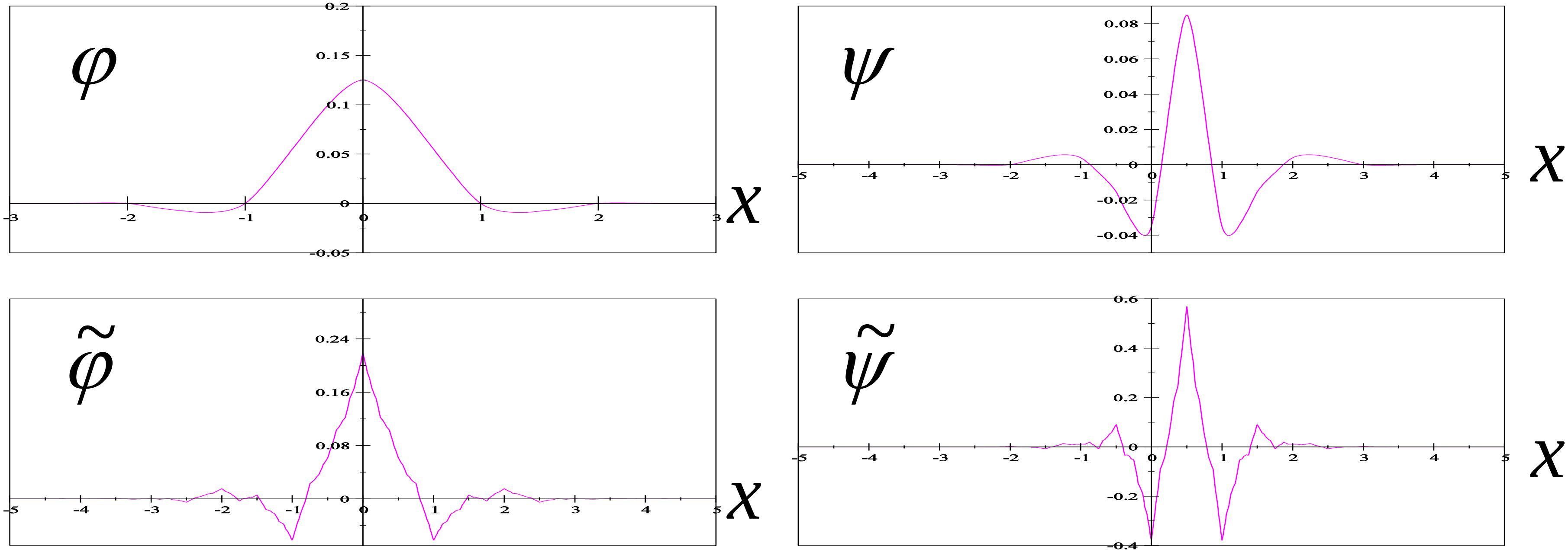
- fits 4th order polynomials
- multipole expansion → monopole

Compact in both real and Fourier space



- compact support in x } simultaneously
- localized in k.
- Potential V(x) sparse
- Kinetic Energy T(k) sparse

Bi-orthogonality



completeness: $$\mathbf{1} = \sum_k \left|\varphi_{0,k}\right\rangle\left\langle\tilde{\varphi}_{0,k}\right| + \sum_{j,k}\left|\psi_{j,k}\right\rangle\left\langle\tilde{\psi}_{j,k}\right|$$

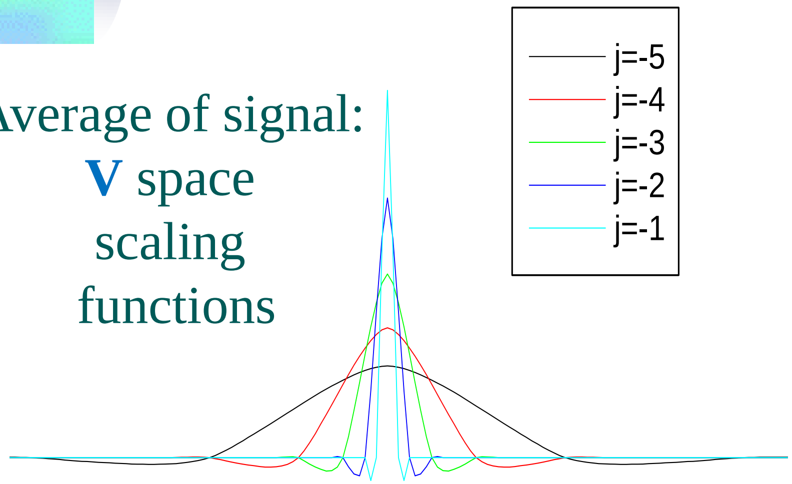
biorthogonality: $$\left\langle\tilde{\varphi}_{0,k}\middle|\varphi_{0,k'}\right\rangle = \delta_{k,k'} \quad \left\langle\tilde{\psi}_{j,k}\middle|\varphi_{0,k'}\right\rangle = 0$$

$$\left\langle\tilde{\varphi}_{0,k}\middle|\psi_{j,k'}\right\rangle = 0 \quad \left\langle\tilde{\psi}_{j,k}\middle|\psi_{j,k'}\right\rangle = \delta_{j,j'}\delta_{k,k'}$$

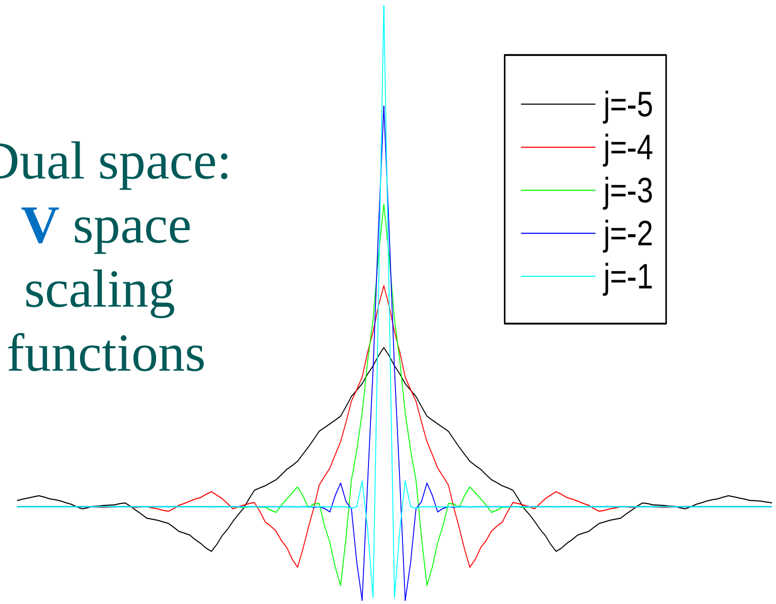
Duals of wavelets are also wavelets.

Bi-orthogonality

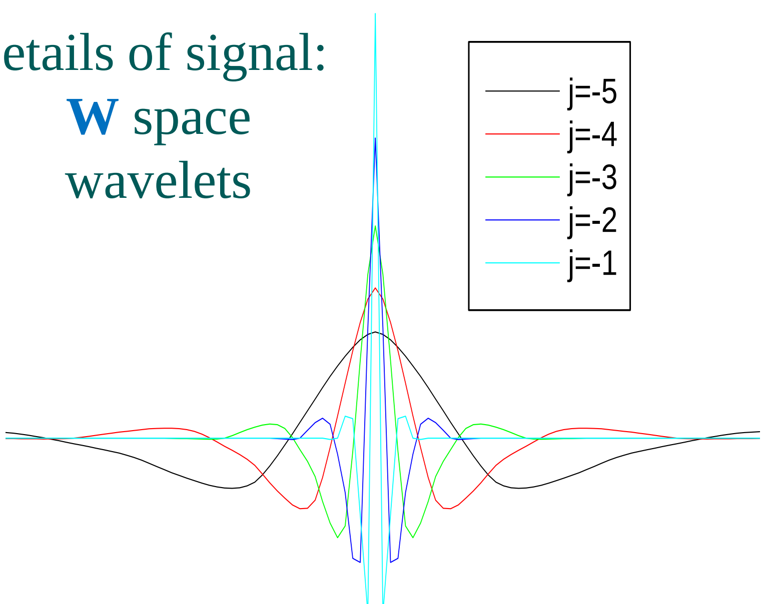
Average of signal:
V space
scaling
functions



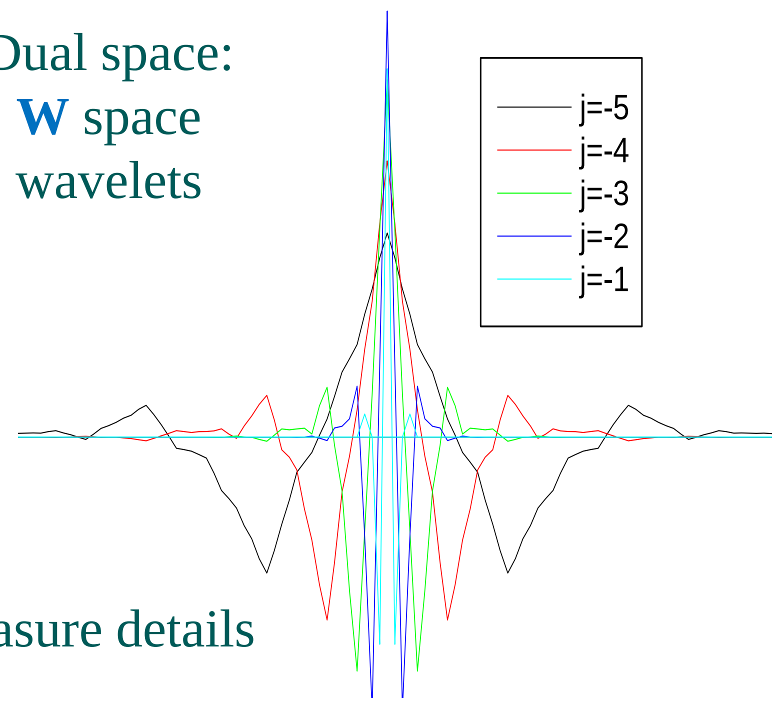
Dual space:
V space
scaling
functions



Details of signal:
W space
wavelets

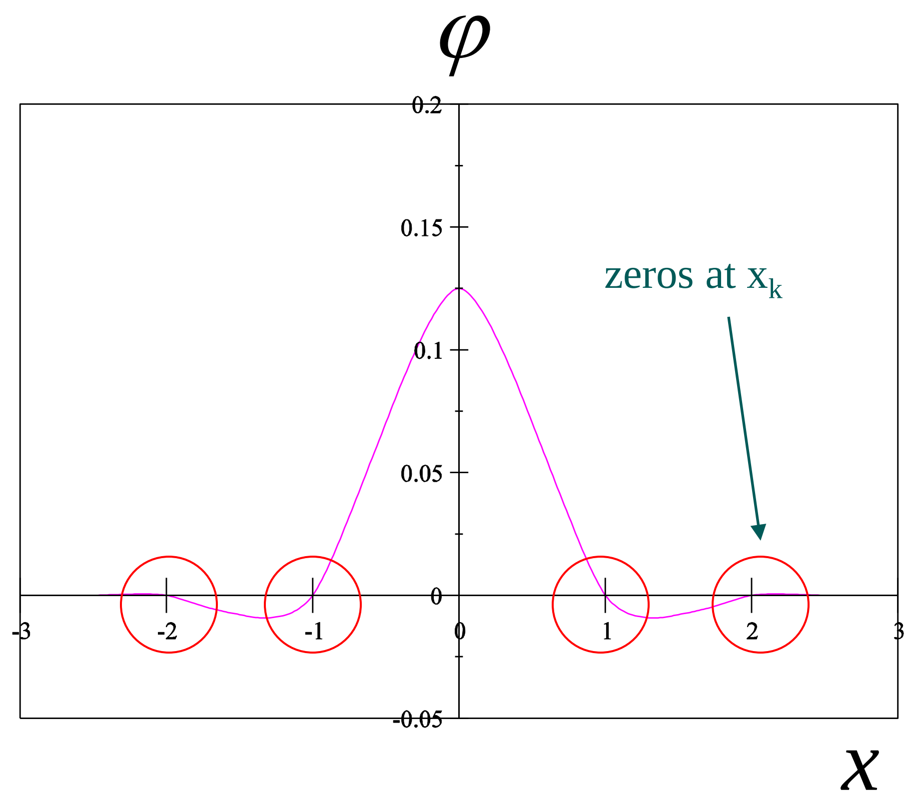


Dual space:
W space
wavelets



all wavelets have zero average: coeffs measure details

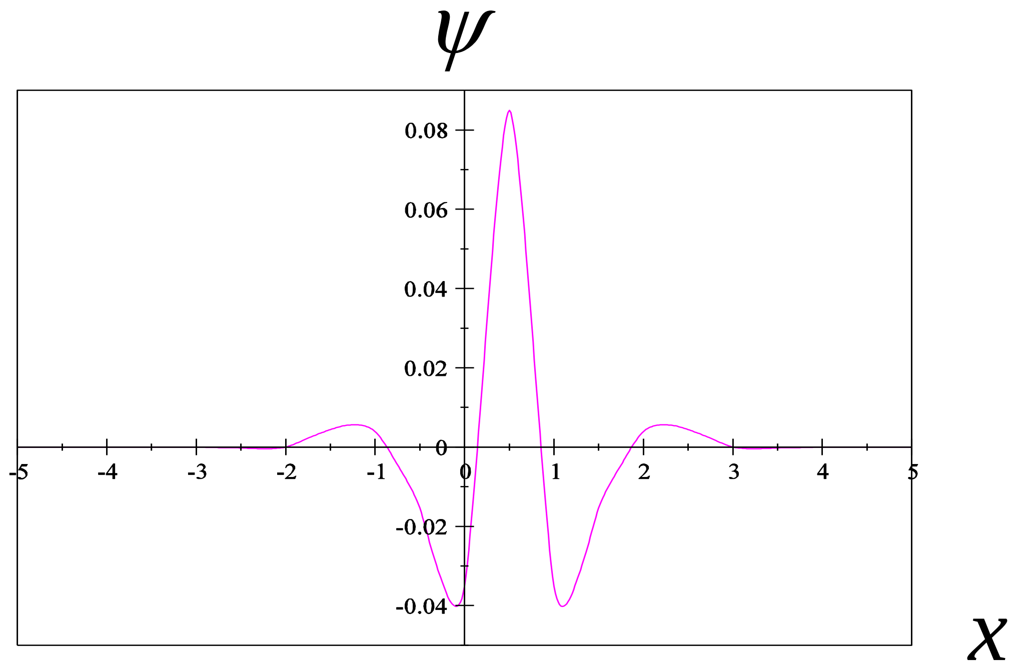
CDF(*N*,*N'*) interpolating wavelets



φ has zeros at x_k so
coefficienk s_k equals value of function at grid points at this scale.

$$f(x) = \sum_k s_k \varphi_k(x) \qquad \varphi_{k_1}(x_{k_2}) = \delta_{k_1,k_2} \qquad f(x_k) = s_k$$

Moment conservation of CDF(*N*,*N'*) wavelets



DD(4,4) wavelet ψ

- interpolates polynomials up to x^3
- has zero moments up to 3rd order.

Coulomb interaction trivial and efficient.

- Only 0^{th} moment of φ contributes.
- Acts like small number of point charges.

$$\int \psi\, dx = 0 \quad \int x\psi\, dx = 0 \quad \int x^2\psi\, dx = 0 \quad \int x^3\psi\, dx = 0$$

$$\boxed{\int \varphi\, dx = 1} \quad \int x\varphi\, dx = 0 \quad \int x^2\varphi\, dx = 0 \quad \int x^3\varphi\, dx = 0$$

Example: significant reduction of multipole expansion

$$\Phi(x) = \int \frac{\rho(x')}{|x - x'|} d^3x'$$

$$\Phi(x) = \frac{q}{r} + \frac{p \bullet x}{r^3} + \frac{1}{2}\sum_{i,j} Q_{i,j} \frac{x_i x_j}{r^5} + \text{higher} - \text{order}$$

$$Q_{i,j} = \int \left(3x_i' x_j' - r'^2 \delta_{i,j}\right) \rho(x') d^3x'$$

for ρ represented by CDF44 wavelets,

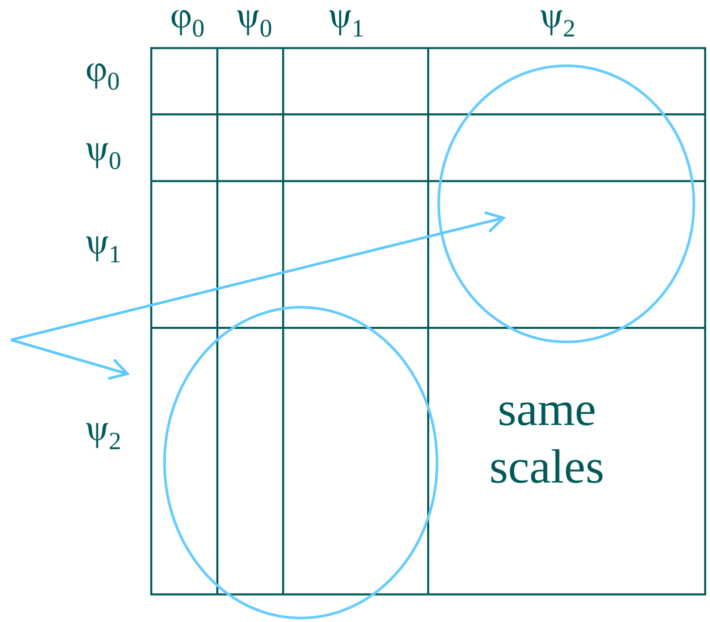
first 3 moments are zero, so

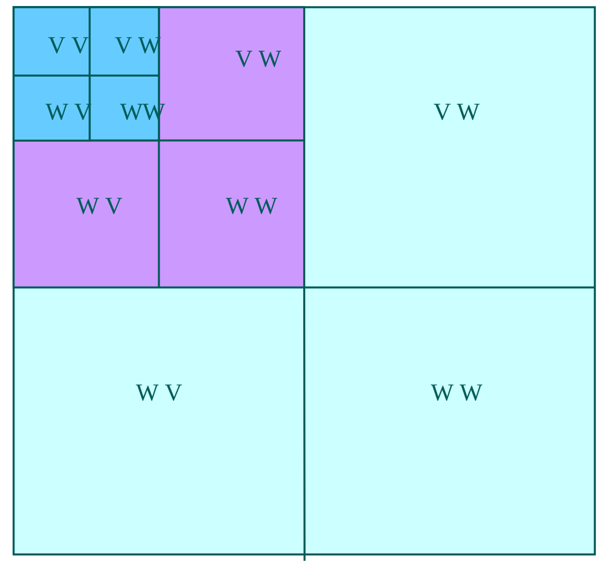
$q,\ p,\ Q_{i,j}$ are computed from the coarse scale data only :

(scaling function coefficients)

There is much less data to compute.

Higher dimension: tensor wavelets in nonstandard form





separate scales treated separately;

no mixed scales

Standard Form:
Forward Transform X and Y
Recur on whole row/col
Disadvantage:
mix scales; Operator matrix *not simple*

Nonstandard Form:
Forward Transform X and Y
Recur on V V average data
Advantage:
Data sparse; Operator matrix sparse

Operator Matrix (Laplacian):
recur on V V block. Do not mix scales
COMPACT SUPPORT → O(N): within each scale, matrices are banded
All operations O(N)

$$\text{Block of Matrix} = \left\langle \psi_{j,k1} \middle| \nabla^2 \middle| \psi_{j,k2} \right\rangle = \left\langle \psi_{j,k1-k2} \middle| \nabla^2 \middle| \psi_{j,0} \right\rangle$$

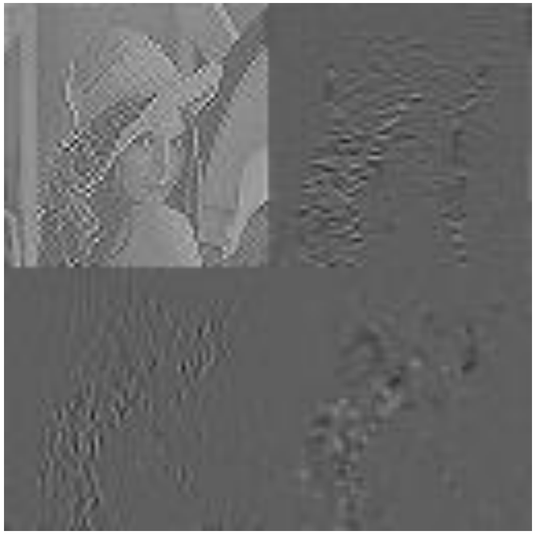
Example: 2D cubic spline forward transform

Original 512x512

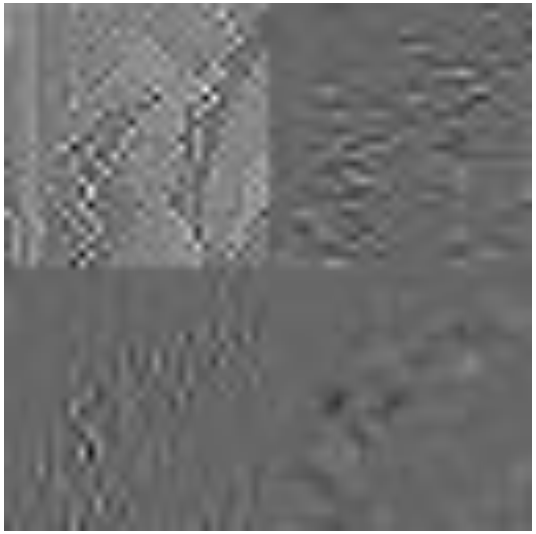
Level 4 256x256

Level 3 128x128

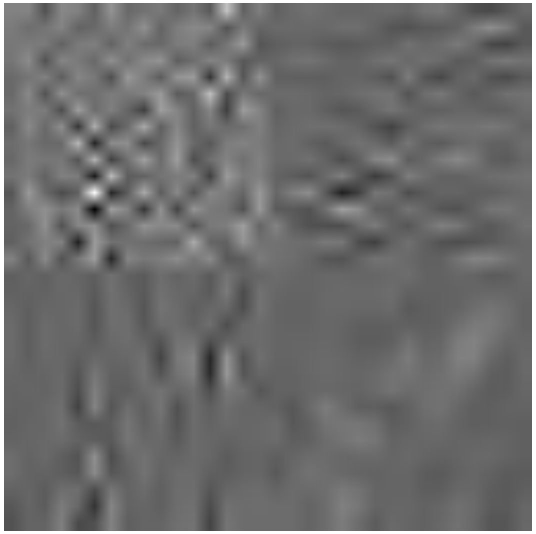
Level 2 64x64



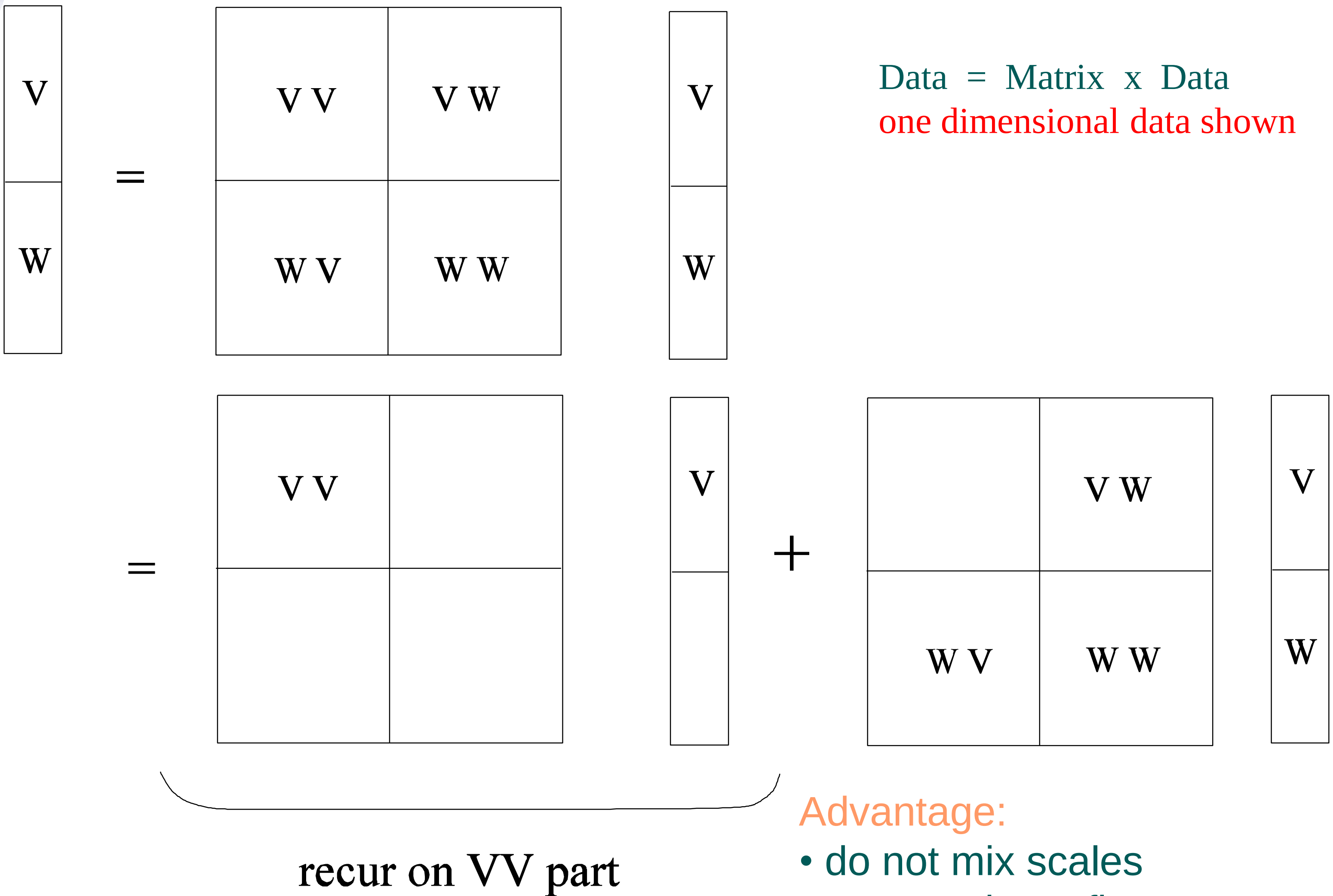
Level 1 32x32



Level 0 16x16



Linear algebra: matrix vector multiplication



Data = Matrix x Data

one dimensional data shown

Advantage:

- do not mix scales
- progressive refinement
- for translationally invariant matrix,
  blocks are simple filters: O(N)

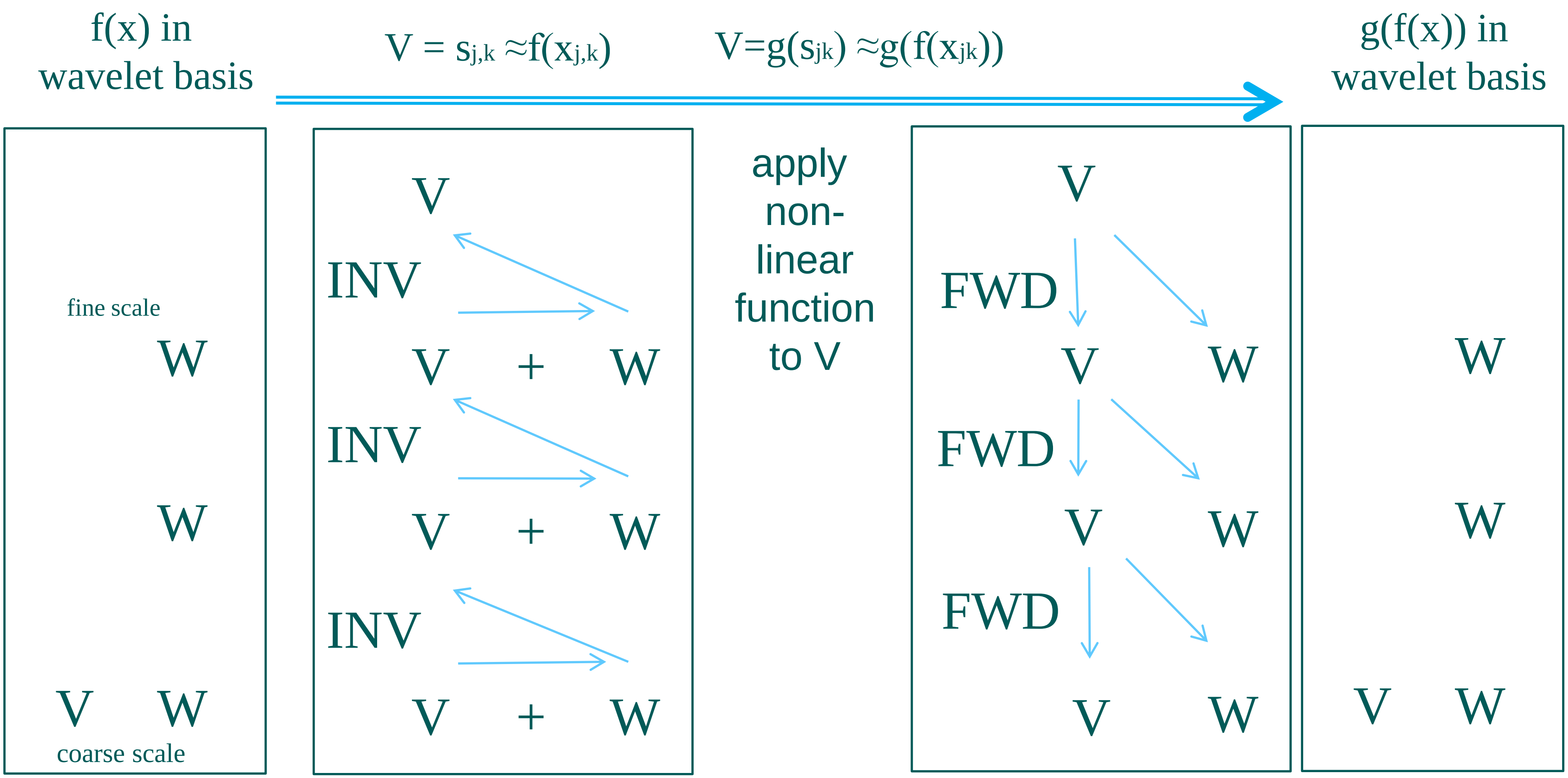
Timing: Laplacian operator

j	Size, m x m	Time, sec		**Speed = m^2/T (10^6/s)**		**Speed, Sparse/ Dense**
		Dense	Sparse	**Dense**	**Sparse**	
2	1024x1024	2.9	1.4	0.36	0.75	2.1 x faster
3	2048x2048	11.5	4.1	0.36	1.02	2.8 x faster
4	4096x4096	83	21.5	0.20	0.78	3.9 x faster
5	8192x8192	837 (swaps)	98	0.080	0.68	8.5 x faster

- Sparse wavelets faster than dense
- Handles larger problem with same amount of memory

Non-linear algebra with interpolating wavelets

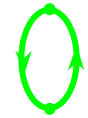
Example : $f = \frac{1}{r}\psi$; $E_{ion} = \langle \psi | f \rangle$



- interpolating property: average data V ≈ value of function at grid points
- remain within sparse representation
- wavelet transform: COMPACT SUPPORT → O(N)

An example for many-body perturbation theory

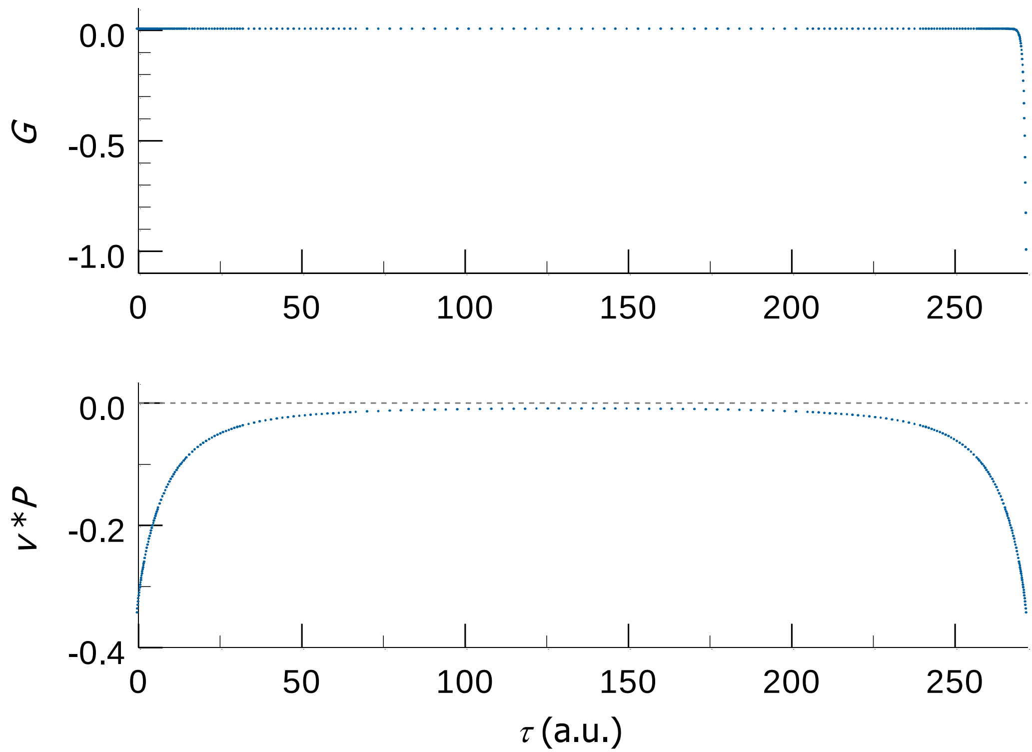
- convolution involving $1/\omega$ tail of $G(\omega)$:



$$P(1,2) = G(1,2) \cdot G(2,1)$$

$$P(\omega_n) = \sum_{i=0}^{\infty} G(\omega_n) \cdot G(\omega_n + \omega_i)$$

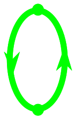
$$P(\tau) = G(\tau) \cdot G(-\tau)$$



- explicit inclusion of $\tau = 0^+$ & 0^- (2^{nd} generation of wavelets)

Non-uniform grid in Matsubara time

- convolution involving $1/\omega$ tail of $G(\omega)$:



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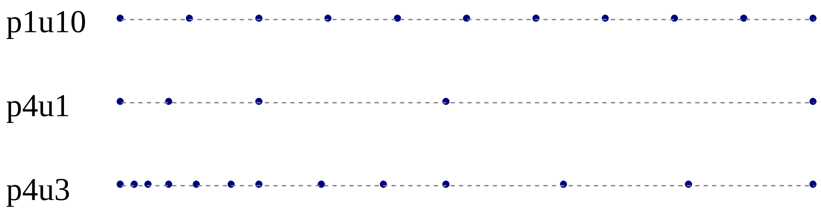

- This is the same as using the scaling function across level as basis
- Easy to handle mismatched grid point (inverse wavelet transform)

$$W(\tau) = v\cdot\delta(\tau) + \int_0^{\beta} v\cdot P(\tau-\tau')W(\tau')d\tau'$$

Wavelet++ package

Why Use Wavelets:

- compact support in space x
- localized in scale k:
  - high res detail, low res averages
  - systematic control of error
- sparse representation:
  - identify, compute with, store only critical data
  - All operations done without leaving sparse represent.
- conservation of moments
- interpolating properties
- fast O(N) algorithms for
  - wavelet transform
  - differential operators (Laplacian; Kinetic Energy)
  - nonlinear operations (External Potential)
  - products

Applications:

- physical problems
- biorthogonal bases (bra/ket)
- large data sets
- high resolution

Wavelet library

Data Structures:

- Filter
  basic convolution
- LiftingStep
  WaveletDef:
  define wavelet coeff h,g
  provide transform
- WaveletRepDense
  WaveletRepSparse
  store data

Operations:

- forward transform
- inverse transform
- function composition
- product
- convert to dense
- convert to sparse

Vector Space library

Data Structures:

- VectorSpaceDense
  VectorSpaceSparse
  Overlap Matrix for finding Duals
  Explicit treatment of crystal
  translational symmetry
- Bivector
  Wrapper associating
  WaveletRep with VectorSpace
- TranslationalyInvariantMatrix

Operations:

- Inherit Wavelet operations
- DualConj
- AddMult: Matrix Multiply
- InnerProduct

Wavelet++ library is easy to use:
Example of 2D cubic spline forward transform

```
WDEF wav = &cubic_spline;
BASIS basis(wav);
TinyI extent(512,512);
WREP wrep(extent, basis);

loadPhoto(wrep, fnamePhotoIn);
while(nlev-- > 0) {
  string fname = "photo”; fname += nlev + ".dat";
  wrep.transFwd(1);
  savePhoto(wrep, fnamePhoto);
}
```

Wavelet++ library is flexible: define your own class of wavelets

```
typedef WaveletDef<double>          WDEF;
typedef WaveletDefLiftStep<double> LSTEP;

// Haar Wavelet with Lifting Steps
WDEF haar("haar", 1/sq2, sq2,
       LSTEP(LS_PREDICT, 1, 1, -1.0),
       LSTEP(LS_UPDATE,  0, 1, 0.5));

// Daubechies Wavelet as Convolution
h = (1+sq3)*sq2/8,
    (3+sq3)*sq2/8, // Filter coefficients
    (3-sq3)*sq2/8,
    (1-sq3)*sq2/8;
g = h(3), -h(2), h(1), -h(0);
std::vector<LSTEP> v;
v[0] = LSTEP(h,g,h,g);  // convolution step
WDEF daubechies("daubechies", 1, 1, v);
```

Vector space library is easy to use: algebra & interface

dense or sparse:

```
ip = InnerProduct(v1, v2);
ip = InnerProductShift(v1, v2, deltaCell);
vz = AddMult(vy, LaplacianMatrix, vx);
vz = DualConj(vy, vx);
vz = Product(v1, v2, v3);
vz.FunctionComp(vx, functionToApply);
```

summary: using blitz++ algebra on blitz::Array base class

```
v1 += v2 + Product(v3, v4, v5)
         + InnerProduct(v3,v4) * v5
         + AddMult(v6, mat, v7);
```

Vector space library is easy to use: Laplacian operator

```
// constructors
BASIS basis(WAV);
BOXS geometry(fnameBox);
VECSPACE_SPARSE vecspaces(basisp, geometry);
VECSPACE_DENSE  vecspaced(basisp, geometry.extent());

BIVEC_SPARSE VEC1(vecspaces, VEC_BRA);
BIVEC_SPARSE VEC2(vecspaces, VEC_BRA);
BIVEC_DENSE  vec1(vecspaced, VEC_BRA);
BIVEC_DENSE  vec2(vecspaced, VEC_BRA);

LAPLACIAN mat(vecspaces);

// input data
storePolyDenseTopLevel(VEC1, vec1, function);

// convert to sparse
convertToSparse(VEC1, vec1);

// VEC2 += mat * VEC1;
AddMult(VEC2, mat, VEC1);

// convert to dense
convertToDense(VEC2, vec1);

// plot
string fnameOut = "denseout.dat";
plotBox(fnameOut, vec1);
```

Generic Algorithm

CG

Supporting Objects

Functional	Constraint	Boundary	Convergence
• Information on the energy functional used • Easy implementation of new fucntionals • get_gradient() • get_dE_2nd_order_corr()	• Information on the constraints used • Lagrange matrix • apply() • modify_gradient()	• Information on the boundaries within unit cell • Information on the crystal periodicity • apply()	• Information on the convergence criteria • apply()

```
function CG_minimization {
  boundary.apply(s);
  constraint.apply(s);
  h = functional.gradient(s);
  h = constraint.modify_gradient(h, s); // get lambda
  boundary.apply(h);
  g = h;
  dE = functional.dE_2nd_order_corr(s, h, g, lambda);
  s = s + h * dE;
  constraint.apply(s);

  until(converged) {

    g = functional.gradient(s);
    g = constraint.modify_gradient(g, s); // get lambda
    boundary.apply(g);
    h = h * (<g|g>/<gold|gold>) - g;
    dE = functional.dE_2nd_order_corr(s, h, g, lambda);
    s = s + h * dE;
    constraint.apply(s);
  }
}

class boundary {
  apply(s) {
    // set s to zero outside domain
  }
};

class constraint {
  modify_gradient(hs, ss) {
    states_unpartitioned su(s);
    states_unpartitioned hu(h);
    // actual code exploits symetry
    // only one row needed
    lambda(j,i) = InnerProduct(su(j),hu(i));
    hu = hu - lambda(j,i) su(j)
  }
  apply(ss) {
    // apply symmetric orthogonalization to ss in place.
  }
};
```

```
class functional {
  gradient(hs, ss) {
    hs = wavelet_Hamiltonian_functor(ss);
  }
  dE_2nd_order_corr(ss, hs, gs, constraint, dE) {
    // H represents hamiltonian functor in get_gradient
    dE = <gs|gs> / (<hs | H | hs> - lambda(i,i) <hs|hs>);
  }
};

class states_unpartitioned {
  int nstates;
  TinyI ncells;
  int superindex(nstate, cell) { } // map indices
  int nstate(superindex) { }
  TinyI cell(superindex) { }
  // algebra on states incorporating shift between cells
  // inner product
  // overlap matrix
};
```