Perspectives of wavelet bases in simulation of lattice theories

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Abstract

We consider the perspectives of using orthogonal wavelet expansion with Daubechies wavelets for lattice theories. The discrete wavelet transform have been already applied to simulate the Landau-Ginzburg/Φ⁴ theory with the assumption that the wavelet coefficients of the order parameter Φ(x) are delta-correlated Gaussian processes in the scale-position space. This reduces the autocorrelation time of simulation, and is not the only merit of wavelet transform. By construction the wavelet transform represents the snapshot of a field at a given scale, and therefore can be used as a tool to study the correlations between fluctuations of different scales. For the same reason the relation of wavelet transform to the renormalization group are considered. We also discuss the prospective of wavelet transform to improve the Metropolis algorithm and the simulated annealing procedure.
References:
This talk is based on


C. Best, A. Schäfer and W. Greiner. Wavelets as a variational basis of the XY model. *NPB (P.S.)* 34(1994)780


Mikhail V. Altaisky

Perspectives of wavelet bases in simulation of lattice theories
References
...and also related author’s works:

Continuous and discrete wavelet transform
Continuous and discrete wavelet transform
Wavelet transform in quantum field theory
Subjects

- Continuous and discrete wavelet transform
- Wavelet transform in quantum field theory
- Resolution-dependent fields
Continuous and discrete wavelet transform
Wavelet transform in quantum field theory
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Wavelets and Monte Carlo
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- Sampling in amplitude vs. sampling in space
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- Wavelet transform in quantum field theory
- Resolution-dependent fields
- Wavelets and Monte Carlo
- Sampling in amplitude vs. sampling in space
- Gauge theories
Continuous Wavelet Transform

CWT in $L^2$-norm:

\[
\phi(x) = \frac{1}{C_g} \int \frac{1}{a^{d/2}} g \left( \frac{x-b}{a} \right) \phi_a(b) \frac{da d^d b}{a^{d+1}},
\]

\[
\phi_a(b) = \int \frac{1}{a^{d/2}} g \left( \frac{x-b}{a} \right) \phi(x) d^d x,
\]

For isotropic wavelets $g$ the normalization constant $C_{\psi}$ is readily evaluated using Fourier transform:

\[
C_g = \int_0^{\infty} |\tilde{g}(ak)|^2 \frac{da}{a} = \int |\tilde{g}(k)|^2 \frac{d^d k}{S_d |k|} < \infty,
\]

where $S_d = \frac{2\pi^{d/2}}{\Gamma(d/2)}$ is the area of unit sphere in $\mathbb{R}^d$.

\[
G : x' = ax + b, \quad U(a, b)g(x) = a^{-d/2} g \left( \frac{x-b}{a} \right), \quad d\mu(a, b) = \frac{da d^d b}{a^{d+1}}
\]
Basic wavelets for CWT

Examples

Vanishing Momenta Family: wavelets $g_1 - g_4$

$$g_n(x) = (-1)^{n+1} \frac{d^n}{dx^n} e^{-\frac{x^2}{2}}$$
Discrete Wavelet Transform

Wavelet transform on a sublattice

\[ a = a_0^m, \ b = n b_0 a_0^m, \quad n, m \in \mathbb{Z} \]

often choice \( a_0 = 2 \)

\[ \psi^m_n(x) = a_0^{-\frac{m}{2}} \psi \left( a_0^{-m} - n b_0 \right) \]

Wavelet coefficients

\[ d^m_n = \langle \psi^m_n | f \rangle \equiv \int a_0^{-\frac{m}{2}} \bar{\psi}(a_0^{-m} x - n b_0) f(x) \, dx \]

Reconstruction

\[ f(x) = \sum \tilde{\psi}^m_n(x) d^m_n + \text{error term} \]
Consider a Hilbert space of $L^2(\mathbb{R})$ functions, then the Mallat multi-resolution analysis (MRA), is an increasing sequence of subspaces \( \{ V_j \}_{j \in \mathbb{Z}}, V_j \in L^2(\mathbb{R}), \) such that

1. \( \ldots \subset V_1 \subset V_0 \subset V_{-1} \subset V_{-2} \subset \ldots \)
2. \( \text{clos } \cup_{j \in \mathbb{Z}} V_j = L^2(\mathbb{R}) \)
3. \( \cap_{j \in \mathbb{Z}} V_j = \emptyset \)
4. The spaces \( V_j \) and \( V_{j-1} \) are similar in a sense that \( f(x) \in V_j \iff f(2x) \in V_{j-1}, \quad j \in \mathbb{Z} \).
5. \( V_j = \text{linear span } \{ \phi^j_k(x), j, k \in \mathbb{Z} \}, \quad \phi^0_k(x) = \phi(x - k) \)

Since \( V_j \) and \( V_{j+1} \) are different in resolution, some details are lost in projection \( f \in V_N \) on a ladder of spaces \( V_{N+1}, V_{N+2}, \ldots \). The details can be stored in orthogonal complements \( W_j = V_{j-1} \setminus V_j \), \( Q_m = P_{m-1} - P_m \). \( \psi^m_n \) is a basis in \( W_m \).

Explicitly: \( V_0 = V_1 \oplus W_1, \quad V_1 = V_2 \oplus W_2, \ldots \)

Hence \( V_0 = W_1 \oplus W_2 \oplus W_3 \oplus \ldots \oplus V_N \)
The numerical implementation of the decomposition of a function $f \in L^2([0, 1])$ is based on the truncation of the Mallat sequence with certain finest resolution level $V_0$. The unit interval in $N = 2, 4, 8, 16, 32, \ldots$ points. The initial data vector is then denoted as $s^0 = (s^0_0, \ldots, s^0_{N-1}) \in V_0$. The projections onto the spaces $V_1, W_1, V_2, W_2, \ldots$ are sequentially performed

$$s^0 \Downarrow h \Updownarrow g \Downarrow d^1$$

$$s^1 \Downarrow h \Updownarrow g \Downarrow d^2$$

$$s^2 \Downarrow h \Updownarrow g \Downarrow d^3$$

$$\vdots$$

where $N$ denotes the size of current data vector.
Low-pass filter is a pair-averaging, high-pass filter is a difference

\[ h_1 = h_2 = \frac{1}{\sqrt{2}} \]

**Decomposition**

\[ s_k^j = \frac{s_{2k}^{j-1} + s_{2k+1}^{j-1}}{\sqrt{2}}, \quad d_k^j = \frac{s_{2k}^{j-1} - s_{2k+1}^{j-1}}{\sqrt{2}} \]

**Reconstruction**

\[ s_{2k}^{j-1} = \frac{s_k^j + d_k^j}{\sqrt{2}}, \quad s_{2k+1}^{j-1} = \frac{s_k^j - d_k^j}{\sqrt{2}} \]
Orthogonal wavelets with compact support - the Daubechies wavelets - are given not explicitly, but recursively, by functional scaling equation:

\[
\phi(x) = \sqrt{2} \sum_{k=0}^{N-1} h_k \phi(2x - k)
\]

The coefficients \(h_k\) give complete definition of the wavelet

\[
\psi(x) = \sqrt{2} \sum_{k=0}^{N-1} g_k \phi(2x - k)
\]

The coefficients \(h_k\) and \(g_k\) are referred to as low- and high-pass filter coefficients. They are related by

\[
g_k = (-1)^k h_{N-1-k}, \quad 0 \leq k < N
\]
Scaling and wavelet functions for DAUB4 wavelet

Graphs of $\phi(x)$ and $\psi(x)$ obtained at recursion level 8 for DAUB4 wavelet

"grf.dat" u 1:2
"grf.dat" u 1:3
2 and more dimensions
from M.V.Altaisky, Wavelets: Theory, Implementation, Applications, 2005

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Two ways of use

- Coordinate resolution: a microscope at a given point

\[ \phi(x, \xi) = \sum_{jk} d^j_k(\xi) \psi^j_k(x) \]
Two ways of use

- Coordinate resolution: a microscope at a given point

\[ \phi(x, \xi) = \sum_{jk} d^j_k(\xi) \psi^i_k(x) \]

- Amplitude resolution (Generalized Polynomial Chaos)


\[ \phi(x, \xi) = \sum_{jk} d^j_k(x) \psi^i_k(P(\xi)) \]

\[ P(\xi) = \int_{-\infty}^{\xi} p(s) ds \equiv u \in [0, 1] \]

\[ d^j_k(x) = \langle \phi(x) \psi^j_k(P(\xi)) \rangle_\xi \]
Partition function

\[ Z[J] = \int \exp \left( -\beta H[\phi] + \int d^d x J(x) \phi(x) \right) D\phi, \]

\[ H[\phi] = \int d^d x \left[ \frac{1}{2} (\partial \phi)^2 + \frac{1}{2} m^2 \phi^2 + V(\phi) \right] \]

Integration over a finite set of wavelet coefficients \( d^j_k \) instead of infinite set \( D\phi \)
Ginzburg-Landau Hamiltonian

\[ H[\phi] = \int d^d x \left[ \frac{1}{2} (\partial \phi(x))^2 + \frac{r_0}{2} (\phi(x))^2 + \frac{u_0}{2} (\phi(x))^4 \right] \]

Decomposition with respect Daubechies wavelets

\[ \phi(x) = \sum_{j, x'} d_{j, x'}^t \psi_{x'}^j(x) + \phi_0, \quad \langle \phi \rangle = \phi_0 \]

Fluctuating wavelet coefficients \( \langle d_{t, x}^j \psi_{x'}^j(x) \rangle = \delta_{jj'} \delta_{xx'} \delta_{tt'} A_t^j \),

\( t = (h_1, \ldots, h_d) \) is the d-dimensional filter multiindex. Thus the correlations of fluctuating wavelet coefficients depend on scale only. For Daubechies wavelets the matrix elements of the Laplacian are known analytically

\[ \int d^d x \psi_{t, x_1}^j(x) \Delta \psi_{t', x_1}^j(x) = 2^{-2j} C_{tt'} \]

Latto, Resnikoff, Tenenbaum, 1991
The correlations $A^j$ can be found by minimizing the free energy
C.Best, A.Schäfer and W.Greiner. *NPB (P.S.)*34(1994)780

$$F = U - S/\beta, \quad U = Z^{-1} \text{Tr}(He^{-\beta H}), \quad S = -k_B \sum p(u) \ln p(u)$$

This gives

$$\frac{U}{N} = -\frac{1}{2} \sum_{jt} 2^{-j(d+2)} C_{tt} A^n_t + r_0 A + \frac{3u_0}{2} A^2$$

$$+ 3u_0 \phi_0^2 A + \frac{r_0}{2} \phi_0^2 + \frac{u_0}{2} \phi_0^4,$$

$$A = \sum_{j,t} 2^{-jd} A^j_t$$

Minimizing the free energy with respect to magnetization $\phi_0$ gives

$$\phi_0 = 0 \quad \text{or} \quad \phi_0 = \sqrt{-\frac{r_0}{2u_0} - 3A}$$

The spontaneous symmetry breaking occurs then $A$ exceeds $-\frac{r_0}{6u_0}$. The minimization of the free energy with respect to $A_t^i$ gives

$$A_t^i = \frac{1}{\beta} \frac{1}{2^{-2n-1}C_{tt}} + \frac{1}{2} r_0 + 3u_0(A + \phi_0^2)$$
Fourier Path Integral

\[ x(u) = x + (x' - x)u + \sum_{k=1}^{\infty} a_k \sin \pi k u \]

\[ 0 \leq u = \frac{\tau}{\beta \hbar} \leq 1 \]

In analogy with Fourier transform one can introduce

Wavelet Path Integral Monte Carlo

\[ x(u) = x + (x' - x)u + s_0 \phi(u) + \sum_{j,k} w_j^i \psi_k^j(u) + \alpha u + \delta \]

Mean coordinate averaged in \( u \):

\[ \langle x \rangle = \frac{x + x'}{2} + s_0 + \frac{\alpha}{2} + \delta \]
\[ S[x(u)] = \beta \int_0^1 du \left\{ \frac{m}{2\beta^2 \hbar^2} \left[ x' - x + \alpha \right] + s_0 \phi'(u) + \sum_{j,k} w_j^k \psi_j^k(u) \right\}^2 + V(x(u)) \]

Kinetic term cannot be evaluated analytically. Numerical integration over \( w = (s_0, w_j^k) \) gives averages

\[ \langle A \rangle = \frac{\int dx dwe^{-S(x,w)} A(x,x)}{\int dx dwe^{-S(x,w)}} \]
Multiresolution analysis in statistical mechanics

Ising model Hamiltonian

\[-\beta H = \sum h_i s_i + \sum_{i,j} J_{ij} s_i s_j, \quad s_i \in \{-1, +1\}, \beta = (k_B T)^{-1}\]

Orthogonal wavelet transform \(W^T W = I, u = (s_1, \ldots, s_N)\):

\[-\beta H = (h^T W^T)(W u) + (u^T W^T)(W J W^T)(W u)\]

Hamiltonian in wavelet space

\[-\beta \tilde{H}[\tilde{u}] = \tilde{h}\tilde{u} + \tilde{u}^T \tilde{J}\tilde{u}\]

Configuration space of \(\tilde{u}\) is wider than that of \(u\).

Partition function

\[\tilde{Z} = \sum \omega(\tilde{u}) e^{-\beta \tilde{H}}\]
Restrictions and Results

- Only averages contribute, but not details

\[ \langle s^j_k A(\cdot) \rangle \neq 0, \langle d^j_k A(\cdot) \rangle = 0 \]

- The restriction \( u \rightarrow s \) ignoring \( d \) prevents unique reconstruction and results in Kadanoff-like blocking procedure

Left curve corresponds to Metropolis MC, right – to wavelets
Just see correlations of 2D Ising with wavelets

$64 \times 64$

"64-1.5.corr" u 1:2:3
"64-2.5.corr" u 1:2:3
1D

\[-H = J \sum_i s^0_i s^0_{i+1}, \quad s^j_{2k} = \frac{s^j_k + d^j_k}{\sqrt{2}}, \quad s^j_{2k+1} = \frac{s^j_k - d^j_k}{\sqrt{2}}\]

\[-H/J = \frac{1}{2} \sum_k (s^1_k - d^1_k)(s^1_k + s^1_{k+1} + d^1_k + d^1_{k+1})\]

\[= -\frac{1}{2} \sum_k (d^1_k)^2 + d^1_k d^1_{k+1} + \frac{1}{2} \sum_i (s^1_{2i})^2 + (s^1_{2i+1})^2 + s^1_{2i}s^1_{2i+1} + s^1_{2i+1}s^1_{2i+2}
\]

\[\quad - d^1_{2i}s^1_{2i+1} - d^1_{2i+1}s^1_{2i+2} + s^1_{2i}d^1_{2i+1} + s^1_{2i+1}d^1_{2i+2} = \ldots\]

Case of hierarchic harmonic oscillators is easier and is considered in M. Altaisky, *PLA* 374(2009)522
Example of Haar wavelet

Haar wavelet:

\[ h = \left( \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}} \right), \quad g = \left( \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}} \right) \]

The finest level variables (block size 1) admit the values

\[ s^0 \in \{-1, 1\}, \]

the second level variables (block size 2)

\[ s^1, d^1 \in \{0, \pm \sqrt{2}\}, \]

the third level variables (block size 4)

\[ s^2, d^2 \in \{0, \pm 1, \pm 2\}, \]

the fourth level variables (block size 8)

\[ s^3, d^3 \in \{0, \pm \frac{1}{\sqrt{2}}, \pm \sqrt{2}, \pm 2\sqrt{2}\}, \]

etc.
For $M = 2$ the finest resolution space $V_0$ is the span of a four spinor product

$$\Psi = \psi_0 \psi_1 \psi_2 \psi_3,$$

which transforms according to $(D^{1/2}_{1/2} \otimes D^{1/2}_{1/2}) \otimes (D^{1/2}_{1/2} \otimes D^{1/2}_{1/2})$. We define $V_1$ as a linear span of the states of maximal spin of each block:

$$V_1 = D_1 \otimes D_1 = D_2 \oplus D_1 \oplus D_0.$$

In this case the detail space $W_1$ is

$$W_1 = V_0 \setminus V_1 = D_1 \otimes D_0 + D_0 \otimes D_1 + D_0 \otimes D_0.$$

Similarly, the $V_2$ space is the maximal spin state of a next level block, which transforms according to $D_2$. The corresponding detailed space is

$$W_2 = V_1 \setminus V_2 = D_1 \oplus D_0.$$

The total number of degrees of freedom is conserved. $V_0 = W_1 \oplus W_2 \oplus V_2$. Their dimensions are $16 = 7 + 4 + 5$. 

\[
\frac{dx_1(t)}{dt} = A_1 x_2(t) x_3(t), \quad \frac{dx_2(t)}{dt} = A_2 x_1(t) x_3(t), \quad \frac{dx_3(t)}{dt} = A_3 x_1(t) x_2(t),
\]

describing convective processes, subjected to the incompressibility condition \( A_1 + A_2 + A_3 = 0 \). In our study we set \( A_1 = A_2 = 1, A_3 = -2 \).

The KO system is badly treated by Wiener-Hermite expansion: If the initial perturbation is Gaussian \( \xi_k \), the second order terms \( \xi_i \xi_j \) will always affect it. This results in its failure to describe equipartition and causes numerical oscillations.
MC simulation of KO system with random initial conditions from Altaisky, Popova, Saraev in Proc. DD’09

Mean values for the KO system with normally distributed initial conditions. \( \sigma(x(0)) = \sigma(y(0)) = \sigma(z(0)) = 0.1 \).

\[ x(0) = 0.07, y(0) = 0.01, z(0) = -1.0; \] 5000 MC trajectories.
PC solution for the KO system, obtained with Hermitean polynomials up to the second order and normally distributed initial conditions, \( \sigma(x(0)) = \sigma(y(0)) = \sigma(z(0)) = 0.1 \).
\[
x(0) = 0.07, y(0) = 0.01, z(0) = -1.0
\]
In terms of wavelet transform the random initial conditions
\[ x_i(0, \xi) = \langle x_i(0) \rangle + \sigma \xi \]
gives \( \alpha d_{jk}^i(0) \) to be the wavelet coefficients of \( \langle x_i(0) \rangle + \sigma P^{-1}(u) \). The KO system with gPC-wavelet substitution leads to the system of ODE for the wavelet coefficients \( d_{jk}(t) \).

\[
\begin{align*}
\dot{d}_{jk}^1 &= d_{j_1 k_1}^2 d_{j_2 k_2}^3 \langle \psi_{jk} \psi_{j_1 k_1} \psi_{j_2 k_2} \rangle \\
\dot{d}_{jk}^2 &= d_{j_1 k_1}^1 d_{j_2 k_2}^3 \langle \psi_{jk} \psi_{j_1 k_1} \psi_{j_2 k_2} \rangle \\
\dot{d}_{jk}^3 &= -2 d_{j_1 k_1}^1 d_{j_2 k_2}^2 \langle \psi_{jk} \psi_{j_1 k_1} \psi_{j_2 k_2} \rangle,
\end{align*}
\]

where the connection coefficients
\[
\langle \psi_{jk} \psi_{j_1 k_1} \psi_{j_2 k_2} \rangle \equiv \int_{-\infty}^{\infty} \psi_{jk}(x) \psi_{j_1 k_1}(x) \psi_{j_2 k_2}(x) dx
\]
are evaluated using the connections
\[
\Lambda_{k,m} \equiv \int \phi(t) \phi(t - k) \phi(t - m) dt
\]
Mean values for the KO system with normally distributed initial conditions. \( \sigma = 0.1 \). \( x(0) = 0.07, y(0) = 0.01, z(0) = -1.0 \). DAUB4 wavelet transform with 3 scales was used.
Variances for the KO system with normally distributed initial conditions. \( \sigma = 0.1 \). \( x(0) = 0.07, y(0) = 0.01, z(0) = -1.0 \). DAUB4 wavelet transform with 3 scales was used.
Mean values for the KO system with normally distributed initial conditions. \( \sigma = 0.1 \). \( x(0) = 0.07, y(0) = 0.01, z(0) = -1.0 \)

DAUB6 wavelet transform with 3 scales was used.
KO: variance with DAUB6

Variances for the KO system with normally distributed initial conditions. \( \sigma = 0.1. \) \( x(0) = 0.07, y(0) = 0.01, z(0) = -1.0. \) DAUB6 wavelet transform with 3 scales was used.
To flip entire blocks by random change of bigger level coefficients $d_k^j, j > 0$, rather than $s_k^j$.

If the energy of the new configuration obtained in this way is less than the energy of initial configuration, then the new configuration is accepted.

If not, then the Metropolis algorithm is applied to the coarse scales first, i.e. to spin configuration constructed for only the coarse coefficients are present;

If the configuration is accepted at the coarse level then the Metropolis algorithm goes one level down.

The procedure should be continued up to the finest resolution level. The temperature may depend on the level $T = T(t, j)$. 

\[ \text{The temperature may depend on the level } T = T(t, j). \]
The wavelet transform of the matrix $J_{ij}$ is performed only once. Having this done the Metropolis algorithm will not spend unnecessary calculations of small scale details in case the large scale block was flipped.

We also expect that the block structure of matrix to vector multiplication in wavelet space provides for effective parallelization.

We expect that some information about the coupling matrix $J_{ij}$ will enable for choosing different temperatures at different levels of the wavelet transform to speed up the simulated annealing procedure.
Gauge fixing
T. Draper and C. McNeile. hep-lat/9312044

Coulomb gauge fixing

\[ F = \frac{1}{2n_c3V} \sum_x \sum_{k=1}^3 \text{Tr}(U_k^g(x) + U_k^g(x)^\dagger), \quad U_k^g(x) = G(x)U_k(x)G^\dagger(x+k) \]

Single iteration \( G(x) = \exp(\omega_a(x) T_a \alpha), \) where \( \alpha \) is a step size, \( T_a \) are the \( SU(3) \) generators,

\[ \omega_a(x) = -i \sum_{k=1}^3 \text{Tr} T_a \Delta_{-k}(U_k(x) - U_k(x)^\dagger) \]

Find maximum of \( F \) using \textbf{fast matrix multiplication} CTH Davies et al. PRD 37(1988)1581

**FFT**

\[
G(x) = \exp \left( \hat{F}^{-1} \frac{\hat{p}_x^2}{\hat{p}^2} \hat{F} \omega_a(x) T_a \alpha \right)
\]

**FWT**

\[
G(x) = \exp \left( \hat{W}^{-1} \hat{P} \hat{W} \omega_a(x) T_a \alpha \right)
\]
Thank You for Your Attention!