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/ Φ^4 theory with the assumption that the wavelet coefficients of the order parameter $\Phi(x)$ 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.

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• Continuous and discrete wavelet transform

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- Wavelet transform in quantum field theory

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- Resolution-dependent fields

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- Gauge theories

Continuous Wavelet Transform

CWT in L^2 -norm:

$$\begin{split} \phi(x) &= \frac{1}{C_g} \int \frac{1}{a^{d/2}} g\left(\frac{x-b}{a}\right) \phi_a(b) \frac{dad^d b}{a^{d+1}}, \\ \phi_a(b) &= \int \frac{1}{a^{d/2}} \overline{g\left(\frac{x-b}{a}\right)} \phi(x) d^d x, \end{split}$$

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

$$C_g = \int_0^\infty | ilde{g}(ak)|^2 rac{da}{a} = \int | ilde{g}(k)|^2 rac{d^d k}{S_d |k|} < \infty,$$

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

$$G: x'=ax+b, \quad U(a,b)g(x)=a^{-d/2}g\left(rac{x-b}{a}
ight), \quad d\mu(a,b)=rac{dad^db}{a^{d+1}}$$

Basic wavelets for CWT

Vanishing Momenta Family: wavelets g1 - g4



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

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Discrete Wavelet Transform

Wavelet transform on a sublattice

$$a = a_0^m, b = nb_0a_0^m, \quad n,m \in Z$$

often choice $a_0 = 2$

$$\psi_{n}^{m}(x) = a_{0}^{-\frac{m}{2}}\psi\left(a_{0}^{-m} - nb_{0}\right)$$



Wavelet coefficients

$$d_n^m = \langle \psi_n^m | f \rangle \equiv \int a_0^{-\frac{m}{2}} \overline{\psi}(a_0^{-m}x - nb_0)f(x)dx$$

Reconstruction

$$f(x) = \sum ilde{\psi}_n^m(x) d_n^m + ext{error term}$$

Multi-Resolution Analysis

Consider a Hilbert space of $L^2(\mathbb{R})$ functions, then the Mallat multiresolution analysis (MRA), is an increasing sequence of subspaces $\{V_j\}_{j\in\mathbb{Z}}, V_j \in L^2(\mathbb{R})$, such that

$$... \subset V_1 \subset V_0 \subset V_{-1} \subset V_{-2} \subset ...$$

2 clos
$$\cup_{j\in\mathbb{Z}} V_j = L^2(\mathbb{R})$$

• The spaces V_j and V_{j-1} are similar in a sense that $f(x) \in V_j \Leftrightarrow f(2x) \in V_{j-1}, \quad j \in \mathbb{Z}.$

• $V_j = \text{linear span } \{\phi_k^j(x), j, k \in \mathbb{Z}\}, \quad \phi_k^0(x) = \phi(x-k)$

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 $W_j = V_{j-1} \setminus V_j$, $Q_m = P_{m-1} - P_m$. ψ_n^m is a basis in W_m Explicitly: $V_0 = V_1 \oplus W_1$, $V_1 = V_2 \oplus W_2, \ldots$ Hence $V_0 = W_1 \oplus W_2 \oplus W_3 \oplus \ldots \oplus V_N$

Fast Wavelet Transform

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, ... points. The initial data vector is then denoted as $s^0 = (s_0^0, \ldots, s_{N-1}^0) \in V_0$. The projections onto the spaces $V_1, W_1, V_2, W_2, \ldots$ are sequentially performed ⁰ $\begin{array}{ccc} h \Downarrow & g \searrow \\ s^1 & & d^1 \end{array}$ $\begin{array}{ccc} h \Downarrow & g \searrow & \\ s^2 & d^2 & \\ \end{array} \qquad \begin{array}{ccc} s_i^j = \sum_{k=0}^{N-1} h_k s_{k+2i}^{j-1}, \\ d_i^j = \sum_{k=0}^{N-1} g_k s_{k+2i}^{j-1}, \end{array}$ $\begin{array}{c}h\Downarrow g\searrow\\s^3\end{array}$

where N denotes the size of current data vector.

Haar wavelet algorithm Scaling function $\phi(x) = \chi_{[0,1)}(x)$

Low-pass filter is a pair-averaging, high-pass filter is a difference

$$h_1 = h_2 = \frac{1}{\sqrt{2}}$$

Decomposition

$$s_k^j = rac{s_{2k}^{j-1} + s_{2k+1}^{j-1}}{\sqrt{2}}, \quad d_k^j = rac{s_{2k}^{j-1} - s_{2k+1}^{j-1}}{\sqrt{2}}$$

Reconstruction

$$s_{2k}^{j-1} = rac{s_k^j + d_k^j}{\sqrt{2}}, \quad s_{2k+1}^{j-1} = rac{s_k^j - d_k^j}{\sqrt{2}}$$

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

$$g_k = (-1)^k h_{N-1-k}, \quad 0 \le k < N$$

Scaling and wavelet functions for DAUB4 wavelet



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Two ways of use

 Coordinate resolution: a microscope at a given point

$$\phi(x,\xi) = \sum_{jk} d_k^j(\xi) \psi_k^j(x)$$



Two ways of use

 Coordinate resolution: a microscope at a given point

$$\phi(x,\xi) = \sum_{jk} d_k^j(\xi) \psi_k^j(x)$$

 Amplitude resolution (Generalized Polynomial Chaos)
 [O.P. Le Maitre et al. J. Comp. Phys. 197(2004)28]

$$egin{aligned} \phi(x,\xi) &=& \sum_{jk} d^j_k(x) \psi^j_k(P(\xi)) \ P(\xi) &=& \int_{-\infty}^{\xi} p(s) ds \equiv u \in [0,1] \ d^j_k(x) &=& \langle \phi(x) \psi^j_k(P(\xi))
angle_{\xi} \end{aligned}$$



Partition function

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

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

Integration over a finite set of wavelet coefficients d_k^j instead of infinite set $\mathcal{D}\phi$



Landau-Ginzburg Φ⁴ model simulation C.Best. *Nucl. Phys. B Proc. Suppl.*83(2000)848

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

$$\phi(\mathbf{x}) = \sum_{j,\mathbf{x}'} d^j_{\mathbf{x}'} \psi^j_{\mathbf{x}'}(\mathbf{x}) + \phi_0, \quad \langle \phi \rangle = \phi_0$$

Fluctuating wavelet coefficients $\langle d_{t,x}^{j} d_{t',x'}^{j'} \rangle = \delta_{jj'} \delta_{xx'} \delta_{tt'} \mathcal{A}_{t}^{j}$, $t = (h_1, \ldots, h_d)$ 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

$$\int d^d x \psi^j_{t,x_1}(x) \Delta \psi^j_{t',x_1}(x) = 2^{-2j} C_{tt'}$$

Latto, Resnikoff, Tenenbaum, 1991

Variational ansatz

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

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

This gives

$$\begin{aligned} \frac{U}{N} &= & -\frac{1}{2} \sum_{jt} 2^{-j(d+2)} C_{tt} \mathcal{A}_t^n + r_0 \mathcal{A} + \frac{3u_0}{2} \mathcal{A}^2 \\ &+ & 3u_0 \phi_0^2 \mathcal{A} + \frac{r_0}{2} \phi_0^2 + \frac{u_0}{2} \phi_0^4, \\ \mathcal{A} &= & \sum_{j,t} 2^{-jd} \mathcal{A}_t^j \end{aligned}$$

C.Best. Nucl. Phys. B Proc. Suppl.83(2000)848

Fluctuation strength in Landau-Ginzburg Φ^4 wavelet model C.Best. Nucl. Phys. B Proc. Suppl.83(2000)848

Minimizing the free energy with respect to magnetization ϕ_0 gives

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

The spontaneous symmetry breaking occures then \mathcal{A} exceeds $-\frac{r_0}{6u_0}$. The minimization of the free energy with respect to \mathcal{A}_t^j gives

$$\mathcal{A}_{t}^{j} = \frac{1}{\beta} \frac{1}{-2^{-2n-1}C_{tt} + \frac{1}{2}r_{0} + 3u_{0}(\mathcal{A} + \phi_{0}^{2})}$$



Figure 1. Wavelet fluctuation strengths at different scales as a function of the inverse temperature β , measured in a Monte Carlo simulation



Figure 2. Wavelet fluctuation strengths at different scales as a function of the inverse temperature β , calculated from minimizing the effective inter₂ $_{\circ}$ $_{\circ}$

Wavelet Path Integral Monte Carlo A.E.Cho et al. J.Chem.Phys.117(2002)5971

Fourier Path Integral $x(u) = x + (x' - x)u + \sum_{k=1}^{\infty} a_k \sin \pi ku$ $0 \le u = \frac{\tau}{\beta \hbar} \le 1$

In analogy with Fourier transform one can introduce

Wavelet Path Integral Monte Carlo

$$x(u) = x + (x' - x)u + s_0\phi(u) + \sum_{j,k} w_k^j \psi_k^j(u) + \alpha u + \delta$$

Mean coordinate averaged in u:

$$\langle x \rangle = \frac{x + x'}{2} + s_0 + \frac{\alpha}{2} + \delta$$

Imaginary time path action

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

 $t_{WPI} = 35000$ s, $t_{FPI} = 72000$ s

Kinetic term cannot be evaluated analytically. Numerical integration over $w = (s_0, w_k^j)$ gives averages

$$\langle A \rangle = \frac{\int dx dw e^{-S(x,w)} A(x,x)}{\int dx dw e^{-S(x,w)}}$$

FIG. 3. Plot of density matrix element for particle in a box problem at 10 000 K. For both WPIMC and FPI, only the first eight path variables are used in the expansion.



FK3. 6. Plot of density matrix element for particle in a box problem at 10 K. The first eight path variables are used for both WPIMC and FPI.

Multiresolution analysis in statistical mechanics A.E.Ismail et al. J. Chem. Phys. 118(2003)4414;4424

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 $\mathbf{W}^T \mathbf{W} = \mathbf{I}, \mathbf{u} = (s_1, \dots, s_N)$:

$$-\beta H = (\mathbf{h}^T \mathbf{W}^T)(\mathbf{W}\mathbf{u}) + (\mathbf{u}^T \mathbf{W}^T)(\mathbf{W}\mathbf{J}\mathbf{W}^T)(\mathbf{W}\mathbf{u})$$

Hamiltonian in wavelet space

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

Configuration space of $\tilde{\mathbf{u}}$ is wider than that of \mathbf{u} .

Partition function

$$ilde{Z} = \sum_{ ilde{u}} \omega(ilde{u}) e^{-eta ilde{H}}$$

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• Only averages contribute, but not details

 $\langle s_k^j A(\cdot) \rangle \neq 0, \langle d_k^j A(\cdot) \rangle = 0$

 The restriction u → 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 $_{64 \times 64}$



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Example of Ising model with Haar wavelet

1D

$$-H = J \sum_{i} s_{i}^{0} s_{i+1}^{0}, \quad s_{2k}^{j-1} = rac{s_{k}^{j} + d_{k}^{j}}{\sqrt{2}}, \quad s_{2k+1}^{j-1} = rac{s_{k}^{j} - d_{k}^{j}}{\sqrt{2}}$$

$$-H/J = \frac{1}{2} \sum_{k} (s_{k}^{1} - d_{k}^{1})(s_{k}^{1} + s_{k+1}^{1} + d_{k}^{1} + d_{k+1}^{1})$$

$$= -\frac{1}{2} \sum_{k} (d_{k}^{1})^{2} + d_{k}^{1} d_{k+1}^{1} + \frac{1}{2} \sum_{i} (s_{2i}^{1})^{2} + (s_{2i+1}^{1})^{2}$$

$$+ s_{2i}^{1} s_{2i+1}^{1} + s_{2i+1}^{1} s_{2i+2}^{1}$$

$$- d_{2i}^{1} s_{2i+1}^{1} - d_{2i+1}^{1} s_{2i+2}^{1} + s_{2i}^{1} d_{2i+1}^{1} + s_{2i+1}^{1} d_{2i+2}^{1} = \dots$$

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.

Why not construct MRA on Clebsch-Gordan coefficients? M.V.Altaisky and N.E.Kaputkina. Int. J. Quant. Inf.10(2012)1250026

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 $(D_{\frac{1}{2}} \otimes D_{\frac{1}{2}}) \otimes (D_{\frac{1}{2}} \otimes D_{\frac{1}{2}})$. 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 $16 = 7 \oplus 4 + 5$. The original Kraichnan-Orszag system: R.H.Kraichnan,*Phys. Fluids*6(1963)1603; S.A.Orszag and L.R.Bissonnette, *ibid.* 10(1967)2603 is the system of three coupled first order differential equations

$$\frac{dx_1(t)}{dt} = A_1x_2(t)x_3(t), \frac{dx_2(t)}{dt} = A_2x_1(t)x_3(t), \frac{dx_3(t)}{dt} = A_3x_1(t)x_2(t),$$

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 ξ_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



PC solution of KO system from Altaisky,Popova,Saraev in Proc. DD'09



polynomials up to the second order and normally distributed initial conditions, $\sigma(x(0)) = \sigma(y(0)) = \sigma(z(0)) = 0.1$. $\overline{x(0)} = 0.07, \overline{y(0)} = 0.01, \overline{z(0)} = -1.0$

Initial conditions and Galerkin system from Altaisky, Popova, Saraev in Proc. DD'09

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 $d_{jk}(t)$.

$$egin{array}{rcl} \dot{d}_{jk}^1 &=& d_{j_1k_1}^2 d_{j_2k_2}^3 \langle \psi_{jk}\psi_{j_1k_1}\psi_{j_2k_2}
angle \ \dot{d}_{jk}^2 &=& d_{j_1k_1}^1 d_{j_2k_2}^3 \langle \psi_{jk}\psi_{j_1k_1}\psi_{j_2k_2}
angle \ \dot{d}_{jk}^3 &=& -2d_{j_1k_1}^1 d_{j_2k_2}^2 \langle \psi_{jk}\psi_{j_1k_1}\psi_{j_2k_2}
angle, \end{array}$$

where the connection coefficients

$$\langle \psi_{jk}\psi_{j_1k_1}\psi_{j_2k_2}\rangle \equiv \int_{-\infty}^{\infty}\psi_{jk}(x)\psi_{j_1k_1}(x)\psi_{j_2k_2}(x)dx$$

are evaluated using the connections

$$\Lambda_{k,m} \equiv \int \phi(t)\phi(t-k)\phi(t-m)dt \Rightarrow \forall \exists h \in \mathbb{R}$$
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KO: mean with DAUB4 from Altaisky,Popova,Saraev in Proc. DD'09





KO: mean with DAUB6





Multi-scale Metropolis?

- To flip entire blocks by random change of bigger level coefficients d^j_k, j > 0, rather than s^j_k.
- 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).

- 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

$$F = \frac{1}{2n_c 3V} \sum_{x} \sum_{k=1}^{3} \operatorname{Tr}(U_k^g(x) + U_k^g(x)^{\dagger}), U_k^g(x) = G(x)U_k(x)G^{\dagger}(x+\mathbf{k})$$

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

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

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



Thank You for Your Attention !

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