Spin-Orbital Motion: Symmetry, Dynamics, Multiresolution

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Abstract

We present an application of the variational multiscale approach to a nonlinear model for spin-orbital motion in the rational approximation: orbital dynamics and Thomas-BMT equations for the classical spin vector. As the first step, we present the solution of this dynamical system by means of periodization procedure via the variational approach in multiresolution framework. At the next step, we consider a more flexible biorthogonal localized representation via the invariant Hamiltonian (loop) approach. In the last part, we outline the combination of the projection method together with the power technique of non-regular (vs. r-regular) multiresolution analysis to provide the careful evaluation of nonlinearities at each scale of resolution of the underlying functional space by the action of the internal hidden symmetry.

Introduction

In this paper, we consider the applications of our numerical-analytical technique [1]–[12] based on the methods of local nonlinear harmonic analysis (LNHA) or wavelet analysis (in the particular case of internal affine symmetry of the underlying functional space) to the modeling of the dynamics of spin-orbital motion. LNHA is a relatively novel universal set of mathematical methods, which allows to work with well-localized/best localized bases in functional spaces and provides the maximum sparse form for the general type of operators (differential, integral, pseudodifferential) in such bases. In this paper, our approach is based on some generalization of our variational-multiresolution approach applied in [1]-[12] to a variety of dynamical problems with polynomial nonlinearities, which allows to consider not only the polynomial but rational type of nonlinearities.

The general solution has the following multiscale decomposition:

$$z(t) = z_N^{slow}(t) + \sum_{j\geq N} z_j(\omega_j t), \quad \omega_j \sim 2^j \tag{1}$$

which corresponds to the full multiresolution expansion in all time (or space) scales. Formula (1) gives us exact expansion in the corresponding funtional space into a slow part z_N^{slow} and fast oscillating parts for arbitrary N. So, we may move from coarse scales of resolution to the finest one to obtain more detailed information about our dynamical process. The first term in the RHS of equation (1) corresponds on the global level of function space decomposition to resolution space and the second one to detail space. In this way, we contribute to our full solution from each scale of resolution or each time scale. The same is correct for the contribution to power spectral density (energy spectrum): we can take into account contributions from each level/scale of resolution. Using tensor product technique for localized bases, the generalization for the multidimensional case can be made too.

In Section 1, we consider the classical Thomas-BMT (Bargmann-Michel-Telegdi) representation for spin-orbital motion.

Starting from the variational formulation in Section 2, we construct the explicit representation for dynamical variables in the base of compactly supported periodized wavelets via multiscale decomposition.

In Section 3, we present more flexible framework based on the variational formulation via the invariant Hamiltonian (loop) approach in the biorthogonal bases of compactly supported wavelets, demonstrating, e.g., the acceleration of convergence for multiscale decompositions.

In Section 4, we outline the combination of the projection method together with the power technique of non-regular (vs. r-regular) multiresolution analysis to provide the careful evaluation of nonlinearities at each scale of the resolution of the underlying functional space by the action of internal hidden symmetry.

In Section 5, we consider the results of numerical modeling.

1 Spin-orbital motion

Let us consider the system of equations for the orbital motion and the Thomas-BMT (Bargmann-Michel-Telegdi) representation for the classical spin vector [13]:

$$\mathrm{d}q/\mathrm{d}t = \partial H_{orb}/\partial p, \quad \mathrm{d}p/\mathrm{d}t = -\partial H_{orb}/\partial q, \quad \mathrm{d}s/\mathrm{d}t = w \times s, \tag{2}$$

where

$$\begin{aligned} H_{orb} &= c\sqrt{\pi^2 + m_0 c^2} + e\Phi, \\ w = &- \frac{e}{m_0 c\gamma}(1+\gamma G)\vec{B} + \frac{e}{m_0^3 c^3 \gamma}\frac{G(\vec{\pi}\cdot\vec{B})\vec{\pi}}{(1+\gamma)} + \frac{e}{m_0^2 c^2\gamma}\frac{G+\gamma G+1}{(1+\gamma)}[\pi \times E], \end{aligned} \tag{3}$$

$q = (q_1, q_2, q_3), p = (p_1, p_2, p_3)$ are canonical position and momentum, $s = (s_1, s_2, s_3)$ is the classical spin vector of length $\hbar/2$, $\pi = (\pi_1, \pi_2, \pi_3)$ is kinetic momentum vector.

We may introduce, in 9-dimensional phase space $z = (q, p, s)$, the Poisson brackets

$$\{f(z), g(z)\} = f_q g_p - f_p g_q + [f_s \times g_s] \cdot s$$

corresponding to the Hamiltonian equations

$$\mathrm{d}z/\mathrm{d}t = \{z, H\} \tag{4}$$

with the Hamiltonian

$$H = H_{orb}(q, p, t) + w(q, p, t) \cdot s. \tag{5}$$

More explicitly we have

$$\begin{aligned} \frac{\mathrm{d}q}{\mathrm{d}t} &= \frac{\partial H_{orb}}{\partial p} + \frac{\partial (w\cdot s)}{\partial p}, \\ \frac{\mathrm{d}p}{\mathrm{d}t} &= -\frac{\partial H_{orb}}{\partial q} - \frac{\partial (w\cdot s)}{\partial q}, \\ \frac{\mathrm{d}s}{\mathrm{d}t} &= [w \times s]. \end{aligned} \tag{6}$$

We considered such a dynamical system in [7] via an invariant approach, based on investigation of Lie-Poison structures on semidirect products, but here we present another symplectic invariant "loop" framework. Anyway, in this paper we mostly concentrate on the analytical aspects of multiresolution representation for the case of rational dynamics. We will present invariant consideration in a separate paper.

2 Variational wavelet approach for periodic trajectories

We start with the extension of our approach [1]–[12] to the case of periodic trajectories. The equations of motion corresponding to our problem may be formulated as a particular case of the general system of ordinary differential equations $dx_i/dt = f_i(x_j, t)$, $(i, j = 1, ..., n)$, $0 \leq t \leq 1$, where f_i are not more than rational functions of dynamical variables x_j and have an arbitrary time dependence but with periodic boundary conditions. According to our variational-multiresolution approach we have the solution in the following form

$$x_i(t) = x_i(0) + \sum_k \lambda_i^k \varphi_k(t), \qquad x_i(0) = x_i(1), \tag{7}$$

where λ_i^k are the roots of reduced algebraical systems of equations, Generalized Dispersion Relations (GDR), with the same degree of nonlinearity and $\varphi_k(t)$ correspond to the proper type of wavelet bases (or frames). It should be noted that the coefficients of the reduced algebraical system are the solutions of an additional linear problem and also depend on the particular type of wavelet construction and the type of bases we chose.

Our representations are based on multiresolution approach. Because the affine group of translation and dilations is inside the approach, this method resembles the action of a microscope. We contribute to the final result from each scale of resolution from the whole infinite scale of spaces. More exactly, the closed subspace $V_j (j \in \mathbf{Z})$ corresponds to level j of resolution, or to scale j. We consider a r-regular multiresolution analysis of $L^2(\mathbf{R}^n)$ (of course, we may consider any different functional space) which is a sequence of increasing closed subspaces V_j:

$$...V_{-2} \subset V_{-1} \subset V_0 \subset V_1 \subset V_2 \subset ... \tag{8}$$

Then just as V_j is spanned by dilation and translations of the scaling function, so W_j are spanned by translations and dilation of the mother wavelet $\psi_{jk}(x)$, where

$$\psi_{jk}(x) = 2^{j/2}\psi(2^j x - k). \tag{9}$$

All expansions we used are based on the following decomposition for the underlying functional space:

$$L^2(\mathbf{R}) = \overline{V_0 \bigoplus_{j=0}^{\infty} W_j} \tag{10}$$

We need also to find, as in general situation, the following generic objects

$$\Lambda^{d_1 d_2 ... d_n}_{\ell_1 \ell_2 ... \ell_n} = \int_{-\infty}^{\infty} \prod \varphi^{d_i}_{\ell_i}(x) \mathrm{d}x, \tag{11}$$

but now in the case of periodic boundary conditions. Now we consider the procedure of their calculations in case of periodic boundary conditions in the base of periodic wavelet functions on the interval [0,1] and the corresponding expansions (1), (7) inside our variational approach. The periodization procedure according to [14], [15] gives us:

$$\begin{aligned} \hat{\varphi}_{j,k}(x) &\equiv \sum_{\ell \in Z} \varphi_{j,k}(x - \ell) \qquad (12) \\ \hat{\psi}_{j,k}(x) &= \sum_{\ell \in Z} \psi_{j,k}(x - \ell) \end{aligned}$$

So, $\hat{\varphi}, \hat{\psi}$ are periodic functions on the interval [0,1]. Because $\varphi_{j,k} = \varphi_{j,k'}$ if $k = k' \mathrm{mod}(2^j)$, we may consider only $0 \le k \le 2^j$ and as a consequence our multiscale decomposition has the form: $\bigcup_{j\ge 0} \hat{V}_j = L^2[0,1]$ with $\hat{V}_j = \mathrm{span}\{\hat{\varphi}_{j,k}\}_{k=0}^{2j-1}$ [14], [15]. Integration by parts and periodicity gives useful relations between objects (10) in the particular quadratic case ($d = d_1 + d_2$):

$$\begin{aligned} \Lambda^{d_1,d_2}_{k_1,k_2} &= (-1)^{d_1}\Lambda^{0,d_2+d_1}_{k_1,k_2}, \\ \Lambda^{0,d}_{k_1,k_2} &= \Lambda^{0,d}_{0,k_2-k_1} \equiv \Lambda^d_{k_2-k_1}. \end{aligned} \tag{13}$$

So, any 2-tuple can be represented by Λ^d_k. Then our second additional linear problem is reduced to the eigenvalue problem for $\{\Lambda^d_k\}_{0\le k\le 2^j}$ by creating a system of 2^j homogeneous relations in Λ^d_k and inhomogeneous equations. So, if we have dilation equation in the form $\varphi(x) = \sqrt{2}\sum_{k\in Z} h_k\varphi(2x-k)$, then we have the following homogeneous relations [15]

$$\Lambda^d_k = 2^d \sum_{m=0}^{N-1}\sum_{\ell=0}^{N-1} h_m h_\ell \Lambda^d_{\ell+2k-m}, \tag{14}$$

or in such a form $A\lambda^d = 2^d\lambda^d$, where $\lambda^d = \{\Lambda^d_k\}_{0\le k\le 2^j}$. Inhomogeneous equations are:

$$\sum_\ell M^d_\ell \Lambda^d_\ell = d! 2^{-j/2}, \tag{15}$$

where objects $M^d_\ell(|\ell| \le N-2)$ can be computed by recursive procedure

$$\begin{aligned} M^d_\ell &= 2^{-j(2d+1)/2}\tilde{M}^d_\ell, \\ \tilde{M}^k_\ell &= < x^k, \varphi_{0,\ell} > = \sum_{j=0}^{k}\binom{k}{j} n^{k-j} M^j_0, \quad \tilde{M}^\ell_0 = 1. \end{aligned} \tag{16}$$

So, we have reduced our generic algebraic problems encoded important information about the analytical properties of a hierarchy of multiscales to a standard set of linear algebraical problems (huge, but solvable in principle) to provide the explicit construction for key ingredient of our scheme, GDR. Then by using our regular variational methods, we have obtained the explicit exact multiscale representations (1), (7) in proper functional spaces for closed periodic trajectories for rational spin-orbital dynamics in the base of periodized wavelets (12). The particular case is demonstrated on Fig. 1.

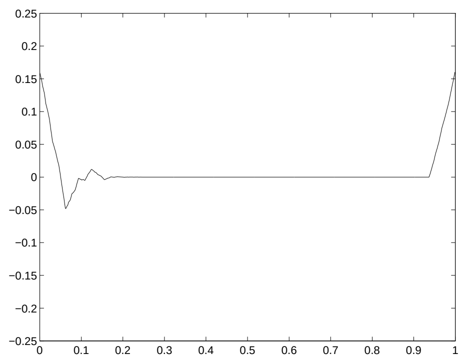

Figure 1: Periodic wavelet

3 Variational approach in biorthogonal wavelet bases

Usually the integrand of variational functionals is represented by a bilinear form (scalar product), so it seems more reasonable to consider a modified multiresolution construction taking into account all features of that structure.

The invariant action functional for loops in the phase space is [16]:

$$F(\gamma) = \int_\gamma pdq - \int_0^1 H(t,\gamma(t))dt. \tag{17}$$

The critical points of F are those loops γ, which solve the Hamiltonian equations associated with the Hamiltonian H and hence are periodic orbits. By the way, all critical points of F are the saddle points of the infinite Morse index, but fortunately this approach is actually effective. This was demonstrated using several variational techniques starting from minimax due to Rabinowitz and ending with Floer homology.

So, (M,ω) is a symplectic manifold, $H: M \to R$ is a Hamiltonian, X_H is the unique Hamiltonian vector field defined by $\omega(X_H(x),\upsilon) = -dH(x)(\upsilon), \quad \upsilon \in T_xM, \quad x \in M$, where ω is a symplectic structure.

A T-periodic solution $x(t)$ of Hamiltonian equations $\dot{x} = X_H(x)$ on M is the solution satisfying the boundary conditions $x(T) = x(0),\ T > 0$.

We consider the loop space $\Omega = C^\infty(S^1, R^{2n})$, where $S^1 = R/\mathbf{Z}$, of smooth loops in R^{2n}. We define a (variational) function $\Phi: \Omega \to R$ by setting

$$\Phi(x) = \int_0^1 \frac{1}{2} < -J\dot{x}, x > dt - \int_0^1 H(x(t))dt, \quad x \in \Omega, \tag{18}$$

where J is a quasicomplex structure.

The critical points of Φ are the periodic solutions of Hamiltonian equations $\dot{x} = X_H(x)$. Computing the derivative at $x \in \Omega$ in the direction of $y \in \Omega$, we find

$$\Phi'(x)(y) = \frac{d}{d\epsilon}\Phi(x+\epsilon y)|_{\epsilon=0} = \int_0^1 < -J\dot{x} - \bigtriangledown H(x), y > dt. \tag{19}$$

Consequently, $\Phi'(x)(y) = 0$ for all $y \in \Omega$ iff the loop x satisfies the equation

$$-J\dot{x}(t) - \bigtriangledown H(x(t)) = 0, \tag{20}$$

i.e. $x(t)$ is a solution of Hamiltonian equations, which also satisfies $x(0) = x(1)$, i.e. periodic with period 1. Periodic loops may be represented by their Fourier series: $x(t) = \sum e^{k2\pi Jt}x_k,\ x_k \in R^{2k}$, where J is a quasicomplex structure. We will consider the detailed multiresolution analysis of quasicomplex structures in a separate paper but here we are interested, first of all, to take into account all analytical features of the bilinear representation of integrands in such a multiscale approach. Let us start with two hierarchical sequences of approximation spaces [14]:

$$\dots V_{-2} \subset V_{-1} \subset V_0 \subset V_1 \subset V_2 \dots, \quad \dots \widetilde{V}_{-2} \subset \widetilde{V}_{-1} \subset \widetilde{V}_0 \subset \widetilde{V}_1 \subset \widetilde{V}_2 \dots, \tag{21}$$

where as usually, W_0 is a complement to V_0 in V_1, but now not necessarily orthogonal complement. New orthogonality conditions have now the following form:

$$\widetilde{W}_0 \perp V_0, \quad W_0 \perp \widetilde{V}_0, \quad V_j \perp \widetilde{W}_j, \quad \widetilde{V}_j \perp W_j, \tag{22}$$

where translates of ψ span W_0, translates of $\tilde{\psi}$ span $\widetilde{W}_0$. Biorthogonality conditions are

$$< \psi_{jk}, \tilde{\psi}_{j'k'} > = \int_{-\infty}^{\infty} \psi_{jk}(x)\tilde{\psi}_{j'k'}(x)\mathrm{d}x = \delta_{kk'}\delta_{jj'}, \tag{23}$$

where $\psi_{jk}(x) = 2^{j/2}\psi(2^j x - k)$. Our generic functions $\varphi(x), \tilde{\varphi}(x-k)$ form dual pair:

$$< \varphi(x-k), \tilde{\varphi}(x-\ell) >= \delta_{kl}, \quad < \varphi(x-k), \tilde{\psi}(x-\ell) >= 0$$

and generate a different version of multiresolution analysis. Here $\varphi(x-k)$, $\psi(x-k)$ are synthesis functions, $\tilde{\varphi}(x-\ell)$, $\tilde{\psi}(x-\ell)$ are analysis functions. Synthesis functions are biorthogonal to analysis functions. Scaling spaces are orthogonal to dual wavelet spaces. Two multiresolutions are intertwining $V_j + W_j = V_{j+1}$, $\quad \widetilde{V}_j + \widetilde{W}_j = \widetilde{V}_{j+1}$. These are direct sums but not orthogonal sums. The modified representation for solution has the following form

$$f(t) = \sum_{j,k} \tilde{b}_{jk}\psi_{jk}(t), \tag{24}$$

where synthesis base wavelets are used to synthesize the function. At the same time $\tilde{b}_{jk}$ come from inner products with analysis wavelets. Biorthogonality yields

$$\tilde{b}_{\ell m} = \int f(t)\tilde{\psi}_{\ell m}(t)\mathrm{d}t. \tag{25}$$

So, now we can apply this more sophisticated construction to our (invariant) variational approach. We need to modify it on the level of computing coefficients of generic reduced nonlinear algebraical system (GDR) only. Definitely, this new construction is more flexible, e.g., the biorthogonal point of view is more stable under the action of a large class of operators while the orthodox orthogonal one (one scale for multiresolution) is fragile, all computations are more simpler and, finally, we provide the acceleration of convergence. In all types of such "Hamiltonian" calculations, which are based on some bilinear structures (symplectic or Poissonian structures, the bilinear form of integrand in variational integral), such a framework provides additional positive features. It should be noted that according to standard LNHA reasons we prefer the so called wavelet packets [14],15],[17],[18] (Fig. 1)as a generic set of perfectly localized bases functions.

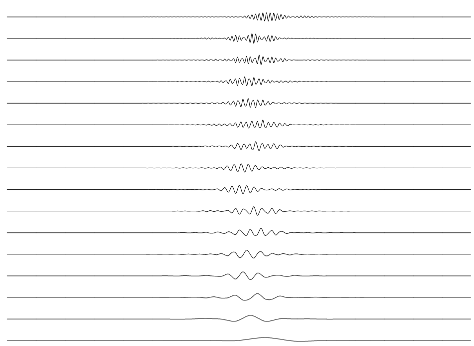

Figure 2: Wavelet packets.

4 Evaluation of nonlinearities scale by scale. Non-regular approximation.

According to construction, the base wavelet functions $\psi(x)$ have K vanishing moments $\int x^k\psi(x)\mathrm{d}x = 0$, or equivalently $x^k = \sum c_\ell\varphi_\ell(x)$ for each k, $0 \le k \le K$. Let P_j be an orthogonal projector on subspace V_j corresponding to scale j. For any $u \in L^2(\mathbf{R})$ and $\ell \in \mathbf{Z}$, the tree algorithm [14] provides us by wavelet coefficients of $P_\ell(u)$, i.e. the set $\{< u, \psi_{j,k} >, j \leq \ell - 1, k \in \mathbf{Z}\}$ can be computed using hierarchical algorithms based on a set of scaling coefficients in V_ℓ, i.e. the set $\{< u, \varphi_{\ell,k} >, k \in \mathbf{Z}\}$ [14], [17]. For the scaling function φ we have in general only one relation $\int \varphi(x)\mathrm{d}x = 1$, therefore for any function $u \in L^2(\mathbf{R})$ we have the following asymptotic evaluation:

$$\lim_{j\to\infty, k2^{-j}\to x} \mid 2^{j/2} < u, \varphi_{j,k} > - u(x) \mid = 0. \tag{26}$$

If the integer $n(\varphi)$ is the largest one such that

$$\int x^\alpha \varphi(x)\mathrm{d}x = 0 \qquad \text{for} \qquad 1 \leq \alpha \leq n, \tag{27}$$

then if $u \in C^{(n+1)}$ with $u^{(n+1)}$ bounded we have for $j \to \infty$ uniformly in k:

$$\mid 2^{j/2} < u, \varphi_{j,k} > - u(k2^{-j}) \mid = O(2^{-j(n+1)}). \tag{28}$$

Such scaling functions with zero moments are very useful for us from the point of view of time-frequency localization: for Fourier component $\hat{\varphi}(\omega)$ of them there exists some $C(\varphi) \in \mathbf{R}$, such that for $\omega \to 0 \quad \hat{\varphi}(\omega) = 1 + C(\varphi) \mid \omega \mid^{2r+2}$ (remember, that we consider r-regular multiresolution analysis). The using of such a type of scaling functions leads to superconvergence properties for the general Galerkin approximation [17], a particular case of our general scheme. Now we are interested in very important for us estimates in each scale for non-linear terms of type $u \mapsto f(u) = f \circ u$, where f is C^∞ (definitely we will consider n-germs, i.e. actions of truncated Taylor series). According to [17], let us consider non regular space of approximation $\widetilde{V}$ of the form

$$\widetilde{V} = V_q \oplus \sum_{q \leq j \leq p-1} \widetilde{W_j}, \tag{29}$$

with $\widetilde{W_j} \subset W_j$. We need the efficient and precise estimate of $f \circ u$ on $\widetilde{V}$. Let us consider the following approximation for $q \in \mathbf{Z}$ and $u \in L^2(\mathbf{R})$

$$\prod f_q(u) = 2^{-q/2} \sum_{k\in\mathbf{Z}} f(2^{q/2} < u, \varphi_{q,k} >) \cdot \varphi_{q,k}. \tag{30}$$

According to the construction in [17], we have the following important for us estimation (uniformly in q) for $u, f(u) \in H^{(n+1)}$:

$$\|P_q\left(f(u)\right) - \prod f_q(u)\|_{L^2} = O\left(2^{-(n+1)q}\right). \tag{31}$$

For non regular spaces (29) we have

$$\prod f_{\widetilde{V}}(u) = \prod f_q(u) + \sum_{\ell=q,p-1} P_{\widetilde{W_j}} \prod f_{\ell+1}(u) \tag{32}$$

and as a result the following estimate as a byproduct:

$$\|P_{\widetilde{V}}\left(f(u)\right) - \prod f_{\widetilde{V}}(u)\|_{L^2} = O(2^{-(n+1)q}) \tag{33}$$

uniformly in q and $\widetilde{V}$ (29). This estimate depends on q, not p, i.e. on the scale of the coarse grid, not on the finest grid used in the definition of $\widetilde{V}$. As a result we can evaluate the total error

$$\|f(u) - \prod f_{\widetilde{V}}(u)\| = \|f(u) - P_{\widetilde{V}}(f(u))\|_{L^2} + \|P_{\widetilde{V}}(f(u) - \prod f_{\widetilde{V}}(u))\|_{L^2} \tag{34}$$

and since the projection error in $\widetilde{V}$: $\|f(u) - P_{\widetilde{V}}(f(u))\|_{L^2}$ is much smaller than the projection error in V_q we have more flexible evaluation (33) instead of limited one (31). In advanced evaluations and estimations it is more effective to consider approximations in the special case of c-structured space to provide, scale-by-scale, the careful evaluation of the action of nonlinear terms in the situation where the dynamics of localied modes dominates:

$$\widetilde{V} = V_q + \sum_{j=q}^{p-1} span\{\psi_{j,k},\ k \in [2^{(j-1)} - c, 2^{(j-1)} + c] \mod 2^j\}. \tag{35}$$

5 Numerical Calculations

In this part we consider numerical illustrations of previous analytical approaches. Our numerical calculations are based on periodic compactly supported Daubechies wavelets and related wavelet/wavepackets families (Fig. 1, Fig. 2). Also in our modelling we added noise as perturbation to our spin–orbit configurations. On Fig. 3, according to formulas (1),(7), (8), we present contributions to the full multiscale approximation of our dynamical evolution (top row on Fig. 4) starting from the coarse approximation corresponding to scale 2^0 (bottom row) to the finest one corresponding to the scales from 2^1 to 2^5 or from coarse slow modes to fast ones (5 high frequencies) as finest details for approximation. Then on Fig. 4, from bottom to top, we demonstrate the summation of contributions from the corresponding levels of multiresolution given on Fig. 3 and, as result, we restore the final approximation of our dynamical process (top row on Fig. 4) by taking into account five scales (frequencies)/levels of resolution from the whole tower. We also made the same decomposition/approximation on the level of power spectral density in the process with noise (Fig. 5). All that demonstrates the power methods of LNHA allowing to investigate nonlinear dynamics on the orbits of representations of internal hidden symmetry in physically motivated functional spaces.

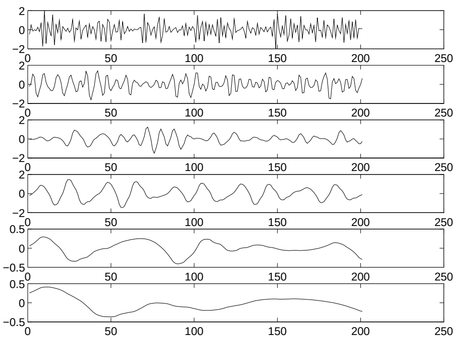

Figure 3: Contributions to approximation: from scale 2^1 to 2^5 (with noise).

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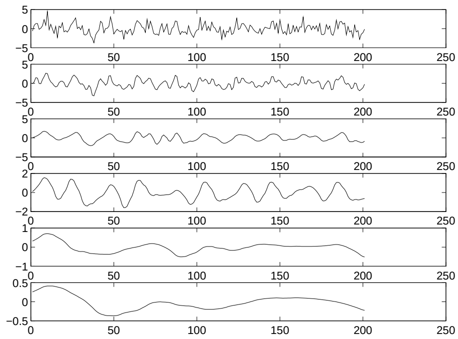

Figure 4: Approximations: from scale 2^1 to 2^5 (with noise).

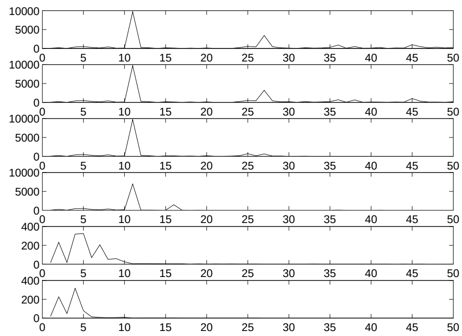

Figure 5: Power spectral density: from scale 2^1 to 2^5 (with noise)

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