Quasiclassics in Wigner-Moyal-von Neumann framework via Multiresolution

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Abstract

We present the application of our variational-multiscale approach to numerical/analytical calculations in the general quasi-classical set-up. The starting points are Wigner-Weyl-von Neumann framework as well as Moyal (naive) deformation quantization. Our technique allows to cover all complicated underlying features of compex quantum dynamics based on the proper choice of background functional spaces which determine dynamical properties together with the internal structure of pseudo-differential operators incorporated in the full hierarchy of Wigner-like equations describing the evolution of the quasiprobability beyond trivial gaussian-like area with pure postitive Wigner functions. The choice of hidden underlying symmetry and its representation on the orbits of proper actions provide us with the filtration of the background Hilbert space of states which implies the whole tower of internal hidden scales by using multiresolution decomposition. All that allows to consider maximally localized quantum states and most sparse representation for all set of observables. At the same time the orbit structure allows to consider basic nonlocal phenomena like entanglement with possible subsequent decoherence. Our main applications in this consideration are related with a description of quantum properties in nonlinear beam dynamics, both in accelerator and plasma physics but such general background provides all possibilities to describe the modeling of prototypes of any future quantum devices.

1 Introduction

In this paper we consider some starting points in the applications of a new numerical-analytical technique which is based on local nonlinear harmonic analysis (wavelet analysis, generalized coherent states analysis) to the quantum/quasiclassical (nonlinear) beam/accelerator physics calculations. The reason for this treatment is that recently a number of problems appeared in which one needs take into account quantum properties of particles/beams.Our starting point is the general point of view of deformation quantization approach at least on naive Moyal/Weyl/Wigner level (part 2). The main point is that the algebras of quantum observables are the deformations of commutative algebras of classical observables (functions) [1]. So, if we

have the Poisson manifold M (symplectic manifolds, Lie coalgebras, etc.) as a model for classical dynamics then for quantum calculations we need to find an associative (but non-commutative) star product $*$ on the space of formal power series in $\hbar$ with coefficients in the space of smooth functions on M such that

$$f * g = fg + \hbar\{f, g\} + \sum_{n\geq 2} \hbar^n B_n(f, g), \tag{1}$$

where $\{f, g\}$ is the Poisson brackets, B_n are bidifferential operators $C^\infty(X) \otimes C^\infty(X) \to C^\infty(X)$. There is also an infinite-dimensional gauge group on the set of star-products

$$f \mapsto f + \sum_{n\geq 2} \hbar^n D_n(f), \tag{2}$$

where D_n are differential operators. Kontsevich gave the solution to this deformation problem in terms of formal power series via sum over graphs [1]. He also proved that for every Poisson manifold M there is a canonically defined gauge equivalence class of star-products on M. Also there is the nonperturbative corrections to power series representation for $*$ [1]. In naive calculations we may use simple formal rules:

$$* \equiv \exp\Big(\frac{i\hbar}{2}(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x)\Big) \tag{3}$$

$$f(x,p) * g(x,p) = f(x, p - \frac{i\hbar}{2}\overrightarrow{\partial}_x) \cdot g(x, p + \frac{i\hbar}{2}\overleftarrow{\partial}_x) \tag{4}$$

$$= f(x + \frac{i\hbar}{2}\overrightarrow{\partial}_p, p - \frac{i\hbar}{2}\overrightarrow{\partial}_x) g(x,p) \tag{5}$$

In this paper we consider calculations of Wigner functions (WF) as the solution of Wigner equations [2] (part 3):

$$i\hbar\frac{\partial}{\partial t} W(x,p,t) = H * W(x,p,t) - W(x,p,t) * H \tag{6}$$

and especially stationary Wigner equations:

$$H * W - W * H = Ef \tag{7}$$

Our approach is based on extension of our variational-wavelet approach [3]-[14]. Wavelet analysis is some set of mathematical methods, which gives us the possibility to work with well-localized bases (Fig. 1) in functional spaces and gives maximum sparse forms for the general type of operators (differential, integral, pseudodifferential) in such bases. These bases are natural generalization of standard coherent, squeezed, thermal squeezed states [2], which correspond to quadratical systems (pure linear dynamics) with Gaussian Wigner functions. So, we try to calculate quantum corrections to classical dynamics described by polynomial nonlinear Hamiltonians

such as orbital motion in storage rings, orbital dynamics in general multipolar fields etc. from papers [3]-[13]. The common point for classical/quantum calculations is that any solution which comes from full multiresolution expansion in all space/time (or phase space) scales represents expansion into a slow part and fast oscillating parts (part 4). So, we may move from the coarse scales of resolution to the finest one for obtaining more detailed information about our dynamical classical/quantum process. In this way we give contribution to our full solution from each scale of resolution. 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. Because affine group of translations and dilations (or more general group, which acts on the space of solutions) is inside the approach (in wavelet case), this method resembles the action of a microscope. We have contribution to final result from each scale of resolution from the whole underlying infinite scale of spaces. In part 5 we consider numerical modelling of Wigner functions which explicitly demonstrates quantum interference of the generalized "coherent" states.

2 Quasiclassical evolution

Let us consider classical and quantum dynamics in phase space $\Omega = R^{2m}$ with coordinates (x, ξ) and generated by Hamiltonian $\mathcal{H}(x, \xi) \in C^\infty(\Omega; R)$. If $\Phi_t^{\mathcal{H}} : \Omega \longrightarrow \Omega$ is (classical) flow then time evolution of any bounded classical observable or symbol $b(x, \xi) \in C^\infty(\Omega, R)$ is given by $b_t(x, \xi) = b(\Phi_t^{\mathcal{H}}(x, \xi))$. Let $H = Op^W(\mathcal{H})$ and $B = Op^W(b)$ are the self-adjoint operators or quantum observables in $L^2(R^n)$, representing the Weyl quantization of the symbols $\mathcal{H}, b$ [1]

$$(Bu)(x) = \frac{1}{(2\pi\hbar)^n} \int_{R^{2n}} b\left(\frac{x+y}{2}, \xi\right) \cdot e^{i<(x-y),\xi>/\hbar} u(y) \mathrm{d}y \mathrm{d}\xi, \tag{8}$$

where $u \in S(R^n)$ and $B_t = e^{iHt/\hbar} B e^{-iHt/\hbar}$ be the Heisenberg observable or quantum evolution of the observable B under unitary group generated by H. B_t solves the Heisenberg equation of motion $\dot{B}_t = (i/\hbar)[H, B_t]$. Let $b_t(x, \xi; \hbar)$ is a symbol of B_t then we have the following equation for it

$$\dot{b}_t = \{\mathcal{H}, b_t\}_M, \tag{9}$$

with the initial condition $b_0(x, \xi, \hbar) = b(x, \xi)$. Here $\{f, g\}_M(x, \xi)$ is the Moyal brackets of the observables $f, g \in C^\infty(R^{2n})$, $\{f, g\}_M(x, \xi) = f\sharp g - g\sharp f$, where $f\sharp g$ is the symbol of the operator product and is presented by the composition of the symbols f, g

$$(f\sharp g)(x, \xi) = \frac{1}{(2\pi\hbar)^{n/2}} \int_{R^{4n}} e^{-i<r,\rho>/\hbar + i<\omega,\tau>/\hbar} \cdot f(x+\omega, \rho+\xi) \cdot g(x+r, \tau+\xi) \mathrm{d}\rho \mathrm{d}\tau \mathrm{d}r \mathrm{d}\omega \tag{10}$$

For our problems it is useful that $\{f, g\}_M$ admits the formal expansion in powers of $\hbar$:

$$\{f, g\}_M(x, \xi) \sim \{f, g\} + 2^{-j} \cdot \sum_{|\alpha+\beta|=j\geq 1} (-1)^{|\beta|} \cdot (\partial_\xi^\alpha f D_x^\beta g) \cdot (\partial_\xi^\beta g D_x^\alpha f), \tag{11}$$

where $\alpha = (\alpha_1, \ldots, \alpha_n)$ is a multi-index, $|\alpha| = \alpha_1 + \cdots + \alpha_n$, $D_x = -i\hbar\partial_x$. So, evolution (9) for symbol $b_t(x, \xi; \hbar)$ is

$$\dot{b}_t = \{\mathcal{H}, b_t\} + \frac{1}{2^j} \sum_{|\alpha+\beta|=j\geq 1} (-1)^{|\beta|} \cdot \hbar^j (\partial_\xi^\alpha \mathcal{H} D_x^\beta b_t) \cdot (\partial_\xi^\beta b_t D_x^\alpha \mathcal{H}). \tag{12}$$

At $\hbar = 0$ this equation transforms to classical Liouville equation. Equation (12) plays the key role in many quantum (semiclassical) problems. We consider its particular case–Wigner equation–in the next section.

3 Wigner equations

According to Weyl transform quantum state (wave function or density operator) corresponds to Wigner function, which is analog of classical phase-space distribution [2]. We consider the following form of differential equations for time-dependent WF

$$\partial_t W(p, q, t) = \frac{2}{\hbar} \sin\Big[\frac{\hbar}{2}(\partial_q^H \partial_p^W - \partial_p^H \partial_q^W)\Big] \cdot H(p, q) W(p, q, t) \tag{13}$$

Let

$$\hat{\rho} = |\Psi_\epsilon >< \Psi_\epsilon| \tag{14}$$

be the density operator or projection operator corresponding to the energy eigenstate $|\Psi_\epsilon >$ with energy eigenvalue ϵ. Then time-independent Schroedinger equation corresponding to Hamiltonian

$$\hat{H}(\hat{p}, \hat{q}) = \frac{\hat{p}^2}{2m} + U(\hat{q}) \tag{15}$$

where $U(\hat{q}$ is arbitrary polynomial function (related beam dynamics models considered in [3]-[13]) on $\hat{q}$ is [2]:

$$\hat{H}\hat{\rho} = \epsilon\hat{\rho} \tag{16}$$

After Weyl-Wigner mapping we arrive at the following equation on WF in c-numbers:

$$H(p + \frac{\hbar}{2i}\frac{\partial}{\partial q}, q - \frac{\hbar}{2i}\frac{\partial}{\partial p}\Big) W(p, q) = \epsilon W(p, q) \tag{17}$$

or

$$\Big(\frac{p^2}{2m} + \frac{\hbar}{2i}\frac{p}{m}\frac{\partial}{\partial q} - \frac{\hbar^2}{8m}\frac{\partial^2}{\partial q^2}\Big) W(p, q) + U\Big(q - \frac{\hbar}{2i}\frac{\partial}{\partial p}\Big) W(p, q) = \epsilon W(p, q)$$

After expanding the potential U into the Taylor series we have two real partial differential equations

$$\Big(- \frac{p}{m}\frac{\partial}{\partial q} + \sum_{m=0}^{\infty} \frac{1}{(2m+1!)} \Big(\frac{i\hbar}{2}\Big)^{2m} \frac{\mathrm{d}^{2m+1} U}{\mathrm{d}q^{2m+1}} \frac{\partial^{2m+1}}{\partial p^{2m+1}}\Big) W(p, q) = 0 \tag{18}$$

$$\Big(\frac{p^2}{2m}+U(q)-\frac{\hbar^2}{8m}\frac{\partial^2}{\partial q^2}+\sum_{n=1}^{\infty}\frac{1}{(2n)!}\Big(\frac{i\hbar}{2}\Big)^{2n}\frac{\mathrm{d}^{2n}U}{\mathrm{d}q^{2n}}\frac{\partial^{2n}}{\partial p^{2n}}\Big)W(p,q)=$$
$$\epsilon W(p,q) \tag{19}$$

In the next section we consider variation-wavelet approach for the solution of these equations for the case of arbitrary polynomial $U(q)$, which corresponds to a finite number of terms in equations (18), (19) up to any order of $\hbar$.

4 Variational multiscale representation

Let L be arbitrary (non)linear differential operator with matrix dimension d, which acts on some set of functions $\Psi \equiv \Psi(x,y) = \Big(\Psi^1(x,y),...,\Psi^d(x,y)\Big), \quad x,y \in \Omega \subset \Re^2$ from $L^2(\Omega)$:

$$L\Psi \equiv L(Q,x,y)\Psi(x,y) = 0, \tag{20}$$

where

$$Q \equiv Q_{d_1,d_2,d_3,d_4}(x,y,\partial/\partial x,\partial/\partial y) = \sum_{i,j,k,\ell=1}^{d_1,d_2,d_3,d_4} a_{ijk\ell}x^i y^j\Big(\frac{\partial}{\partial x}\Big)^k\Big(\frac{\partial}{\partial y}\Big)^\ell \tag{21}$$

Let us consider now the N mode approximation for solution as the following ansatz (in the same way we may consider different ansatzes):

$$\Psi^N(x,y) = \sum_{r,s=1}^{N} a_{r,s}\Psi_r(x)\Phi_s(y) \tag{22}$$

We shall determine coefficients of expansion from the following Galerkin conditions (different related variational approaches are considered in [3]-[13]):

$$\ell^N_{k\ell} \equiv \int (L\Psi^N)\Psi_k(x)\Phi_\ell(y)\mathrm{d}x\mathrm{d}y = 0 \tag{23}$$

So, we have exactly dN^2 algebraical equations for dN^2 unknowns a_{rs}.
But in the case of equations for WF (18), (19) we have overdetermined system of equations: $2N^2$ equations for N^2 unknowns a_{rs} (in this case $d=1$). In this paper we consider non-standard method for resolving this problem, which is based on biorthogonal wavelet expansion. So, instead of expansion (22) we consider the following one:

$$\Psi^N(x,y) = \sum_{r,s=1}^{N} a_{r,s}\Psi_r(x)\Psi_s(y) + \sum_{i,j=1}^{N}\widetilde{a}_{ij}\widetilde{\Psi}_i(x)\widetilde{\Phi}_j(y), \tag{24}$$

where $\widetilde{\Psi}_i(x)\widetilde{\Phi}_j(y)$ are the bases dual to initial ones. Because wavelet functions are the generalization of coherent states we consider an expansion on this overcomplete set of bases wavelet functions as a generalization of standard coherent states expansion.
So, variational/Galerkin approach reduced the initial problem (20) to the problem of solution of functional equations at the first stage and some algebraical problems at the second stage. We consider now the multiresolution expansion as the second main part of our construction. Because affine group of translation and dilations is inside the approach, this method resembles the action of a microscope. We have contribution to final result from each scale of resolution from the whole infinite scale of increasing closed subspaces V_j:

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

The solution is parametrized by solutions of two reduced algebraical problems, one is linear or nonlinear (23) (depends on the structure of operator L) and the second one is some linear problem related to computation of coefficients of algebraic equations (23). These coefficients can be found by the method of Connection Coefficients (CC) [15] or related method [16]. We use compactly supported wavelet basis functions for expansions (22), (24). We may consider different types of wavelets including general wavelet packets (section 5 below). These coefficients depend on the wavelet-Galerkin integrals. In general we need to find ($d_i \geq 0$)

$$\Lambda^{d_1 d_2 ... d_n}_{\ell_1 \ell_2 ... \ell_n} = \int\limits_{-\infty}^{\infty} \prod \varphi^{d_i}_{\ell_i}(x) dx \tag{25}$$

According to CC method [15] we use the next construction for quadratic case. When N in scaling equation is a finite even positive integer the function $\varphi(x)$ has compact support contained in $[0, N-1]$. For a fixed triple (d_1, d_2, d_3) only some $\Lambda^{d_1 d_2 d_3}_{\ell m}$ are nonzero: $2 - N \leq \ell \leq N - 2, \quad 2 - N \leq m \leq N - 2, \quad |\ell - m| \leq N - 2$. There are $M = 3N^2 - 9N + 7$ such pairs (ℓ, m). Let $\Lambda^{d_1 d_2 d_3}$ be an M-vector, whose components are numbers $\Lambda^{d_1 d_2 d_3}_{\ell m}$. Then we have the following reduced algebraical system : Λ satisfy the system of equations ($d = d_1 + d_2 + d_3$)

$$A\Lambda^{d_1 d_2 d_3} = 2^{1-d}\Lambda^{d_1 d_2 d_3}, \quad A_{\ell,m;q,r} = \sum_p a_p a_{q-2\ell+p} a_{r-2m+p} \tag{26}$$

By moment equations we have created a system of $M + d + 1$ equations in M unknowns. It has rank M and we can obtain unique solution by combination of LU decomposition and QR algorithm. For nonquadratic case we have analogously additional linear problems for objects (25). Solving these linear problems we obtain the coefficients of reduced main linear/nonlinear algebraical system (23) and after its solution we obtain the coefficients of wavelet expansion (22), (24). As a result we obtained the explicit solution of our problem in the base of compactly supported wavelets (22).
Also in our case we need to consider the extension of this approach to the case of any type of variable coefficients (periodic, regular or singular). We can produce such approach if we add in our construction additional refinement equation, which

encoded all information about variable coefficients [16]. So, we need to compute only additional integrals of the form

$$\int_D b_{ij}(t)(\varphi_1)^{d_1}(2^m t - k_1)(\varphi_2)^{d_2}(2^m t - k_2)\mathrm{d}x, \tag{27}$$

where $b_{ij}(t)$ are arbitrary functions of time and trial functions φ_1, φ_2 satisfy the refinement equations:

$$\varphi_i(t) = \sum_{k\in\mathbf{Z}} a_{ik}\varphi_i(2t - k) \tag{28}$$

If we consider all computations in the class of compactly supported wavelets then only a finite number of coefficients do not vanish. To approximate the non-constant coefficients, we need choose a different refinable function φ_3 along with some local approximation scheme

$$(B_\ell f)(x) := \sum_{\alpha\in\mathbf{Z}} F_{\ell,k}(f)\varphi_3(2^\ell t - k), \tag{29}$$

where $F_{\ell,k}$ are suitable functionals supported in a small neighborhood of $2^{-\ell}k$ and then replace b_{ij} in (27) by $B_\ell b_{ij}(t)$. To guarantee sufficient accuracy of the resulting approximation to (27) it is important to have the flexibility of choosing φ_3 different from φ_1, φ_2. So, if we take $\varphi_4 = \chi_D$, where χ_D is characteristic function of D, which is again a refinable function, then the problem of computation of (27) is reduced to the problem of calculation of integral

$$H(k_1, k_2, k_3, k_4) = H(k) = \int_{\mathbf{R}^s} \varphi_4(2^j t - k_1) \cdot \\ \varphi_3(2^\ell t - k_2)\varphi_1^{d_1}(2^r t - k_3)\varphi_2^{d_2}(2^s t - k_4)\mathrm{d}x \tag{30}$$

The key point is that these integrals also satisfy some sort of algebraical equation [16]:

$$2^{-|\mu|}H(k) = \sum_{\ell\in\mathbf{Z}} b_{2k-\ell}H(\ell), \qquad \mu = d_1 + d_2. \tag{31}$$

This equation can be interpreted as the problem of computing an eigenvector. Thus, the problem of extension of our approach to the case of variable coefficients is reduced to the same standard algebraical problem as in case of constant coefficients. So, the general scheme is the same one and we have only one more additional linear algebraic problem. After solution of these linear problems we can again compute coefficients of wavelet expansions (22), (24).

Now we concentrate on the last additional problem which comes from overdeterminity of equations (18), (19), which demands to consider expansion (24) instead of expansion (22). It leads to equal number of equations and unknowns in reduced algebraical system of equations (23). For this reason we consider biorthogonal wavelet analysis. We started with two hierarchical sequences of approximations spaces [16]:

$$\ldots V_{-2} \subset V_{-1} \subset V_0 \subset V_1 \subset V_2 \ldots,$$

$$\ldots \widetilde{V}_{-2} \subset \widetilde{V}_{-1} \subset \widetilde{V}_0 \subset \widetilde{V}_1 \subset \widetilde{V}_2 \ldots,$$

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

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

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

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

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

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

Functions $\varphi, \tilde{\varphi}$ generate a multiresolution analysis. $\varphi(x-k)$, $\psi(x-k)$ 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. So, our representation for solution has now the form

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

where synthesis wavelets are used to synthesize the function. But $\tilde{b}_{jk}$ come from inner products with analysis wavelets.

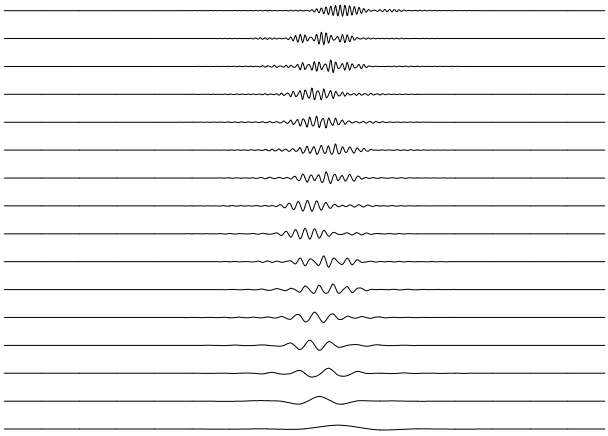

Figure 1: Localized contributions to beam motion.

Biorthogonal point of view is more flexible and stable under the action of large class of operators while orthogonal (one scale for multiresolution) is fragile, all computations are much more simple and we accelerate the rate of convergence of our expansions (24). By analogous anzatzes and approaches we may construct also the multiscale/multiresolution representations for solution of time dependent Wigner equation (13) [14].

5 Numerical Modelling

So, our constructions give us the following N-mode representation for solution of Wigner equations (18)-(19):

$$W^N(p,q) = \sum_{r,s=1}^{N} a_{rs}\Psi_r(p)\Phi_s(q), \tag{32}$$

where $\Psi_r(p)$, $\Phi_s(q)$ may be represented by some family of (nonlinear) eigenmodes with the corresponding multiresolution/multiscale representation in the high-localized wavelet bases (Fig. 1):

$$\Psi_k(p) = \Psi^{M_1}_{k,slow}(p) + \sum_{i\geq M_1} \Psi^i_k(\omega^1_i p), \quad \omega^1_i \sim 2^i, \tag{33}$$

$$\Phi_k(q) = \Phi^{M_2}_{k,slow}(q) + \sum_{j\geq M_2} \Phi^j_k(\omega^2_j q), \quad \omega^2_j \sim 2^j. \tag{34}$$

Our (nonlinear) eigenmodes are more realistic for the modelling of nonlinear classical/quantum dynamical process than the corresponding linear gaussian-like coherent states. Here we mention only the best convergence properties of expansions based on wavelet packets, which realize the so called minimal Shannon entropy property (Fig. 1). On Fig. 2 we present numerical modelling [17] of Wigner function for a simple model of beam motion, which explicitly demonstrates quantum interference property. On Fig. 3 we present the N-mode multiscale/multiresolution decomposition (32)-(34) for solution of Wigner equation. It demonstrates a variety of possible quantum states/patterns generated inside "deformed" Wigner-Moyal dynamics by means of action of internal hidden symmetry on the Hilbert space of states provided by a base set of fundamental localized (nonlinear) eingenmodes. The full zoo includes chaotic, entangled and decoherent states. Qualitative aspects will be considered elsewhere. Some novel approach to the description of quantum problems can be found in our recent papers [18] and at web pages below.

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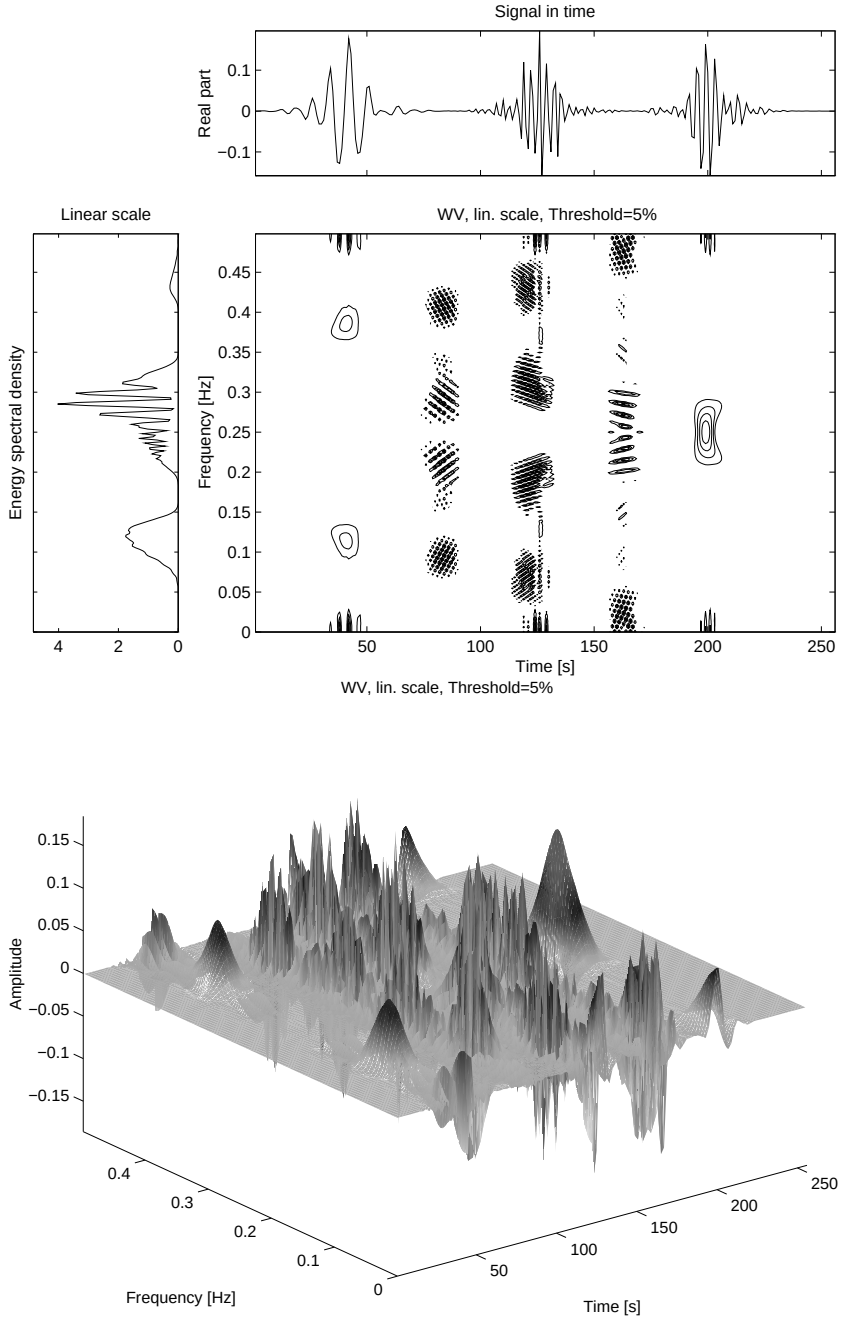

Figure 2: Wigner function for 3 wavelet packets.

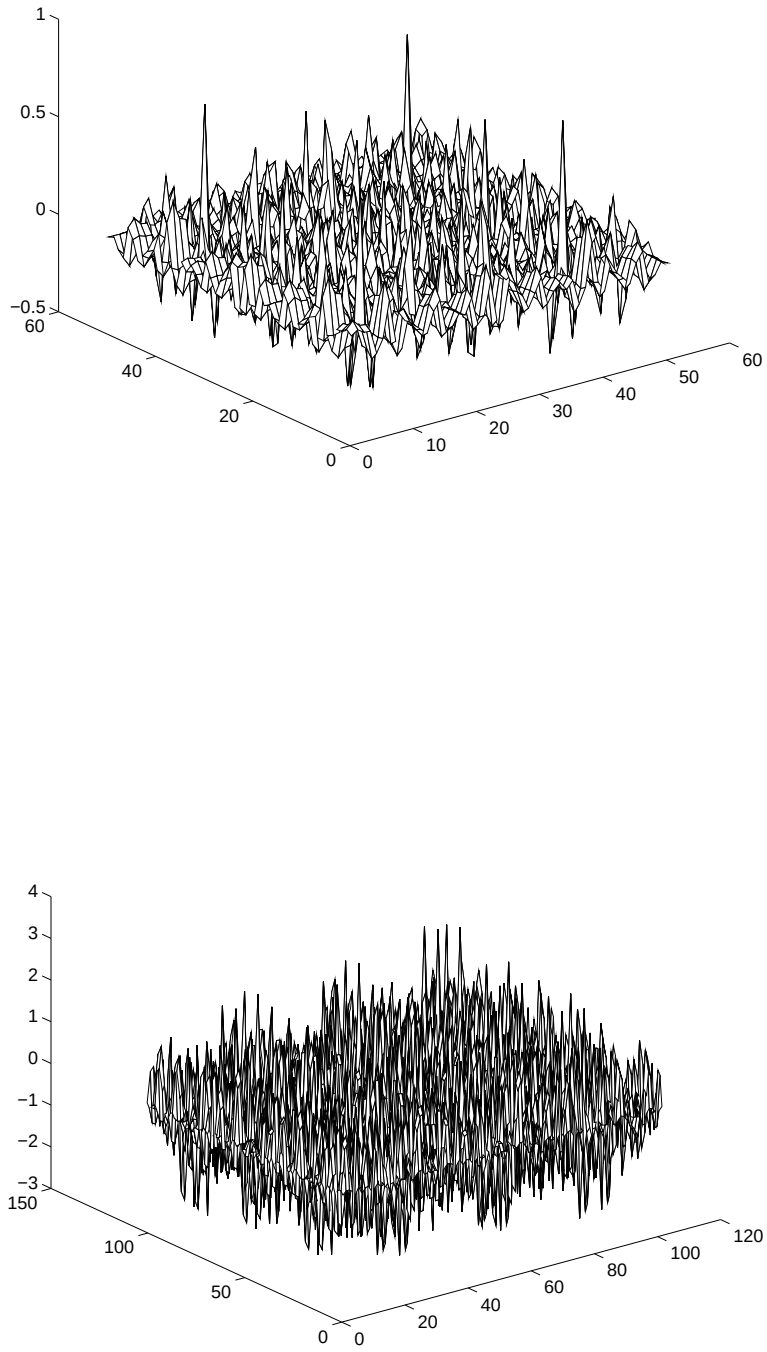

Figure 3: Multiresolution/multiscale representations for Wigner functions.