Space-Frequency Adaptive Approximation for Quantum Hydrodynamic Models

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Abstract

We introduce two space-frequency adaptive strategies for the numerical approximation of the solutions of *quantum hydrodynamic models* for semiconductors, based respectively on wavelets and wavelet packets. The two strategies are compared on a test case, and wavelet packets perform better in approximating with fewer degrees of freedom the high frequency dispersive oscillations of the solution.

1 Introduction

The quantum hydrodynamic model (QHD) for semiconductors has been recently introduced (see e.g. [1, 13, 14]) in order to describe with macroscopic fluid-type unknowns phenomena, such as negative differential resistance in a resonant tunneling diode, which are due to quantum effects and cannot be modeled with classical or semi–classical descriptions. Mathematically, the QHD system is a dispersive regularization of the so–called hydrodynamic equations (HD) for semiconductors (a hyperbolic system of conservation laws coupled self–consistently with the Poisson equation). As usual in macroscopic semiconductor models, the electron position density or some of its derivatives may present strong variation or even blow up in some points. Moreover, the dispersive character of the QHD system implies that the solution may develop high frequency oscillations, which are localized in regions not a priori known. Therefore, numerical simulations of the QHD system with uniform discretizations require an extremely high number of grid points, also when the "pathology" of the solution, which enforces the mesh size, is localized in a small percentage of the simulation domain. This leads to unnecessarily time consuming computations.

Due to the possible dispersive oscillations, an efficient approximation demands the use of a discretization where not only the spatial grid, but also the frequency distribution is adaptively adjusted to the behavior of the solution. One way of achieving such a goal is to use bases with good localization both in space and frequency. Wavelet type bases, which display such a property, have already been successfully used in the design of efficient adaptive schemes in various application fields (see e.g. [5, 3, 2, 6, 12, 18, 20, 19]). Due to their characteristics, the definition of criteria for driving the adaptive procedure (refining and coarsening) *both in space and in frequency* is quite natural. In particular, wavelet based adaptive algorithms have been introduced by the authors ([4]) for the semiconductor hydrodynamic model, where, after performing a diffusive regularization, the adaptive strategy is aimed at well approximating solutions with steep gradients.

Here we study the feasibility of an adaptive algorithm based on wavelets and wavelet packets for the QHD model. Wavelet packets have better frequency localization properties and consequently they are superior to wavelets in drastically diminishing the required number of degrees of freedom for well approximating solutions which exhibit high frequency oscillations.

The outline of the paper is the following. Section 2 contains the QHD equations and a description of the dispersive behavior of the solution. The general adaptive algorithm is presented in Section 3 and specialized to the wavelet basis case in Section 4 and to the wavelet packet case in Section 5.

2 QHD Equations

We consider the isothermal, stationary, one dimensional quantum hydrodynamic (QHD) equations in the domain $(0, 1)$

$$
(P_\varepsilon) \qquad \begin{cases} J^\varepsilon_x = 0, \\ \left(\dfrac{(J^\varepsilon)^2}{u^\varepsilon} + u^\varepsilon\right)_x + u^\varepsilon V_x - \dfrac{\varepsilon^2}{2} u^\varepsilon \left(\dfrac{\sqrt{u^\varepsilon_{xx}}}{\sqrt{u^\varepsilon}}\right)_x = -\dfrac{J^\varepsilon}{\tau}, \\ -\lambda^2 \Delta V = u^\varepsilon - C(x). \end{cases}
$$

Here u^ε (which we will also at times denote by $u(\varepsilon)$) denotes the electron density, J^ε the current density, V the electrostatic potential. The parameter ε is the scaled Planck constant, the function $C(x)$ represents the (prescribed) doping profile of the semiconductor device, the parameter λ is the scaled Debye length and τ is the relaxation time.

As pointed out before, equations (P_ε) are a dispersive regularization of the classical isothermal hydrodynamic (HD) equations

$$
\begin{cases} J_x = 0, \\ \left(\dfrac{J^2}{u} + u\right)_x + uV_x = -\dfrac{J}{\tau}, \\ -\lambda^2 \Delta V = u - C(x), \end{cases}
$$

and, in the **formal** limit, the QHD equations tend to the HD equations. However, due to the dispersive term and the non-linearity, if the HD system exhibits a shock discontinuity, the solution of the QHD system is expected to develop dispersive oscillations, which are not damped as ε goes to zero. In that case only a weak convergence can hold as ε goes to zero and the limiting system is not expected to be the HD system. In [22] a numerical study shows evidence of this fact. A complete theory on the small dispersion limit for the QHD system is still an open problem. We refer to [15, 16, 17] for partial answers in special cases.

Figures 1–3 present the solution of (P_ε) for different values of ε ($\varepsilon = 0.01$, $\varepsilon = 0.005$ and $\varepsilon = 0.0026$, resp.). The pictures clearly show that the oscillation amplitude and location does not change as ε decreases. Changes in ε affect only the oscillation frequency, which is about the double when ε is halved.

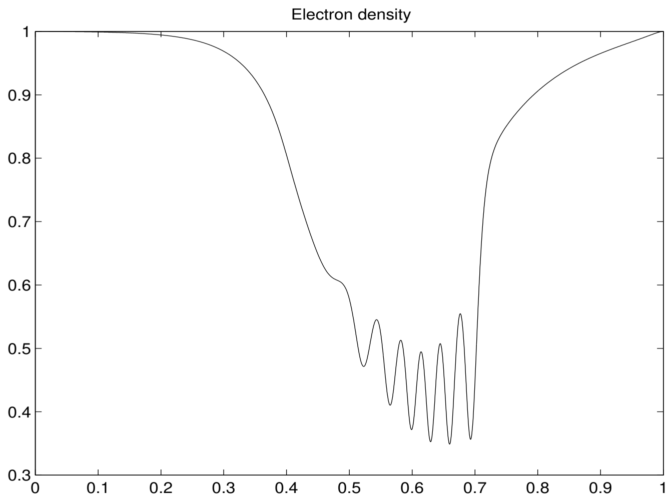

Figure 1: Solution of (P_ε) for $\varepsilon = .01$ ($\lambda = 0.1$, $\tau = 1/8$ and $V_0 = 6.5$, with doping profile C as in figure 5).

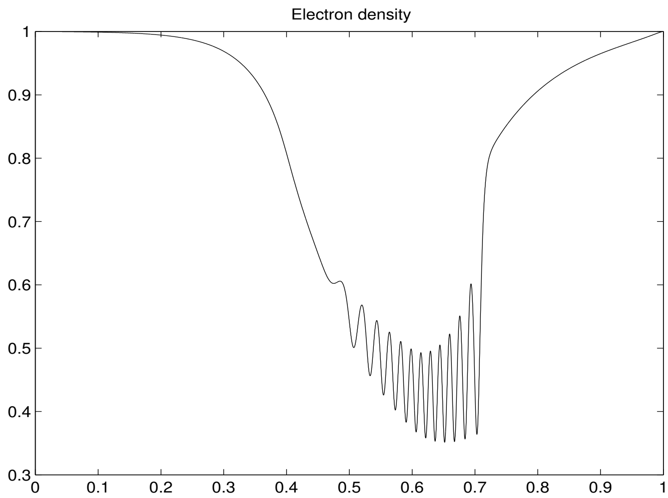

Figure 2: Solution of (P_ε) for $\varepsilon = .01$ ($\lambda = 0.1$, $\tau = 1/8$ and $V_0 = 6.5$, with doping profile C as in figure 5).

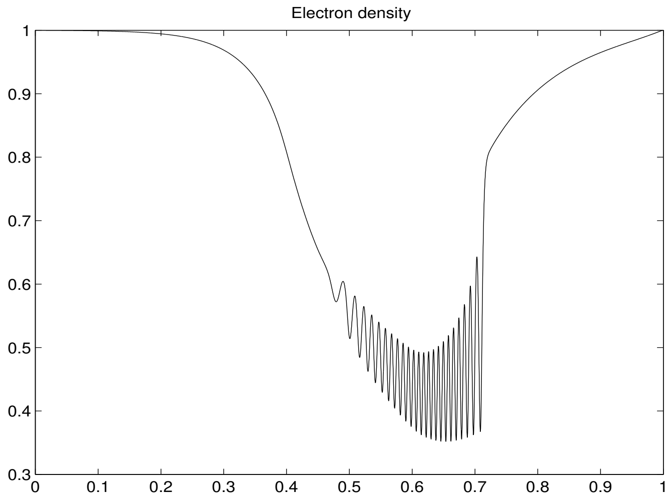

Figure 3: Solution of (P_ε) for $\varepsilon = .01$ ($\lambda = 0.1$, $\tau = 1/8$ and $V_0 = 6.5$, with doping profile C as in figure 5).

An efficient numerical scheme to solve problem (P_ε) when dispersive oscillations occur is a challenging issue. The oscillations must be well resolved in order to keep the correct limiting behavior (for $\varepsilon \longrightarrow 0$) and it is clear that a discretization on a uniform grid requires too many degrees of freedom.

Here we concentrate on the issue of defining proper finite dimensional spaces, adaptely chosen, well suited to approximate the solution of the QHD problem. The regular pattern in dependence of ε will be exploited in the procedure.

The adaptive strategy will then be coupled in a future work with a Galerkin discretization scheme in the selected finite dimensional space. We point out that due to the presence of the dispersive regularization, no special treatment is required to approximate the convection terms in (P_ε). On the contrary, the use of upwind–type schemes would introduce spurious numerical damping of the oscillations and, consequently, further strong restriction on the mesh size in order to describe correctly the oscillations. We refer to [22] for a discussion on this issue.

3 Adaptive Solution of QHD Equations

Problem (P_ε) is highly non–linear, due to the non–linear terms in the second equation of (P_ε) and to the strong coupling to the Poisson equation. A continuation procedure in the parameter ε is an efficient strategy to deal with such problems and it can be coupled, for instance, to a (possibly damped) Newton algorithm for solving the non–linear system for a given ε of the continuation procedure. More precisely, for solving problem (P_ε), with a prescribed $\bar{\varepsilon}$, we define a finite decreasing sequence $\{\varepsilon_n, n = 0, ..., N\}$ with $\varepsilon_0 \sim 1$ and $\varepsilon_N = \bar{\varepsilon}$, and we solve the sequence of problems (P_{ε_n}). For the solution of problem $(P_{\varepsilon_{n+1}})$, the knowledge of the solution of (P_{ε_n}) is exploited in several ways for enhancing the efficiency of the algorithm, for instance it can be used as an initial guess for the Newton scheme. This procedure has been used in [22] for solving (P_ε), there discretized with a finite difference scheme on a uniform grid.

Here, we are interested in designing and testing some strategies for taking advantage of the knowledge of the computed solution of (P_{ε_n}) for reducing the number of degrees of freedom to be used for numerically solving problem $(P_{\varepsilon_{n+1}})$. We aim at an algorithm of the following form.

- Choose a class $\mathcal{B}$ whose elements B are the L^2-orthonormal bases of finite dimensional subspaces V_B of L^2:

  (1) $\mathcal{B} = \{B : \ B \text{ finite orthonormal basis of } V_B =< B >^{span} \subset L^2\}.$

  We assume that the basis functions considered are sufficiently smooth.

- Compute an approximation u_0 to the solution $u(\varepsilon_0)$ of equations (P_ε) for $\varepsilon = \varepsilon_0$ using a coarse uniform grid. This is possible since for $\varepsilon \sim 1$ the solution of (P_ε) is smooth.

- Given the approximation u_n to the solution $u(\varepsilon_n)$ of (P_{ε_n}), an approximation u_{n+1} to the solution $u(\varepsilon_{n+1})$ of $(P_{\varepsilon_{n+1}})$ is obtained as follows:

  – By analyzing u_n select a basis $B_{n+1} \in \mathcal{B}$, *as small as possible*, well suited for approximating $u(\varepsilon_{n+1})$.

  – Compute u_{n+1} in $V_{n+1} =< B_{n+1} >^{span}$ approximate solution of $(P_{\varepsilon_{n+1}})$, by a suitable numerical method (for instance, Galerkin approximation of $(P_{\varepsilon_{n+1}})$).

In this paper we will concentrate on two of the issues to be faced when designing an algorithm of this type:

1. the choice of the class $\mathcal{B}$;

2. the adaptive selection (out of $\mathcal{B}$) of a (small) basis B_{n+1}, well suited for approximating $u(\varepsilon_{n+1})$.

Due to the onset of high frequency oscillations in a possible large (though localized) portion of the domain, in order to be able to approximate the solutions of (P_ε) with few degrees of freedom, it is not enough to work with methods that are adaptive only with respect to the space. We will then rather work with basis functions which display good localization properties also in the frequency domain. In particular we will consider bases B whose elements will be *phase atoms*. *Phase atoms* ([23]) are smooth functions which are well localized in both position and momentum in the sense of quantum mechanics. More precisely, a phase atom ψ needs to satisfy the following properties.

- Finite Energy. Possibly after a re-normalization, it holds

$$\|\psi\|_{L^2} = 1.$$

- Smoothness and decay. Both ψ and $\hat{\psi}$ are smooth ($\hat{\psi}$ being the Fourier transform of ψ).

- Finite *position* and *momentum*.

$$\begin{aligned} x_0 &:= \int x|\psi(x)|^2\,dx < \infty, \\ \xi_0 &:= \int \xi|\hat{\psi}(\xi)|^2\,d\xi < \infty, \end{aligned}$$

  are respectively called *position* and *momentum* (or *frequency*) of ψ.

- Localization in position and momentum. We have

$$\begin{aligned} \Delta x &:= \left(\int (x-x_0)^2|\psi(x)|^2\,dx\right)^{1/2} < \infty, \\ \Delta \xi &:= \left(\int (\xi-\xi_0)^2|\hat{\psi}(\xi)|^2\,d\xi\right)^{1/2} < \infty. \end{aligned}$$

Δx and $\Delta\xi$ are also called *position* and *momentum uncertainty* respectively.

In the following two sections we will consider two classes of phase atoms, namely *wavelets* and *wavelet packets*. In particular we will analyze the performances of such two classes in the framework of adaptive approximation of the solution of (P_ε).

4 Wavelet Adaptivity

The first example of adaptive scheme that we will consider, is the one based on the use of wavelets [21].

In the literature it is possible to find a large number of orthonormal wavelet bases for L^2:

$$L^2 =< \psi_{jk}, j \in \mathbb{Z}^+, k = 1, \cdots, 2^j >^{span} .$$

Such bases consist of functions with the following localization properties:

- The position of ψ_{jk} is $x_{jk} = k/2^j$.
- The momentum of ψ_{jk} is $\xi_{jk} = \alpha 2^j$ ($\alpha \neq 0$ independent of j and k).
- The localization in position of ψ_{jk} is $\Delta x_{jk} \sim 2^{-j}$.
- The localization in frequency (or momentum) of ψ_{jk} is $\Delta\xi_{jk} \sim 2^j$

We remark that, by the Heisenberg uncertainty principle it is not possible to localize a function arbitrarily well both in position and momentum ($\Delta x \cdot \Delta\xi \geq 1$). Therefore the functions ψ_{jk} are localized in the phase space nearly as well as possible.

The construction of such bases is originally performed on $\mathbb{R}$, but it can be carried out also on the interval ([8]) with boundary conditions of different type (homogeneous Dirichlet, periodic, ...). However in this paper we will not explicitely deal with the issue of boundary condition, since the phenomenology we are interested in is in general concentrated far from the boundaries.

Remark 4.1 *Though for simplicity we consider here only orthonormal wavelet bases, the strategy that we are going to present could be applied, without major modifications, in the more general framework of biorthogonal wavelets. [7]*

We recall that the above localization properties imply that a norm equivalence of the form

$$\|f\|_{H^r} \sim \left(\sum_{j,k} 2^{2jr} | < f, \psi_{jk} > |^2 \right)^{1/2}$$

holds for all $f \in H^r$, $r \in (-R, R)$, with the parameter $R > 0$ depending on the particular wavelet basis under consideration. For $f \in H^{-r}$, $r > 0$ the notation $< \cdot, \cdot >$ is to be intended as the duality relation between H^{-r} and H^r.

In the following it will be useful to represent each basis function ψ_{jk} with the rectangle $]k2^{-j}, (k+1)2^{-j}[\times]2^j, 2^{j+1}[$ in the (x, ξ) plane. Using such a representation yields a "tiling" of the phase space which well represents the localization features of such bases.

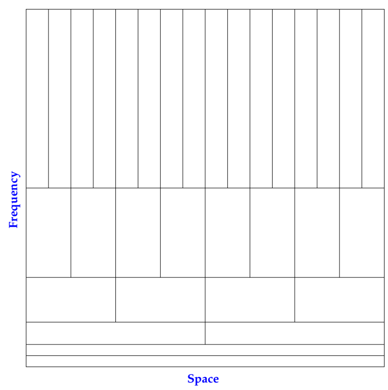

Figure 4: "tiling" of the phase-space corresponding to a wavelet basis

When considering adaptive wavelet methods the class of bases $\mathcal{B}$ takes the form

$$\mathcal{B} = \{B = \{\psi_{jk},\ (j,k) \in \Lambda\},\ \Lambda \text{ finite subset of } \mathbb{Z}^+ \times \mathbb{Z}\}.$$

A simple, yet effective, adaptive strategy based on wavelet bases is the following [20, 3, 4]. Let $u(\varepsilon_n)$ be given:

$$u(\varepsilon_n) = \sum_{j,k} u^n_{j,k} \psi_{jk}.$$

We can construct a basis $B_{n+1} \in \mathcal{B}$ for approximating $u(\varepsilon_{n+1})$ by simply looking at the size of the coefficients $u^n_{j,k}$. If a coefficient is big, the corresponding function is included in the basis B_{n+1}, as well as some "neighboring" (in the phase-space) functions. If, on the other hand, a coefficient is very small, the corresponding function will not belong to the basis B_{n+1}.

More precisely, we define B_{n+1} as follows. We choose two tolerances δ_r and δ_a, as well as a number N_{add} of "relevant neighbors", and we set

$$B^r_{n+1} = \left\{ \psi_{jk} : \quad 2^{\frac{3}{2}j} |u^n_{j,k}| > \delta_r \right\}. \tag{2}$$

Moreover, we set

$$\begin{aligned} I^{add}_{n+1} &= \{(j,k) : \ 2^{\frac{3}{2}j} |u^n_{j,k}| > \delta_a\}, && (3)\\ N_{jk} &= \{(j+\zeta, 2^\zeta k + \eta), \zeta = 0, 1, \quad \eta = -N_{add}, \cdots, N_{add}\}, && (4)\\ B^a_{n+1} &= \bigcup_{(j,k)\in I^{add}_{n+1}} \{\psi_{jk}, \ (j,k) \in N_{jk}\}. && (5) \end{aligned}$$

The basis B_{n+1} is then defined as

$$B_{n+1} = B^r_{n+1} \cup B^a_{n+1}. \tag{6}$$

We stress out that the above refining and de-refining strategy is tuned in order to give a good approximation in $H^{\frac{3}{2}}$ rather than in L^2. This is reflected by the presence of factor $2^{\frac{3}{2}j}$ in equations (2) and (3). The choice of such a norm is heuristically motivated by the fact that we are dealing with a third order operator.

Remark 4.2 *For simplicity we considered an algorithm where neighbors are added only at the same level j and at the immediately next level $j+1$. A more effective algorithm might sometimes be obtained by adding neighbors chosen in more than two levels.*

To test the effectiveness of adaptive wavelet methods for solving the QHD equations we performed the following test. Let $(\varepsilon_n)_{n=0,\cdots,N}$ be given.

- Compute a reference solution $u(\varepsilon_n)$, $(n = 0, \cdots, N)$, by solving (P_ε) for $\varepsilon = \varepsilon_n$ with a finite difference scheme on a very fine grid ("overkill"). In our case we used a discretization step 2.5 10^{-4}.

- For each $n = 0, \cdots, N-1$, perform the following procedure:

  Step 1. given $\check{u}_n$ (computed at the previous step)

$$\check{u}_n = \sum_{j,k \in \Lambda_n} u^n_{j,k} \psi_{jk},$$

  ($\check{u}_n$ approximation of $u(\varepsilon_n)$), define $B_{n+1} = \{\psi_{jk}, \quad (j,k) \in \Lambda_{n+1}\}$ and the corresponding space $V_{n+1} =< B_{n+1} >^{span}$ by the preceding adaptive strategy (2)–(6).

  Step 2. define $\check{u}_{n+1}$ as the L^2 orthogonal projection of $u(\varepsilon_{n+1})$ onto V_{n+1}

$$\check{u}_{n+1} = \sum_{(j,k) \in \Lambda_{n+1}} < u(\varepsilon_{n+1}), \psi_{jk} > \psi_{jk}.$$

- For all $n = 1, \cdots, N$ evaluate the relative error

$$e_n = \frac{\|u(\varepsilon_n) - \check{u}_n\|_{H^{3/2}}}{\|u(\varepsilon_n)\|_{H^{3/2}}}.$$

We performed the above test for the following data in (P_ε): the doping profile $C(x)$ is chosen as in figure 5, with max(C)=1 and min(C)=0.1, the Debye length is $\lambda = 0.1$, the relaxation time is $\tau = 1/8$ and the applied voltage is $V_0 = 6.5$. The solutions for these values of the parameters are the ones depicted in pictures 1–3.

In the following table we give for each n, the value ε_n, the relative error e_n, the cardinality N_{adapt} of the adaptively selected basis B_n, as well as the "compression ratio" (CR) N_{adapt}/N_{unif} (N_{unif} ($\sim 2^j$ for some j) being the number of degrees of freedom which would be necessary to represent $u(\varepsilon_n)$ with a uniform discretization with the same accuracy).

5 Wavelet-Packets Adaptivity

The results of wavelet adaptivity for the numerical solution of QHD system are not entirely satisfactory. This is mainly due to the fact that wavelet bases

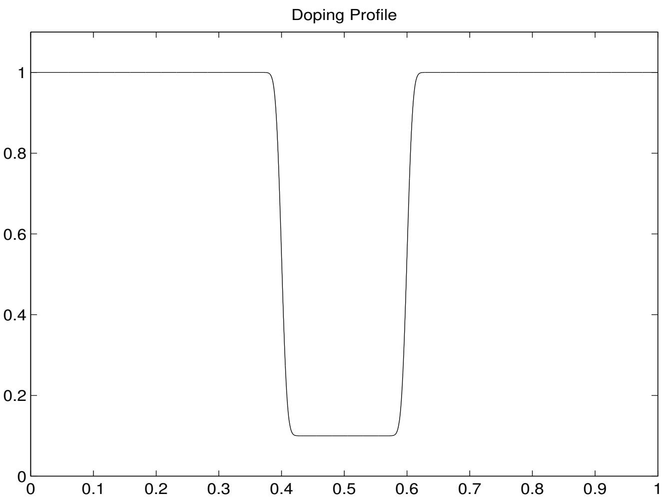

Figure 5: Doping profile $C(x)$

ε_n	e_n	N_{adapt}	CR
.0075	.1535	120	4.27
.007	.0218	156	3.28
.006	.0377	160	3.20
.005	.0202	175	2.93
.004	.0208	195	5.25
.0025	.0230	256	4.00
.002	.0137	353	5.70
.0016	.0111	446	4.51
.0011	.0123	596	6.71
.00102	.0020	858	4.66
.001	.0014	969	4.13

Table 1: Wavelet Adaptive Strategy

approximate high frequencies with basis functions which are highly localized in space. In other words, when approximating an highly oscillating function, the use of wavelets correspond to using (in the region where oscillations occur) an uniform discretization. In order to push the adaptivity even further one needs to use functions which display better localization in momentum even at high frequency. *Wavelet Packets* [9] are a generalization of wavelets which allows one more degree of freedom, as far as phase space localization is concerned. They have been recently applied ([19]) for the adaptive numerical solution of Burgers equation.

Let us briefly review the main features of wavelet packets. A "Wavelet Packet dictionary" $\mathcal{D}$ is a overly redundant (*i.e.* non linearly independent) set of functions, which, by abuse of notation we will call "basis functions". Each basis function $\psi_{p,\omega,s}$ in the set is identified by three parameters: the (scaled) position p, the (scaled) wave number ω and the scale s. Each of these functions is constructed in such a way that its space-localization is $\Delta x \sim 2^{-s}$ with center $p/2^s$ and its frequency-localization is $\Delta\xi \sim 2^s$ with center $\omega 2^s$. Again, in view of the Heisemberg uncertainty principle, the functions $\psi_{p,\omega,s}$ are localized in the phase space nearly as well as possible.

For a given $f \in L^2$ one can define the *wavelet packet transform* of f:

$$w_{p,\omega,s}(f) = \int f\psi_{p,\omega,s}.$$

Out of a given "Wavelet Packet dictionary" it is possible to extract many different orthonormal bases for L^2 of the form $B_\Lambda = \{\psi_{p,\omega,s},\ (p,\omega,s) \in \Lambda\}$, by selecting suitable subsets Λ of the index set $\{(p,\omega,s)\}$. For such subsets the inversion formula holds for any $f \in L^2$:

$$f = \sum_{(p,\omega,s)\in\Lambda} w_{p,\omega,s}(f)\psi_{p,\omega,s}.$$

In particular, for the choice $\Lambda = \{(p,1,s),\ p \in \mathbb{Z}, s \in \mathbb{Z}^+\}$ one obtains the usual wavelet orthonormal basis described in the previous section.

The "basis functions" $\psi_{p,\omega,s}$ can be constructed as follows. We start by choosing two *quadrature mirror filters*, *i.e.* two finite sequences $\{h_n\}$ and $\{g_n\}$, satisfying the following relations:

$$(7)\qquad \sum_n h_{2n} = \sum_n h_{2n+1} = \frac{1}{\sqrt{2}}, \qquad g_n = (-1)^{n-1}h_{1-n} \qquad \forall n \in \mathbb{Z},$$

$$\sum_n h_n h_{n+2m} = \sum_n g_n g_{n+2m} = \begin{cases} 1, & \text{if } m = 0, \\ 0, & \text{otherwise}, \end{cases} \tag{8}$$

$$\sum_n h_n g_n + 2m = 0, \qquad \forall m \in \mathbb{Z}. \tag{9}$$

We can then define a family of functions, depending on an integer parameter $\ell \geq 0$ by

$$W_{2\ell}(x) = \sqrt{2} \sum_n h_n W_\ell(2x - n), \tag{10}$$

$$W_{2\ell+1}(x) = \sqrt{2} \sum_n g_n W_\ell(2x - n). \tag{11}$$

We remark that W_0 satisfies a dilation equation. Conditions (7 – 9) guarantee the existence of a compactly supported solution of such a dilation equation (and therefore they imply the well posedness of definition (10)). W_0 and W_1 are, respectively, the scaling and wavelet functions of the corresponding wavelet basis. The pair $\{h_n\}$ and $\{g_n\}$ can be chosen in such a way that the functions W_ℓ have any prescribed smoothness.

For $p \in \mathbb{Z}, \omega \in \mathbb{Z}^+, s \in \mathbb{Z}^+$, wavelet packets are then defined by

$$\psi_{p,\omega,s} = 2^{s/2} W_\omega(2^s x - p), \tag{12}$$

where ω is the (integer) scaled wave number.

Orthonormal sets can be extracted out of the wavelet packet dictionary by selecting index subsets Λ for which the dyadic intervals $\{[\omega 2^s, (\omega+1)2^s[: (p, \omega, s) \in \Lambda\}$ form a disjoint cover of the positive semi-axis.

More precisely, we will say that an index set Λ is *admissible* if the following condition is satisfied: for Ξ defined by

$$\Xi = \{(\omega, s) : \ \exists p, (p, \omega, s) \in \Lambda\},$$

it holds for each $(\omega, s), (\omega', s') \in \Xi$

$$(\omega, s) \neq (\omega', s') \Rightarrow [\omega 2^s, (\omega+1)2^s[\cap [\omega' 2^{s'}, (\omega'+1)2^{s'}[= \emptyset.$$

It is possible to prove that if the index set Λ is admissible, then $B_\Lambda = \{\psi_{p,\omega,s}, (p,\omega,s) \in \Lambda\}$ forms an orthogonal system.

We say that an admissible index set Λ,

$$\Lambda = \{(p,\omega,s),\ (\omega,s) \in \Xi,\ p \in I_{(\omega,s)}\},$$

is *complete* at scale S on the domain $\mathbb{T}$ if Ξ satisfies

$$\bigcup_{(\omega,s)\in\Xi} [\omega 2^s, (\omega+1)2^s[= [0, 2^S[, \tag{13}$$

and if, for all $(\omega,s) \in \Xi$, the set $I_{(\omega,s)} = \{p : (p,\omega,s) \in \Lambda\}$ satisfies

$$\bigcup_{p \in I_{(\omega,s)}} [p2^{-s}, (p+1)2^{-s}] \supseteq \mathbb{T}. \tag{14}$$

Roughly speaking, a complete index set identifies the orthonormal basis of a discrete subspace of $L^2(\mathbb{T})$ corresponding to a uniform discretization with mesh size 2^{-S}. Condition (13) assures that all the frequencies below 2^S are covered, and condition (14) guarantees that, for all frequency ranges, all the spatial positions are present.

We can then define a class $\mathcal{B}$ of bases as follows:

$$\mathcal{B} = \{B_\Lambda \subset \mathcal{D}, \Lambda \in \mathcal{L}\}, \qquad B_\Lambda := \{\psi_{p,\omega,s}, (p,\omega,s) \in \Lambda\}, \tag{15}$$

with

$$\mathcal{L} = \{\Lambda\ : \Lambda \text{ is admissible and } \#(\Lambda) < +\infty\}.$$

Again, it is useful to visualize the phase-space localization property of each basis function by means of a "tiling" (obtained by representing $\psi_{p,\omega,s}$ by the rectangle $]p2^{-s}, (p+1)2^{-s}[\times]2^s\omega, 2^s(\omega+1)[$.

The redundancy of the wavelet packet dictionary allows for a greater flexibility as far as space frequency localization is concerned. On the other hand, the computation of a good approximation of a function by means of few degrees of freedom needs for a more sophisticated approach.

Let us at first consider the problem of approximating a known function f with as few as possible degrees of freedom. The extraction of a basis well suited for approximating the given function f with few degrees of freedom needs now to be performed in two steps:

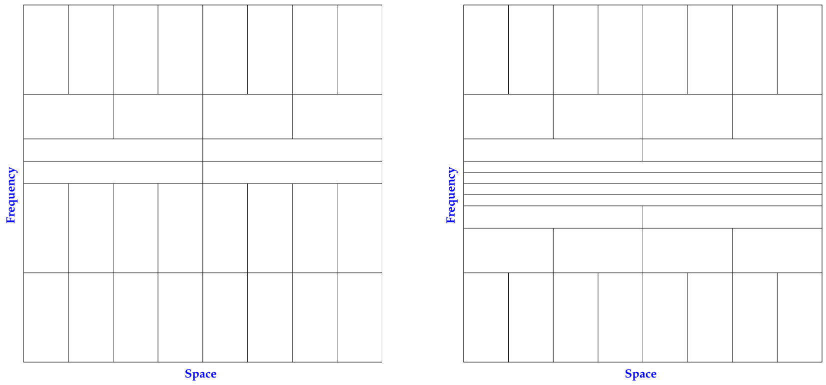

Figure 6: "tilings" corresponding to different wavelet packets orthonormal bases

(i) Select a complete (at scale S if the function is sampled with sampling rate 2^{-S}) index set $\hat{\Lambda} \in \mathcal{L}$.

(ii) Select a subset $\hat{\Lambda}_\delta \subset \hat{\Lambda}$ such that

$$\|f - \sum_{(p,\omega,s)\in\hat{\Lambda}_\delta} w_{p,\omega,s}\psi_{p,\omega,s}\|_{H^{3/2}} \quad \text{is small.}$$

Task (ii) can be performed quite easily thanks to the observation that for all functions $f \in H^{3/2}$ and for any orthonormal basis $B_{\hat{\Lambda}} \in \mathcal{B}$ it holds

$$\|f\|_{H^{3/2}} \sim \left(\sum_{(p,\omega,s)\in\Lambda} |(2^s\omega)^{3/2} w_{p,\omega,s}|^2\right)^{1/2}.$$

As far as task (i) is concerned, the optimal choice is provided by an index set $\hat{\Lambda}$ such that the corresponding basis $B_{\hat{\Lambda}}$ minimizes a suitable additive entropy:

$$H(f, B_{\hat{\Lambda}}) = \min_{B_\Lambda} H(f, B_\Lambda).$$

The basis $B_{\hat{\Lambda}}$ is usually referred to as *best basis* for the function f. If the goal is, as in our case, to approximate f with as few as possible degrees of freedom, then the entropy can be for instance chosen of the following form

(16) $$H(f, B_\Lambda) = \#(\{(p,\omega,s) \in \Lambda : \ |(2^s\omega)^{3/2}\, w_{p,\omega,s}| \geq \delta\}).$$

Once $B_{\hat{\Lambda}}$ has been selected, the subset $\hat{\Lambda}_\delta$ is clearly defined as

(17) $$\hat{\Lambda}_\delta = \{(p,\omega,s) \in \hat{\Lambda} : \ |(2^s\omega)^{3/2}\, w_{p,\omega,s}| \geq \delta\}.$$

The implementation of the wavelet packet transform and of the best basis search algorithm for a given function f is described in detail in [10]. If f is sampled with step h, the entire procedure has complexity $\frac{1}{h}\log\frac{1}{h}$.

If one wants to use wavelet packet dictionaries and the concept of best basis in the framework of the adaptive type algorithm described in section 3, for each ε_{n+1} one must be able to perform tasks (i) and (ii), for $u(\varepsilon_{n+1})$ by analyzing the solution $u(\varepsilon_n)$ at the previous continuation step. We will not deal here with the problem relative to task (ii), *i.e.* the exctraction out of the best basis of a small subset well suited to well approximate $u(\varepsilon_{n+1})$. We refer to [19], where a possible strategy has been proposed, based on a suitable definition of "neighbors" (in the phase space) of a given basis function $\psi_{p,\omega,s}$. We will rather concentrate here on the problem of selecting the best basis - or a close enough basis - for $u(\varepsilon_{n+1})$, by analyzing the solution $u(\varepsilon_n)$ at the previous continuation step.

In order to verify to what extent this is feasible, we performed the following test

- Compute $u(\varepsilon_n)$ $(n = 0, \ldots, N)$ by solving the QHD equations for $\varepsilon = \varepsilon_n$ by finite differences on a very fine grid ("overkill"). In our case we used a discretization step 2.5 10^{-4} (which corresponds to a scale $S \sim 12$)

- Compute the wavelet packet transform $w^n_{p,\omega,s}$ of $u(\varepsilon_n)$

$$w^n_{p,\omega,s} = \int u(\varepsilon_n)\psi_{p,\omega,s},$$

and select the best basis $\hat{B}^n = \{\psi_{p,\omega,s}, (p,\omega,s) \in \hat{\Lambda}^n\}$:

$$H(u(\varepsilon_n), \hat{B}^n) = \min_{B_\Lambda} H(u(\varepsilon_n), B_\Lambda).$$

- Compute the number of coefficients needed for approximating $u(\varepsilon_{n+1})$ using elements of the best basis for $u(\varepsilon_n)$:

$$H(u(\varepsilon_{n+1}), \hat{B}^n)) = \#(\{(p,\omega,s) \in \hat{\Lambda}^n : \ |(2^s\omega)^{3/2}\, w^{n+1}_{p,\omega,s}| \geq \delta\}),$$

  and compare $H(u(\varepsilon_{n+1}), \hat{B}^n))$ with the optimal number of coefficients $H(u(\varepsilon_{n+1}), \hat{B}^{n+1}))$.

- Define an approximation to $u(\varepsilon_{n+1})$, by selecting an index set $\hat{\Lambda}^n_\delta$

$$\hat{\Lambda}^n_\delta = \{(p,\omega,s) \in \hat{\Lambda}^n : \ |(\omega 2^s)^{\frac{3}{2}} w^{n+1}_{p,\omega,s}| \geq \delta\}$$

  and computing

$$\bar{u}_{n+1} = \sum_{(p,\omega,s)\in\hat{\Lambda}^n_\delta} w^{n+1}_{p,\omega,s} \psi_{p,\omega,s}.$$

- Evaluate the relative error

$$e^{n+1}_{wp} = \frac{\|u(\varepsilon_{n+1}) - \bar{u}_{n+1}\|_{H^{3/2}}}{\|u(\varepsilon_{n+1})\|_{H^{3/2}}}.$$

The following table summarizes the results of such test, performed in the same case as in the previous section. We report the values of ε_{n+1}, of the number N_{opt} of significant degrees of freedom when approximating $u(\varepsilon_{n+1})$ by means of the best basis $\hat{B}^{n+1}_\Lambda$, the number N_{est} when approximating $u(\varepsilon_{n+1})$ by means of the best basis $\hat{B}^n_\Lambda$ obtained from the analysis of $u(\varepsilon_n)$ and the error e^{n+1}_{wp}. The table also displays the two compression ratios $CR_{opt} = N_{unif}/N_{opt}$ and $CR_{est} = N_{unif}/N_{est}$ (N_{unif} is defined, as in the previous section, as the number of degrees of freedom which would be necessary to represent the solution with the same accuracy by means of a uniform discretization of wavelet type). By a comparison with the results of the wavelet adaptive algorithm presented in the previous section it is clear that, especially at very high frequencies, wavelet packets perform better, allowing to almost double the compression ratio.

6 Conclusion

We proposed two space–frequency adaptive strategies based respectively on wavelets and wavelet packets for approximating the solution of the QHD

ε_n	N_{opt}	N_{est}	CR_{opt}	CR_{est}	e^n_{wp}
.0075	95	116	5.3	4.4	.0080
.007	102	105	5.0	4.8	.0074
.006	112	122	4.6	4.2	.0067
.005	124	137	4.1	3.7	.0080
.004	150	163	6.8	6.3	.0045
.0025	192	168	6.1	5.3	.0028
.002	253	292	8.0	6.9	.0023
.0016	331	366	6.0	5.5	.0024
.0011	480	585	8.3	6.8	.0012
.00102	525	550	7.6	7.3	.0010
.001	496	503	8.1	8.0	.0011

Table 2: Performance of an adaptive WP algorithm

system. The aim is to couple such strategies with a Galerkin approximation of the equations in a future work. Wavelet packets, due to their better frequency localization property, are superior to wavelets in drastically diminishing the required number of degrees of freedom for well approximating the solution. Clearly they are more costly when used to solve problem (P_ε), due to the higher cost of the WP transform with respect to the FWT, and to the additional cost of the best basis search. Moreover, the intrinsic difficulties connected with the application of wavelets in the framework on non–linear problems [11] are even harder when dealing with Wavelet Packets. However, the strong non–linearity of the problem requires a continuation algorithm in the parameter ε and for each ε_n of the ε-sequence a non–linear system must be solved (for instance with a Newton algorithm). It is then clear that, when (P_ε) is solved for a small ε, a linearized QHD system must be solved many times and the much lower number of degrees of freedom selected with the wavelet packet procedure is expected to largely compensate the higher cost of the basis selection and of the non–linearity treatment and to provide an over all more efficient numerical scheme.

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