Time Dependent Phase Space Filters: Nonreflecting Boundaries for Semilinear Schrödinger Equations (PRELIMINARY VERSION)

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Abstract

We construct an algorithm, the Time Dependent Phase Space Filter (TDPSF), for solving nonlinear time dependent Schrödinger equations on $\mathbb{R}^N$. The algorithm consists of solving the NLS on a box with periodic boundary conditions. After certain intervals, we apply a filter in phase space to remove outgoing waves. Incoming waves are affected minimally. Rigorous error estimates are provided and numerical tests are discussed.

Contents

1 Introduction and Definitions

Consider a semilinear Schrödinger equation on $\mathbb{R}^{N+1}$

$$i\partial_t\psi(x,t) = -(1/2)\Delta\psi(x,t) + g(t,\vec{x},\psi(\vec{x},t))\psi(\vec{x},t) \tag{1.1}$$

where $g(t,\vec{x},\cdot)$ is some semilinear, Lipschitz (in some Sobolev space) nonlinearity. For instance, $g(t,\vec{x},\cdot)$ could be $V(\vec{x},t) + f(|\psi(\vec{x},t)|^2)$ for some smooth function f and (spatially) localized potential $V(\vec{x},t)$.

We assume the initial condition and nonlinearity are such that the nonlinearity remains localized inside some box $[-L_{\text{NL}}, L_{\text{NL}}]^N$. Outside this region the solution is assumed to behave like a free wave (a solution to (1.1) with $g(t,\vec{x},\cdot) = 0$), which is well understood.

One very common method of solving such a problem is domain truncation. That is, one solves the PDE (1.1) numerically on a region $[-L, L]^N$. On the finite domain, of course, boundary conditions must be specified. Dirichlet and Neumann boundaries introduce spurious reflections, while periodic boundaries (which are desirable in order to use fast spectral methods) allow outgoing waves to wrap around the computational domain. In either case, a serious mistake has been made. This causes the numerical solution to become incorrect after a time $T \approx L/k_{\max}$, where $k_{\max}$ is the "maximal velocity" of the solution[1].

It is an interesting and well known problem to find a way to minimize these errors. The simplest way is simply to expand the domain as the support of $\psi(\vec{x},t)$ grows, but this is computationally very expensive.

For the wave equation and other strictly hyperbolic wave equations this problem has a beautiful exact solution (c.f. [18, 16]), namely the Dirichlet-to-Neumann map. The equation (1.1) is solved in a region $[-L_{\text{int}}, L_{\text{int}}]^N$, and the boundary conditions are given by $\psi(\vec{x},t)$ (where $\psi(\vec{x},t)$ is the solution to (1.1) on $\mathbb{R}^N$) on the boundary. Of course, since $\psi(\vec{x},t)$ is not known, it must be approximated. The usual method (used with great success for the wave equatin) is to approximate the exact solution by rational functions in the frequency domain.

[1] There is, in general, no maximal velocity of the solution. However, we will define $k_{\max}$ more precisely later on. $k_{\max}$ will be the frequency such that the energy of $\hat{\psi}(k,t)$ for $k > k_{\max}$ is small.

These correspond to boundary conditions given by a high order differential operator. This result depends strongly on the fact that in the frequency domain, the Dirichlet-to-Neumann map behaves like a polynomial at ∞.

For the Schrödigner equation and other dispersive wave equations, the situation is not so simple. Even in the free case ($g(t, \vec{x}, \psi(\vec{x}, t)) = 0$), it is impossible to construct local (in time and space) approximations to the Dirichlet-Neumann operator. In addition, constructing the Dirichlet-Neumann map in the case $-(1/2)\Delta + V(x)$ is not an easy matter. In the nonlinear case we know of results only in 1 space dimension, and with no rigorous error estimates [41, 42, 43].

Another drawback of the Dirichlet-to-Neumann approach is that it precludes the use of spectral methods to solve the interior problem. Spectral methods (described on page 17) use the FFT (Fast Fourier Transform) to diagonalize the operator $e^{i(1/2)\Delta t}$. This approach naturally imposes periodic boundaries. Spectral methods are desirable, since they are believed to be more accurate than most other methods on periodic domains (for a finite set of spatial frequencies). The error due to boundary conditions, however, makes them unfeasible. Thus, one usually reverts to using FDTD (Finite Difference Time Domain) in their place, but the accuracy of these methods is limited and decreases rapidly with high spatial frequencies.

An ad-hoc approach (described in, e.g. [29]) which is commonly used is to add an absorbing potential, $-iV(x)\psi(\vec{x}, t)$ to the right hand side of (1.1), with $V(x) = 0$ away from the boundary. This potential has the effect of partially dissipating waves as they pass over it. Thus, as waves reach the boundary, they are partially dissipated by the complex potential, reducing the reflection. This approach is far from optimal, but is still the industry standard due to the ease of implementation, compatibility with spectral methods and simplicity.

A variant on this approach is the PML (Perfectly Matched Layer). Proposed originally for Maxwell's equations in [3] and for the Schrödinger equation in [24], it is a variant on the absorbing potential method in which Δ is replaced by $(1 - ia(x))\Delta$ (with $a(x)$ nonzero only in a boundary layer) in such a way so that when $a(x)$ "switches on", there is no reflection at the interface.

1.0.1 Our Approach

We propose an alternative approach to absorbing boundaries. We make the assumption that near the boundary of the box, the solution behaves like a free wave. We make no assumptions on the nonlinearity, beyond the fact that it is localized on the inside of the box and locally Lipschitz. In particular, the nonlinearity could take the form of a complicated time dependent short range potential $V(\vec{x}, t)\psi(\vec{x}, t)$, a polynomial nonlinearity $f(|\psi(\vec{x}, t)|^{2\sigma})\psi(\vec{x}, t)$ (for $f(z)$ a Lipschitz function) or others.

We also assume that the solution remains localized in frequency, that is $\hat{\psi}(\vec{k}, t)$ is small off the box $[-k_{\max}, k_{\max}]^N$ for some large number $k_{\max}$ (the maximal momentum of the problem, which we assume exists).

Our algorithm is as follows. We assume the initial data is localized on a region $[-L_{\text{int}}, L_{\text{int}}]^N$. We solve (1.1) on the box $[-(L_{\text{int}} + w), L_{\text{int}} + w]^N$ on the time interval $[0, T_{\mathrm{step}}]$.

By making T_{step} small enough (smaller than $w/k_{\max}$), we can ensure that $\psi(\vec{x}, t)$ is mostly localized inside box $[-(L_{\mathrm{int}}+w), (L_{\mathrm{int}}+w)]^N$. Thus, since very little mass has actually hit the boundaries, very little has reflected and we have made few errors.

We now decompose the solution $\psi(\vec{x}, t)$ into a sum of gaussians (indexed by $\vec{a}, \vec{b} \in \mathbb{Z}^N$, with x_0, k_0, σ all positive constants satisfying certain constraints to be made precise later):

$$\psi(x, T_{\mathrm{step}}) = \sum_{(\vec{a},\vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N} \psi_{(\vec{a},\vec{b})} \pi^{-N/4} \sigma^{-N/2} e^{ik_0 \vec{b}\cdot\vec{x}} e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2}$$

Because $\hat{\psi}(\vec{k}, t)$ is localized on $[-k_{\max}, k_{\max}]^N$, $\psi(nT_{\mathrm{step}})_{(\vec{a},\vec{b})} \approx 0$ is for $|\vec{b}k_0|_\infty > k_{\max}$. Also, because $\psi(\vec{x}, t)$ is localized on $[-(L_{\mathrm{int}}+w), (L_{\mathrm{int}}+w)]^N$, $\psi_{(\vec{a},\vec{b})} \approx 0$ for $|\vec{a}x_0|_\infty > L_{\mathrm{int}} + w$.

Thus, we find that:

$$\psi(x, T_{\mathrm{step}}) \approx \sum_{\substack{|\vec{a}x_0|_\infty \leq L_{\mathrm{int}}+w \\ |\vec{b}k_0|_\infty \leq k_{\max}}} \psi_{(\vec{a},\vec{b})} \pi^{-N/4} \sigma^{-N/2} e^{ik_0 \vec{b}\cdot\vec{x}} e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2}$$

We then examine the gaussians near the boundary (with $|\vec{a}x_0|_\infty \geq L$) and determine whether they are leaving the box or not (after propagation under the free flow). This is simple enough to do, since elementary quantum mechanics tells us that:

$$e^{i(1/2)\Delta t} \pi^{-N/4} \sigma^{-N/2} e^{ik_0 \vec{b}\cdot\vec{x}} e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2} = \frac{\exp\left(i\vec{b}k_0 \cdot (\vec{x} - \vec{b}k_0 t - \vec{a}x_0)\right)}{\pi^{N/4}\sigma^{N/2}(1+it/\sigma^2)^{N/2}} \exp\left(\frac{-|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{2\sigma^2(1+it/\sigma^2)}\right)$$

Essentially, $e^{i(1/2)\Delta t} \pi^{-N/4} \sigma^{-N/2} e^{ik_0 \vec{b}\cdot\vec{x}} e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2}$ moves along the trajectory $\vec{a}x_0 + \vec{b}k_0 t$, while spreading about it's center at the rate σ^{-1}.

Then, if a given gaussian is leaving the box, we delete it. If it is not, we keep it. Some gaussians spread more quickly than their center of mass moves, and we do not present here an algorithm to deal with these gaussians. We simply assume that there are not many of these, and so they pose little problem.

Thus, after this filtering operation, the only gaussians remaining are either inside the box $[-L_{\mathrm{int}}, L_{\mathrm{int}}]^N$, or inside the box $[-(L_{\mathrm{int}}+w), (L_{\mathrm{int}}+w)]^N$ but moving towards $[-L_{\mathrm{int}}, L_{\mathrm{int}}]^N$. We then repeat the process, and propagate with periodic boundaries until $2T_{\mathrm{step}}$, and filter again at this time.

This description is vague, and we will make it more precise later. In particular, we explain what we mean by "$\approx$", and also provide theoretical justification of the method.

In particular, we prove rigorous error bounds, subject to some relatively general assumptions (most of which can be estimated apriori or verified aposteriori). That is, for $t \in [0, T_{\max}]$ (where $T_{\max}$ is some maximal time interval of interest) we show that:

$$\sup_{t\in[0,T_{\max}]} \left\| \chi_{[-L_{\text{int}},L_{\text{int}}]^N}(x) \left(\psi(\vec{x},t) - \Psi(\vec{x},t)\right) \right\|_{H^s} \leq \tau$$

where $\Psi(\vec{x},t)$ is our approximate solution, τ is some prescribed error, and $H_b^s = H^s([-L_{\text{int}}, L_{\text{int}}]^N)$ a Sobolev space, with $s = 0, 1$. We believe that similar results can be proved for $s > 1$ without much difficulty, although certain calculations will be different (most notably remark 4.6 and the exact calculations in section 4.2, see also remark 4.8 for a more precise explanation of the modifications necessary for higher Sobolev spaces).

1.0.2 Error Bounds

We calculate the error made at each step in the above analysis and then add it all up to get the global error bound.

For a general time-stepping algorithm (with periodic boundaries and no filtering), the error bound would take the following form:

$$\begin{aligned} \sup_{t\in[0,T_{\max}]} \|\mathcal{U}(t)\psi_0(x) - \Psi(x,t)\|_{H_b^s} &\leq \text{BoundaryError}(T_{\max}) \\ &+ \text{HighFrequency}(T_{\max}) + \text{LowFrequency}(T_{\max}) \\ &+ \text{NonlocalNonlinearity}(T_{\max}) + \text{Instability}(T_{\max}) \end{aligned} \tag{1.2}$$

The term BoundaryError($T_{\max}$) encompasses errors due to waves wrapping/reflecting from the boundaries of the box. For many problems, this is the dominant error term. It is directly proportional to the mass which would have (if we were solving the problem on $\mathbb{R}^N$) radiated outside the box $[-L_{\text{int}}, L_{\text{int}}]^N$.

The HighFrequency($T_{\max}$) part stems from waves with momenta too high to be resolved by the discretization. The term LowFrequency($T_{\max}$) encompasses errors due to waves with wavelength that is long in comparison to the box. The term NonlocalNonlinearity($T_{\max}$) stems from that fraction of the nonlinearity itself which is located outside the box. The Instability($T_{\max}$) stems from the possibility that the dynamics of the solution itself might amplify the other errors dramatically (e.g. in strongly nonlinear problems).

Our algorithm reduces the term BoundaryError($T_{\max}$) only. We show, by a discrete variant of the gaussian beam method, that if we filter off the outgoing waves in the manner described previously, the boundary error term can be made arbitrarily small. The cost is increasing the width of the region in which filtering takes place.

The main drawback of our algorithm is that it does not provide us the ability to filter low frequency outgoing waves, that is to say waves for which the wavelength is longer than the buffer region. This is precisely what we would expect from the Heisenberg uncertainty principle.

Since the goal of this work is to reduce the error due to boundary reflection, all the error terms besides the boundary error term are made small by assumption. We provide no bounds on them, since these bound would depend very strongly on the specific form of $g(t, \vec{x}, \psi(\vec{x}, t))\psi(\vec{x}, t)$.

Remark 1.1 At first glance, it would appear that an absorbing boundary layer (either complex potential or PML) would reduce the boundary error nearly to zero, with the error being nothing more than those waves which it fails to absorb. This intuition is false, and a counterexample is provided in section 9.2.

The reason is as follows. Suppose we add an absorbing boundary layer (denoted by A) term to (1.1). Let $\psi_a(x, t)$ solve:

$$i\partial_t \psi_a(x,t) = (-(1/2)\Delta + A)\psi_a(x,t) + g(t, \vec{x}, \psi_{a,b}(\vec{x}, t))\psi_{a,b}(\vec{x}, t)$$

Let $\psi_{a,b}(x, t)$ solve the corresponding periodic problem:

$$i\partial_t \psi_{a,b}(x,t) = (-(1/2)\Delta_b + A)\psi_{a,b}(x,t) + g(t, \vec{x}, \psi_{a,b}(\vec{x}, t))\psi_{a,b}(\vec{x}, t)$$

It is true that $\|\psi_a(x,t) - \psi_{a,b}(x,t)\|_{H_b^s}$ is small (that is, the box problem with an absorber approximates the $\mathbb{R}^N$ problem with an absorber). However, it is not necessarily true that $\|\psi(x,t) - \psi_a(x,t)\|_{H_b^s}$ is small, because the $\mathbb{R}^N$ problem with an absorber may not accurately approximate the $\mathbb{R}^N$ problem with no absorber.

The TDPSF algorithm sidesteps this issue by directly approximating the solution on $\mathbb{R}^N$, and only using the box propagator on regions of phase space where it is guaranteed to be accurate.

1.0.3 Strong Points

Our method is versatile and general, in the sense that it is merely a numerical application of the gaussian beam method. Extensions and modifications to other sorts of equations are likely to be straightforward, although one might prefer to decompose $\psi(\vec{x}, t)$ into some other functions different than gaussians[2].

In particular, we believe this can be extended without much difficulty to the free wave equation, replacing gaussians by curvelets [7, 6].

In addition, if the dynamics on the boundary are non-free, we believe our method can be modified to treat these dynamics effictively. Suppose that instead of propagating along the trajectory $\vec{a}x_0 + \vec{b}k_0 t$, a typical gaussian propagated along the trajectory $\gamma(\vec{a}, \vec{b}, t)$ instead. We could still apply our method, except now we would attempt to determine whether $\gamma(\vec{a}, vb, t)$ is leaving the box rather than $\vec{a}x_0 + \vec{b}k_0 t$ when determining which gaussians to filter. We have no rigorous error bounds on this method at this time, however we believe they could be constructed by methods similar to what we do in this work.

Another advantage to our method is that when it does fail, it fails gracefully. The main mode of failure is for too many gaussian's to fall into the region where

[2]More precisely, for a given equation, one should use a family of coherent states which is also a frame. In addition, the family of coherent states should not make computations too complex.

we cannot determine whether they are incoming or outgoing[3]. However, if this occurs, the algorithm is aware of it and an exception is raised. In addition, if one can determine what to do with these gaussians, one can catch the exception and do that. We are currently developing a novel multiscale algorithm that can be used [37].

We expect proofs of the error bound in cases like this to be simple (albeit long) variations on the proof we give here.

1.0.4 Our Weak Spots

Our method is based strongly on two main assumptions, which will not hold for every equation or every initial condition.

The most important assumption is that the solution behaves like a free wave outside of a certain box $[-L_F, L_F]^N$, and we demand that the computational region encompass this box. If this does not hold, the error bound we provide is no longer valid. An example of this is the case of a moving soliton which leaves the box[4]. The dynamics near the boundary are no longer free, since the free equation has no soliton solutions.

We also assume the existence of some frequency $k_{\min}$, which has the following property. Outside a certain box $[-L_{\min}, L_{\min}]^N$, the majority of the solution is comprised of gaussians with the property that if $\vec{a}_j x_0 \geq L_{\min}$, then $\vec{b}_j k_0 \geq k_{\min}$ (respectively if $\vec{a}_j x_0 \leq -L_{\min}$, then $\vec{b}_j k_0 \leq -k_{\min}$). This implies that any part of the solution which has moved outside the box $[-L_{\min}, L_{\min}]^N$ is moving outward.

Roughly, what this means is that anything which has already reached the boundary must be moving in the direction of the boundary.

Another difficulty of our method is that it requires a buffer region in which we filter outgoing waves. This buffer region needs to have width $O(k_{\min}^{-1})$, and should encompass many data points (in our examples we typically use approximately 128-512 data points). For comparison, most Dirichlet-to-Neumann based approaches will use far fewer (just enough to numerically calculate a few derivatives). However, those approaches are typically nonlocal in time, and instead need to use many data points in t rather than in x.

Regardless, in both cases, the computational cost on the boundary is orders of magnitude smaller than the computational cost simply to solve the problem on the interior region. See also [37].

[3] The other mode of failure is spectral blocking in the frequency domain, a common mode of failure for spectral methods. This problem occurs when the lattice spacing δx is too large to resolve the high frequencies generated by the problem.

[4] Numerical experiments suggest that our method can also filter outgoing solitons in certain cases, with reasonable accuracy. This is, however, more a coincidence than anything else. It would not occur if one applied this scheme to, e.g. the KdV equation.

1.1 Definitions and Notations

For the sake of precision, we give definitions of certain well known objects (Sobolev spaces, Fourier transforms, etc). We do this because most constants in this paper are calculated explicitly, and the constants will vary depending on, e.g., how the Sobolev space is defined.

Variables written in **bold**, e.g. $\mathbf{J}_s$ (defined below), denote constants which vary only with the parameters indicated. For the convenience of the reader, an index of symbols is provided on page 103.

We will solve (1.1) on the region $[-L_{\text{comp}}, L_{\text{comp}}]^N$, which is a larger domain than $[-L_{\text{int}}, L_{\text{int}}]^N$. The extra region $[-L_{\text{comp}}, L_{\text{comp}}]^N \setminus [-L_{\text{int}}, L_{\text{int}}]^N$ is a buffer region in which we will filter the outgoing waves.

Definition 1.2 *We define Δ_b to be the Laplacian on the box $[-L_{\text{comp}}, L_{\text{comp}}]^N$ with periodic boundary conditions.*

Definition 1.3 *We define $\mathcal{U}(t)$ to be the propagator of (1.1) on $\mathbb{R}^N$. That is, $\mathcal{U}(t)$ is the map taking $\psi_0(x) \mapsto \psi(\vec{x},t)$ where $\psi(\vec{x},t)$ solves (1.1) with initial condition $\psi(\vec{x},t) = \psi_0(x)$.*

For an initial condition ψ_0, we define $\mathcal{U}(t|\psi_0(x))$ to be the mapping $\psi_1(x) \mapsto \psi_1(\vec{x},t)$ where $\psi_1(\vec{x},t)$ solves (1.3) with initial condition $\psi_1(x,0) = \psi_1(x)$:

$$\partial_t \psi_1(\vec{x},t) = -(1/2)\Delta\psi_1(\vec{x},t) + g(t,\vec{x},\mathcal{U}(t)\psi_0)\psi_1(\vec{x},t) \tag{1.3}$$

Similarly, $\mathcal{U}_b(t)$ is the propagator associated to (1.1), but with $(1/2)\Delta_b$ replacing $(1/2)\Delta$ and $[-L_{\text{comp}}, L_{\text{comp}}]^N$ replacing $\mathbb{R}^N$.

Definition 1.4 *We make the following conventions regarding notation.*

$$|\vec{x}|_p = \left(\sum_{j=1}^{N} |\vec{x}_j|^p \right)^{1/p} \quad \text{for } \vec{x} \in \mathbb{R}^N$$

We let $d(\vec{x},\vec{y})$ denote the Euclidean metric on $\mathbb{R}^N$, i.e. $d(\vec{x},\vec{y}) = |\vec{x}-\vec{y}|_2$. Also, if $A, B \subseteq \mathbb{R}^N$, then:

$$\begin{aligned} d(\vec{x},A) &= \inf_{\vec{y}\in A} d(\vec{x},\vec{y}) \\ d(A,B) &= \inf_{\vec{x}\in A, \vec{y}\in B} d(\vec{x},\vec{y}) \end{aligned}$$

Definition 1.5 *We use the notation:*

$$\langle x \rangle = (1 + |x|_2^2)^{1/2}$$

We define certain constants related to this notation:

$$\begin{aligned} \mathbf{J}_s &= \sup_{\vec{x}\in\mathbb{R}^N} \langle x \rangle^s / (1 + |\vec{x}|_s^s) \\ \mathbf{J}_d &= \sup_{\vec{x}} \frac{|\nabla \langle \vec{x} \rangle|}{\langle \vec{x} \rangle} \end{aligned}$$

Thus:

$$\langle x \rangle^s \leq \mathbf{J}_s(1 + |\vec{x}|_s^s)$$

Definition 1.6 *We define the Fourier transform by:*

$$\hat{f}(\vec{k}) = (2\pi)^{-N/2} \int_{\mathbb{R}^N} e^{i\vec{k}\cdot\vec{x}} d\vec{x}$$

The inverse Fourier transform is defined by:

$$f(\vec{x}) = (2\pi)^{-N/2} \int_{\mathbb{R}^N} e^{-i\vec{k}\cdot\vec{x}} d\vec{k}$$

Thus, the operator $f(\vec{x}) \mapsto \hat{f}(\vec{k})$ is an isometry from $L^2(\mathbb{R}^N, d\vec{x}) \to L^2(\mathbb{R}^N, d\vec{k})$, and $\|f(\vec{x})\|_{L^2(\mathbb{R}^N, d\vec{x})} = \left\|\hat{f}(\vec{k})\right\|_{L^2(\mathbb{R}^N, d\vec{k})}$.

Definition 1.7 *We define the Sobolev spaces $H^s = H^s(\mathbb{R}^N)$ by the norms:*

$$\|f\|_{H^s}^2 = \|f\|_{L^2(\mathbb{R}^N)}^2 + \sum_{j=1}^{N} \left\|\partial_{x_j}^s f\right\|_{L^2(\mathbb{R}^N)}^2 \tag{1.4}$$

We make this particular choice of definition when we compute the constants. Similarly, we define the Sobolev spaces H_b^s by the norms:

$$\|f\|_{H_b^s}^2 = \|f\|_{L^2([-L_{\mathrm{comp}}, L_{\mathrm{comp}}]^N)}^2 + \sum_{j=1}^{N} \left\|\partial_{x_j}^s f\right\|_{L^2([-L_{\mathrm{comp}}, L_{\mathrm{comp}}]^N)}^2$$

We define the constant

$$\mathbf{h}_s^{\pm} = \sup_{f \in H^s} \left(\|f\|_{H^s} / \left\|\langle\vec{k}\rangle^s \hat{f}(\vec{k})\right\|_{L^2} \right)^{\pm 1} = \sup_{\vec{k} \in H^s} \left((1 + \left|\vec{k}\right|_s^s) / \langle\vec{k}\rangle^s \right)^{\pm 1}$$

This allows us to relate the Sobolev space we use to Sobolev spaces defined by using $\langle\vec{k}\rangle$.

No matter which Sobolev space we work in, we always let $\langle\cdot|\cdot\rangle$ denote the inner product in L^2.

Definition 1.8 *We make use of smoothed out characteristic functions. Let A be a closed set and let w be a positive number. Toward that end, we demand that the function $P_{A;w}^s(\vec{x})$ have the following properties:*

1. *$P_{A;w}^s(\vec{x}) = 1$ for $\vec{x} \in A$, and $P_{A;w}^s(\vec{x}) = 0$ if the euclidean distance between $\vec{x}$ and A is greater than w.*

2. *$\partial_{x_j}^k P_{A;w}^s(\vec{x})$ exists and is continuous for $j = 1..N$, $k = 1..s$.*

3. *$P_{A;w}^s(\vec{x})$ has minimal norm as an operator from $H^s \to H^s$.*

We adopt the convention that $P^0_{A;w}(\vec{x}) = 1_A(\vec{x})$*, that is,* $P^0_{A;w}(\vec{x}) = 0$ *for* $\vec{x} \notin A$ *regardless of* w*.*

Definition 1.9 *We define* $\mathbf{m}_{c,s}(\sigma, N)$*,* $\mathbf{m}_{v,s}(\sigma, N)$ *and* $\mathbf{m}'_{c,s}(\sigma, N)$*,*$\mathbf{m}'_{v,s}(\sigma, N)$ *so that*

$$\int_{\mathbb{R}^N} \langle \vec{x} \rangle^s e^{-|\vec{y}-\vec{x}|/\sigma^2} d\vec{y} \leq \mathbf{m}_{c,s}(\sigma, N) + \mathbf{m}_{v,s}(\sigma, N) |\vec{x}|_2^s$$

$$\int_{\mathbb{R}^N} \langle \vec{x} \rangle^s \left| \nabla e^{-|\vec{y}-\vec{x}|/\sigma^2} \right| d\vec{y} \leq \mathbf{m}'_{c,s}(\sigma, N) + \mathbf{m}'_{v,s}(\sigma, N) |\vec{x}|_2^s$$

1.2 A Brief Discussion of Frames

We first discuss briefly the concept of a frame, which will be crucial to our analysis. A frame is basically an overcomplete basis for a Hilbert space, in our case, $L^2(\mathbb{R}^N)$. A framelet decomposition is the tool we use to break up the solution $\psi(\vec{x}, t)$ into incoming and outgoing components.

Definition 1.10 *A frame is a countable set of functions (in some Hilbert space, e.g.* L^2*)* $\{\phi_j(x)\}_{j \in J}$ *(for some index set* J*) such that* $\exists A_F, B_F$ *such that for any* $f \in L^2(\mathbb{R}^N)$*:*

$$A_F \|f\|_{L^2} \leq \|\langle f(x) | \phi_j(x) \rangle\|_{l^2(J)} \leq B_F \|f\|_{L^2}$$

The framelet analysis operator F *is the map* $f(x) \mapsto \vec{f} \in l^2(J)$*, where* $\vec{f}_j = \langle f | \phi_j(x) \rangle$*.*

The individual vectors $\phi_j(x)$ *are referred to as framelets, and* $j \in J$ *are referred to as framelet indices.*

Definition 1.11 *For a frame* $\{\phi_j(x)\}_{j \in J}$*, the dual frame* $\left\{\tilde{\phi}_j(x)\right\}_{j \in J}$ *is the unique frame such that:*

$$\tilde{\phi}_j(x) = (F^\star F)^{-1} \phi_j(x)$$

where $F^\star : l^2(J) \to L^2(\mathbb{R}^N)$ *is the adjoint of* F*. It is the "best" (see below for an explanation) set of vectors such that for all* $f(x) \in L^2$*:*

$$f(\vec{x}) = \sum_{j \in J} \left\langle \tilde{\phi}_j(x) | f(x) \right\rangle \phi_j(x)$$

The dual frame is also a frame, with frame bounds B_F^{-1} *and* A_F^{-1}*.*

The framelet coefficients of a function $f(x)$, are the "best" set of coefficients such that:

$$f(x) = \sum_{j \in J} f_j \phi_j(x)$$

The framelet coefficients are not unique. By "best", we mean that $\vec{f_j}$ is the collection of framelet indices minimizing

$$\sum_{j\in J} |f_j|^2 .$$

They can be calculated by the formula:

$$f_{(\vec{a},\vec{b})} = \left\langle \tilde{\phi}_j(x) | f(\vec{x}) \right\rangle \tag{1.5}$$

For a function $f(x,t)$ depending on time, we denote by $f_j(t)$ the framelet coefficients of $f(\vec{x},t)$ at time t.

1.2.1 Windowed Fourier Transform

As an example, we can let $J = \mathbb{Z}^N \times \mathbb{Z}^N$ and let the individual framelets $\phi_{(\vec{a},\vec{b})}(\vec{x})$ be given by:

$$\phi_{(\vec{a},\vec{b})}(\vec{x}) = \pi^{-N/4}\sigma^{-N/2}e^{ik_0\vec{b}\cdot\vec{x}}e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2}$$

For $\sigma \in \mathbb{R}^+$ and $x_0, k_0 \in \mathbb{R}^+$ such that $x_0 k_0 \leq 2\pi$, then the set

$$\left\{ \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\}_{(\vec{a},\vec{b})\in\mathbb{Z}^N\times\mathbb{Z}^N}$$

is a frame in $L^2(\mathbb{R}^N)$. This is known as the windowed Fourier transform frame (with Gaussian window), abbreviated WFT frame. We will return to this specific example later, in section 3. This is the frame we use to build the outgoing wave filter.

Subject to additional conditions on x_0, k_0 and σ, the WFT can also form a frame in various Sobolev spaces (see Theorem 3.5, proved in [11], and corollary 3.6).

1.2.2 Phase Space Localization

For the WFT filter, we consider the index set $\mathbb{Z}^N \times \mathbb{Z}^N$ to be a discrete representation of phase space. That is, we consider the point $(\vec{a},\vec{b})$ to represent the point $(\vec{a}x_0, \vec{b}k_0)$ in phase space.

For a frame that is well localized in phase space, it is simple to characterize the flow with respect to $e^{i(1/2)\Delta t}$. Under the free flow, individual framelets behave like classical particles. For instance, the Gaussian framelet $\phi_{(\vec{a},\vec{b})}(\vec{x})$ travels along the trajectory $\vec{a}x_0 + t\vec{b}k_0$ when propagated by $e^{i(1/2)\Delta t}$. Due to the heisenberg uncertainty principle, the framelet also spreads out at the rate t/σ. When $\vec{b}k_0 \gg \sigma$, it is simple to determine whether the framelet is moving inward or outward, and delete it as is necessary. Of course, of $\vec{b}k_0$ is very close to zero, then the spreading will be the dominant mode of transport. This is the largest source of error in our method.

Some other frames also provide good localization in phase space, although in different ways. For instance, frames of wavelets travel consistently along classical trajectories, but with the added cost that more slowly moving framelets are spread out more in space (as opposed to the Gaussian WFT, for which all framelets have the same width).

It appears very likely that one could replace the WFT frame that we use by a frame of wavelets, or other frames, provided they have the appropriate phase space localization properties.

In addition, we remark on one extremely promising possibility for extending our analysis to hyperbolic systems. It was proved recently by Demanet and Candes (c.f. [7]) that a curvelet frame allows for a sparse representation of wave propagators in the high frequency regime. We intend to investigate the possibility of using curvelets to construct a boundary filter for dispersive hyperbolic systems, e.g. Maxwell's equations.

1.2.3 Distinguished Sets of Framelets, Framelet Functionals

We now define certain distinguished sets of framelets, and also two relevant framelet functionals. Namely, we define the per-framelet error, and per-framelet relevance functions. The per framelet error functional is a measure of the difference between the propagators $e^{i(1/2)\Delta t}$ and $\mathcal{U}(t)$ when applied to that particular framelet. Similarly, the per-framelet relevance functional is a measure of how important a particular framelet is to the solution inside the box.

Definition 1.12 *For a frame $\{\phi_j\}$, a Sobolev space H^s and a distance L_{int} (to be specified later), we define a family of functions, the relevance functions to be:*

$$\left\| e^{i(1/2)\Delta t} \phi_j \right\|_{H^s([-L_{\text{int}}, L_{\text{int}}]^N)} = \mathcal{R}_j^s(t) \tag{1.6}$$

We now define the set of bad framelets, that is, those framelets which cause most of the short time error. Ideally, these are the ones we would like to filter (although this will not be possible).

Definition 1.13 *For a frame $\{\phi_j\}$ and a Sobolev space H_b^s, we define a family of functions, the per-framelet error functions to be a set of functions $\mathcal{E}_j^s(t)$ such that:*

$$\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \phi_j \right\|_{[-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N} \leqslant \mathcal{E}_j^s(T) \tag{1.7}$$

These will be computed for the WFT frame later on.

Definition 1.14 *For a frame $\{\phi_j\}$, a Sobolev space H_b^s an error tolerance ε, and a time T (possibly ∞), we define the set of error causing framelets* $\text{BAD}(\varepsilon, s, T)$ *to be:*

$$\text{BAD}(\varepsilon, s, T) = \{ j \in J \mid \exists t < T \,\text{such that}\, \mathcal{E}_j^s(t) > \varepsilon \} \tag{1.8}$$

Definition 1.15 *The Big Box is defined by:*

$$\begin{aligned}&\mathrm{BB}(\delta_{\mathrm{BB}})\\&=([-(L_{\mathrm{int}}+w+\mathbf{X}^s_{\square}(\epsilon,k_{\max},L_{\mathrm{int}}+w)),(L_{\mathrm{int}}+w+\mathbf{X}^s_{\square}(\epsilon,k_{\max},L_{\mathrm{int}}+w))]^N\cap x_0\mathbb{Z}^N)\\&\qquad\times([-k_{\max},k_{\max}]^N\cap k_0\mathbb{Z}^N)\end{aligned}$$

We define the computational width, L_{comp}, by:

$$L_{\mathrm{comp}} = L_{\mathrm{int}} + w + \mathbf{X}^s_{\square}(\epsilon,k_{\max},L_{\mathrm{int}}+w)$$

The number $\mathbf{X}^s_{\square}(\epsilon,k_{\max},L_{\mathrm{int}}+w)$ is an extra buffer region needed due to the widthe of the framelets. We define it precisely.

Definition 1.16 *Let $B_X=[-X,X]^N$, $B_K=[-K,K]^N$ for $X,K<\infty$. Then $\mathbf{X}^s_{\square}(\epsilon,K,X)$ and $\mathbf{K}^s_{\square}(\epsilon,K)X$ are the smallest numbers for which the following estimate holds.*

Let $X'=X-\mathbf{X}^s_{\square}(\epsilon,K,X)$, $K'=K-\mathbf{K}^s_{\square}(\epsilon,K)$. Then:

$$\begin{aligned}&\left\|f(x)-\mathcal{P}_{B_{X'}\times B_{K'}}f(x)\right\|_{H^s}\leq \mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})\\&\times\left(\left\|(1-P^s_{B_X;x_0}(\vec{x}))f(\vec{x})\right\|_{H^s}+\left\|(1-P^0_{B_K;k_0}(\vec{k}))f(\vec{x})\right\|_{H^s}+\epsilon\left\|f\right\|_{H^s}\right)\end{aligned}\tag{1.9}$$

We provide a proof that this definition is not vacuous in Theorem 3.19.

We note that when we solve (1.1) with periodic boundary conditions, we will do so on the box $[-L_{\mathrm{comp}},L_{\mathrm{comp}}]^N$.

The set $\mathrm{NECC}(\varepsilon,s,t)$ is the set of framelets which have a nontrivial incoming component. That is, these are the framelets which will return to the region of interest, at least partially. $\mathrm{NECC}(\varepsilon,s,T)$ should be thought of as "incoming waves", and cannot be filtered without causing error.

Definition 1.17 *For a frame $\{\phi_j\}$, a Sobolev space H^s_b an error tolerance ε, and a time T (possibly ∞), we define the set $\mathrm{NECC}(\varepsilon,s,T)$ to be:*

$$\mathrm{NECC}(\varepsilon,s,T)=\{j\in J|\exists t<T\,\text{such that}\,\mathcal{R}^s_j(t)>\varepsilon\}\tag{1.10}$$

2 Time Dependent Phase Space Filters

We now describe the TDPSF (Time Dependent Phase Space Filter) in more detail. We first begin with a motivating example, namely the case where we consider the semiclassical limit of (1.1).

2.1 The Motivating Example: Phase Space Filters for Classical Transport

Consider the following simple Schrödinger equation, with $V(x)$ a smooth, rapidly decaying potential.

$$\partial_t \psi(\vec{x}, t) = (-\hbar^2 (1/2)\Delta + V(x))\psi(\vec{x}, t) \tag{2.1}$$

In the limit when $\hbar \to 0$, one can derive the following kinetic equation for $\rho(\vec{x}, t) = |\psi(\vec{x}, t)|^2$:

$$\partial_t \tilde{\rho}(\vec{x}, \vec{k}, t) = (\vec{k} \cdot \nabla_x)\tilde{\rho}(\vec{x}, \vec{k}, t) + (\nabla V(\vec{k}) \cdot \nabla_k)\tilde{\rho}(\vec{x}, \vec{k}, t) \tag{2.2a}$$

$$\rho(\vec{x}, t) = \int \tilde{\rho}(\vec{x}, \vec{k}, t) d\vec{k} \tag{2.2b}$$

This equation is simple because it can be solved by the method of characteristics. The characteristic curve of (2.2) passing through the point $(\vec{x}, \vec{k})$ is the classical trajectory of a particle at the point $\vec{x}$ with initial velocity $\vec{k}$. Now, suppose that we are considering (2.2) on a box sufficiently large so that $V(x) \approx 0$ near the edge of the box.

In that case, near the boundary, the characteristic curve at $(\vec{x}, \vec{k})$ is parameterized locally by $(\vec{x} + \vec{k}t, \vec{k})$. Thus, it is easy to determine whether the flow is incoming or outgoing near the boundary. We merely check whether $(\vec{x} + \vec{k}t, \vec{k})$ is moving in or out of the box. The algorithm is, therefore, as follows.

Surround the box $[-L_{\text{int}}, L_{\text{int}}]^N$ with an extra region (in the $\vec{x}$ direction) of width w. We let $L_{\text{buff}} = L_{\text{int}} + w$. We assume that the problem is such that the velocity is bounded above by $k_{\max}$. Then, inside the region $[-(L_{\text{int}} + w), (L_{\text{int}} + w)]^N \setminus [-L_{\text{int}}, L_{\text{int}}]^N$, we filter the outgoing trajectories every time $T_{\text{step}} = w/k_{\max}$. That is, letting $\tilde{\rho}(\vec{x}, \vec{k}, t)$ be the density, we set $\tilde{\rho}(\vec{x}, \vec{k}, t) = 0$ at the points $(\vec{x}, \vec{k})$ (with $\vec{x} \in [-(L_{\text{int}} + w), (L_{\text{int}} + w)]^N \setminus [-L_{\text{int}}, L_{\text{int}}]^N$) where $(\vec{x} + t\vec{k}, \vec{k})$ is a trajectory which is leaving the box in the time interval $[0, T_{\text{step}}]$.

Thus, classical trajectories which are leaving the box are deleted before they reach the boundary, while trajectories which are not leaving the box are retained, and perfectly accurate propagation is achieved.

2.2 The TDPSF

The TDPSF algorithm is an attempt to perform this procedure for (1.1). The primary sticking point is the Heisenberg uncertainty principle. We can no longer localize the solution precisely on outgoing positions and momenta. We can, however, come close. By expanding the solution $\psi(\vec{x}, t)$ in a frame having good phase space localization properties, we can come reasonably close to

Thus, by using a filter with good phase space localization, we can come close to extending this procedure to Schrödinger type equations. The only region of phase space where this works poorly is the region near $\vec{k} = 0$, due to the inability to localize a function only on outgoing trajectories.

Therefore, the algorithm we propose is as follows.

Suppose we have an initial condition $\psi_0(x)$. The initial condition must be well localized in $[-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N$, measured in H^s.

We decompose $\psi_0(x,0)=\sum_{j\in J}\psi_{0j}\phi_j(x)$. We then split ψ_0 up into framelets coming from the regions NECC $\cap$ BB, NECC^C and NECC $\cap$ BB^C.

We remove all framelets outside the set NECC $\cap$ BB.

It turns out that for a frame with good phase space localization, NECC and BAD are nearly mutually exclusive. This occurs because framelets, when propagated under the free flow, almost completely retain their coherence, and move either into the box or out of the box (but not both). Thus, by removing framelets outside NECC $\cap$ BB, we have removed nearly all of the outgoing waves.

Because of this, it is now most likely safe to propagate the remainder under the periodic flow, since the remainder consists of an initial condition that will not leave the box in the near future (with "near future" defined to be $[0,T_{\text{step}}]$).

The only time this is not true for the WFT is if a significant number of slow waves have reached the boundary. Every time T_{step}, we check if this has occurred. If so, we raise an exception.

When we reach time T_{step}, we go back to step one. That is, taking $\mathcal{U}_b(T_{\text{step}})\psi_{0,\text{modified}}$ as the new initial condition, we again filter off the outgoing waves. We repeat for as long as necessary.

We now write out the algorithm in the form of pseudocode.

The variable `grid` is some numerical representation of $\psi(\vec{x},t)$ restricted to the region $[-L_{\text{comp}},L_{\text{comp}}]^N$ with periodic boundaries. In our implementation, we store evenly spaced samples of $\psi(\vec{x},t)$, but other representations (e.g. finite element) can be used.

The function `box_propagator(grid,timestep)}`is some numerical approximation to the propagator $\mathcal{U}_b(t)$, which acts on `grid`. The exact method of implementation is unimportant for our purposes, provided it is sufficiently accurate. We use the FFT/Split Step propagation algorithm, but other methods (e.g. some high order FDTD or finite element scheme for rough problems) can be substituted.

The function `bad_necc_framelet_coefficients(grid)` is a function which computes whether or not there are too many framelets in the region BAD $\cap$ NECC.

The number `Tstep` is the time between filterings. The parameters `frm_params` are some parameters which characterize the frame. For instance, with the WFT, `frm_params` is a tuple `(sdev,xs,ks,wb)` containing the standard deviation of the Gaussian, the lattice spacings x_0,k_0 in position and momentum, and the width of the boundary w.

Finally, the procedure `plotter(grid,t)` is some procedure which reads the data in `grid` and processes it in some useful way (i.e. storing it to a file, plotting a graph based on it, etc). This must be determined by the application.

Algorithm 2.1 *Propagation algorithm*

```
exception CannotFilterException(grid current_grid,
```

```
                                number current_time)

Tstep, frm_params, tolerance

def propagate(psi0, Tmax, plotter)
   grid <- psi0
   for j = 0 ... Tmax / Tstep:
      fcoeffs <- compute_framelet_coefficients(grid,frm_params)
      if norm(bad_necc_framelet_coefficients(grid)) > tolerange:
         raise CannotFilterException
      grid <- (grid - bad_framelets_projection(fcoeffs))
      grid <- box_propagator(grid,Tstep)
      plotter(grid,j*Tstep)
   return ()
```

Because all framelets inside the box $[-L_{\text{int}}, L_{\text{int}}]^N$ are not bad framelets, we actually do not need to compute them when we apply the function `compute_framelet_coefficients(grid)`. Rather, we need only compute the framelet coefficients inside the buffer region, $[-L_{\text{comp}}, L_{\text{comp}}]^N \setminus [-L_{\text{int}}, L_{\text{int}}]^N$.

2.2.1 Implementation: FFT/Split Step Propagation Algorithm

The algorithm we have described is, to a great extend, independent of the particular method of implementation. However, we sketch out one possible method of implementing it here, namely the FFT/Split Step algorithm.

We fix a grid spacing δx, and timestep `DT`. The object `grid` will be an N dimensional array of size $[2L_{\text{comp}}/\delta x]^N$. This corresponds to a lattice spacing in momentum of $2\pi/L_{\text{comp}}$, with maximal momentum $2\pi/\delta x$. A common rule of thumb is that if the problem has a maximal momentum $k_{\max}$, then $\delta x = 4\pi/\delta x$ (the extra factor of 2 being put there for the sake of safety).

Let `FFT` be the Fast Fourier Transform algorithm, and `iFFT` be the inverse FFT. Let `NLIN(grid)` be the numerical implementation of the nonlinearity.

This is the standard split step/Trotter-Kato formula spectral propagator.

Algorithm 2.2 *Split Step Propagation Algorithm*

```
def box_propagator(grid,timestep):
    for j in 0 ... timestep / DT:
        grid <- grid * exp(i * NLIN(grid) * DT/2)
        grid <- FFT(grid)
        grid <- grid * exp(i * (1/2)k^2 * DT)
        grid <- iFFT(grid)
        grid <- grid * exp(i * NLIN(grid) * DT/2)
    return grid
```

Algorithm 2.2 is "spectrally accurate" in x, of order $O(\delta t^2)$ in time (for nonlinear problems, for linear problems it increases to $O(\delta t^3)$), and has cost

$O(M^N \ln M)$ per timestep (where M is the number of data points in the grid, per dimension). For this reason it is a popular method of propagating dispersive waves.

We will defer a discussion on the implementation of the functions `compute_framelet_coefficients(grid)` and `bad_framelets_projection(fcoeffs)` until after we explain the WFT. One possible implementation of `compute_framelet_coefficients(grid)` is described in section 3.3.

2.3 Why This Works: A Heuristic Argument

The framelets in in NECC^C consist of framelets which are moving out of the box under the free flow $e^{i(1/2)\Delta t}$. Thus, there is little error caused by removing them.

For the WFT frame, the framelets in $\text{NECC} \cap \text{BB}^C$ consist of framelets which are outside the box, but are moving inward under the free flow. If the initial condition $\psi(x, 0)$ is well localized, the only way such framelets can exist is if waves moved out of the box, turned around and came back. This is extremely unlikely. Thus, there is little error caused by removing these framelets.

The remainder consist of framelets in $\text{NECC} \cap \text{BB} \cap \text{BAD}$. In general, little can be said about these framelets. But for the WFT, these consist of framelets which are moving slowly, more slowly than a certain velocity k_{min}. We make this term small merely by assuming it to be true. In practice, it may not be, although we outline (non-rigorously) methods of dealing with this.

We now consider the remaining framelets. Apart from the slowly moving ones, the framelets in $\text{NECC} \cap \text{BB}$ are not coming close to the boundaries of $[-L_{\text{comp}}, L_{\text{comp}}]^N$. Thus, the boundary conditions we have chosen (periodic, in this case) are irrelevant. This is true for a short time, say a time T_{step}.

In the event that the slowly moving framelets in $\text{BAD} \cap \text{NECC}$ do reach the boundary, then an exception is raised.

2.4 Possible Improvements

One obvious improvement to our algorithm is useful for dealing with Hamiltonians of the form $H = -(1/2)\Delta + V(x) + f(|\psi(\vec{x}, t)|)$ with $V(x)$ a localized potential (possibly of long range type). Instead of trying to determine whether the free trajectory of a given framelet, namely $\vec{a}x_0 + \vec{b}k_0 t$ is leaving the box sufficiently fast, we try to determine whether the interacting trajectory $\gamma(\vec{a}x_0, \vec{b}k_0, t)$ is leaving the box. The interacting trajectory is the trajectory obeyed by a classical particle with velocity $\vec{b}k_0$, moving in the potential $V(x)$. Intuitively, this is the right thing to do, although we cannot prove this at the moment.

One potential unknown factor in our algorithm is k_{min}, the smallest relevant momentum. If the problem we are given has an unknown k_{min}, all is not lost. We propose two methods, one simpler than the other, to deal with this case.

The problem will appear as follows. Suppose that at some time NT_{step}, we find that the mass sitting on the framelets in $\text{BAD} \cap \text{NECC}$ is not small. We can reduce $k_{\min}$ by increasing σ, the standard deviation of the Gaussian. The only cost to doing this is that it becomes necessary to increase the width of the buffer region w.

We also are investigating a multiscale algorithm, utilizing multiple computational grids which accurately deal with the slower frequencies. More precisely, we use a tower of grids, having width L_{int}, $2L_{\text{int}}$, etc, with each grid having lattice spacing Δx, $2\Delta x$, etc (so that the computational complexity is linear in the number of grids). Then, if slow waves reach the boundary of the first box, they are filtered, and placed on the interior of the 2'nd box. They are now at the physical position L, and can propagate an additional distance L before leaving the second box. If the reach the edge of the second box, they can be placed in the third, and so on.

Numerical experiments suggest that this result can dramatically decrease the error due to slow waves (by a factor of 50 or more), and we plan to investigate this further.

2.5 A word on Exceptions

We explain exceptions briefly for readers unfamiliar with them.

An exception is merely a signal to the program to break out of the current scope, and move upwards through enclosing scopes until it finds itself inside a `try` block. At this point, control is given over to the corresponding `catch` block. A simple example:

```
...
Exception DivByZeroException(num)

def f(x,y):
   if x == 0:
      raise DivByZeroException(y)
   return y/x
...
try:
   print f(3,z)
catch DivByZeroException e:
   print ''Cannot divide by zero''
...
```

In this code, if `z!=0`, the output would be merely be 3/z. If z = 0, the program will merely print "Cannot divide by zero" and then continue.

Consider now this code.

```
...
print f(3,z)
...
```

This program will terminate if z=0, and any commands after `printf(3,z)` will not be executed.

The purpose to using an exception is to allow control to move upward through enough enclosing scopes until a scope is found which is capable of dealing with the exception. If none is found, the program terminates. This avoids cluttering the code with many `if then` statements to handle error checking.

3 Windowed Fourier Transforms and all that...

In this section, we review some basic results on frames and the windowed Fourier transform. More detailed information can be found in [11, 12, 14], for example.

3.1 Basic Definitions and Theorems

The discrete windowed Fourier transform frame is the standard frame of canonical coherent states. We use it because of it's excellent time and frequency localization properties if a Gaussian window is used.

Definition 3.1 *The Gaussian WFT frame is the set of functions*

$$\left\{\phi_{(\vec{a},\vec{b})}(\vec{x}) = \pi^{-N/4}\sigma^{-N/2}e^{ik_0\vec{b}\cdot\vec{x}}e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2}\right\}_{(\vec{a},\vec{b})\in\mathbb{Z}^N\times\mathbb{Z}^N}$$

for some x_0, k_0, σ. To be a frame, $x_0k_0 < 2\pi$, otherwise there exist vectors orthogonal to the span of the WFT frame. The dual frame to the Gaussian WFT frame is also a WFT frame, given by

$$\left\{e^{ik_0\vec{b}\cdot\vec{x}}\tilde{g}(\vec{x}-\vec{a}x_0)\right\}_{(\vec{a},\vec{b})\in\mathbb{Z}^N\times\mathbb{Z}^N}$$

for a certain $\tilde{g} \in L^2(\mathbb{R}^N)$ (clarified later).

We will refer to $\phi_{(\vec{a},\vec{b})}(\vec{x})$ as a framelet localized at $(\vec{a}x_0, \vec{b}k_0)$ in phase space. When we refer to the position or velocity of a framelet, we are referring to $\vec{a}x_0$ and $\vec{b}k_0$, respectively.

The following theorem establishes that the WFT is a frame, in the special case when $x_0k_0 = 2\pi/\mathbf{M}$, for some $\mathbf{M} \in \mathbb{N}$. The number $\mathbf{M}$ is called the oversampling rate. It also explicitly provides the frame bounds.

We remark here that throughout this paper, we will always take $x_0k_0 = 2\pi/\mathbf{M}$, with $\mathbf{M}$ an even integer. We do this in order to use both theorem 3.4 and also theorem 3.11 (which is stated later).

We conjecture that a similar result holds for $\mathbf{M} \in (1,\infty)$. The assumption $\mathbf{M} \in 2\mathbb{Z}$ is made for algebraic simplicity, and very likely is unnecessary.

Definition 3.2 *The Zak transform is the isometry $\mathcal{Z} : L^2(\mathbb{R}^N) \to L^2([0,1]^N \times [0,1]^N)$ defined by:*

$$(\mathcal{Z}f)(\vec{t},\vec{s}) = x_0^{N/2}\sum_{\vec{l}\in\mathbb{Z}^N} e^{2\pi i(\vec{t}\cdot\vec{l})}f(x_0(\vec{s}-\vec{l})) \tag{3.1}$$

and for $\phi(\vec{t},\vec{s}) \in L^2([0,1]^N \times [0,1]^N)$*:*

$$\mathcal{Z}^{-1}\varphi(\vec{x}) = x_0^{N/2} \int_{[0,1]^N} e^{-2\pi i(\vec{t}\cdot\lfloor \vec{x}/x_0 \rfloor)} \phi\left(\vec{t}, \vec{x}/x_0\right) dt \tag{3.2}$$

Note that $(\mathcal{Z}f)(\vec{t},\vec{s})$ *is* 1*-periodic* $\vec{t}$*.*

The Zak transform will be used to diagonalize the operator F^*F in theorem 3.4. We first state some results concerning the $\theta_3(z|\tau)$, which are necessary to proceed.

Definition 3.3 *The elliptic function* $\theta_3(z|\tau)$ *is defined by:*

$$\theta_3(z|\tau) = 1 + 2\sum_{l=1}^{\infty} \cos(2\pi l z) e^{i\pi\tau l^2} \tag{3.3}$$

It has the equivalent definition:

$$\theta_3(z|\tau) = \prod_{n=1}^{\infty} (1 - e^{i2\pi n\tau})(1 + e^{(2n-1)i\pi\tau} e^{2\pi i z})(1 + e^{(2n-1)i\pi\tau} e^{-2\pi i z}) \tag{3.4}$$

It can be analytically continued in z *by the recurrence relation:*

$$\theta_3(z+\tau,\tau) = e^{-\pi i(\tau - 2z)}\theta_3(z,\tau) \tag{3.5}$$

Using the Zak transform, we can now diagonalize the operator F^*F. By computing the inf and sup of the diagonalized operator, we can obtain the frame bounds.

Theorem 3.4 (Daubechies and Grossman) *Let* F *be the framelet analysis operator for a windowed Fourier transform. Suppose that for some integer* $\mathbf{M} \geq 2$*,* $x_0 k_0 = 2\pi/\mathbf{M}$*. Define:*

$$\begin{aligned} S(x_0,\mathbf{M},\vec{t},\vec{s}) &= \left|[\mathcal{Z}e^{-x^2/2}](\vec{s},\vec{t})\right|^2 \\ &= \left(\frac{x_0}{\sqrt{\pi}}\right)^N \sum_{\vec{r}\in\{0,\ldots\mathbf{M}-1\}^N} \left|\sum_{\vec{l}\in\mathbb{Z}^N} \exp\left(2\pi i\vec{l}\cdot(\vec{t}-\vec{r}/\mathbf{M})\right)\exp\left(\frac{-x_0^2}{2}(\vec{s}-\vec{l})^2\right)\right|^2 \\ &= \frac{x_0^N e^{-|s|^2 x_0^2}}{\pi^{N/2}} \sum_{\vec{r}\in\{0,\ldots\mathbf{M}-1\}^N} \prod_{j=1}^{N} \theta_3\left(\vec{t}_j\frac{\vec{r}_j}{\mathbf{M}} + i\frac{x_0^2}{2\pi}\vec{s}_j \middle| \frac{ix_0^2}{2\pi}\right) \times \\ &\qquad \theta_3\left(\vec{t}_j - \frac{\vec{r}_j}{\mathbf{M}} - i\frac{x_0^2}{2\pi}\vec{s}_j \middle| \frac{ix_0^2}{2\pi}\right) \end{aligned} \tag{3.6}$$

Then:

$$[\mathcal{Z}F^*F\mathcal{Z}^{-1}f](\vec{t},\vec{s}) = S(x_0,\mathbf{M},\vec{t},\vec{s})f(\vec{t},\vec{s}) \tag{3.7}$$

This implies that:

$$A_F = \inf_{(\vec{s},\vec{t})\in[0,1]^{N+N}} \left|S(x_0,\mathbf{M},\vec{t},\vec{s})\right| \tag{3.8a}$$

$$B_F = \sup_{(\vec{s},\vec{t})\in[0,1]^{N+N}} \left|S(x_0,\mathbf{M},\vec{t},\vec{s})\right| \tag{3.8b}$$

Proof. This is proved in [13] for the one dimensional case, where $\sigma = 1$. The multidimensional follows by noting that:

$$S(x_0,\mathbf{M},\vec{t},\vec{s}) = \prod_{j=1}^{N} S_{1d}(x_0,\mathbf{M},\vec{t}_j,\vec{s}j)$$

The case when $\sigma \neq 1$ is recovered by scaling. □

The next theorem is taken from [11]. It shows that for a sufficiently oversampled frame, the WFT is a frame in Sobolev spaces as well.

Theorem 3.5 (Daubechies,[11]) *Recall the operator:*

$$F^*Ff(x) = \sum_{(\vec{a},\vec{b})\in\mathbb{Z}\times\mathbb{Z}} e^{ibk_0}g(x-ax_0)\left\langle e^{ibk_0}g(x-ax_0)|f(x)\right\rangle$$

where $g(x)$ is either $e^{-x^2/2}$ or the 1 dimensional dual window $\tilde{g}(x)$. The operator F^*F is bounded above and below, in H^s and H^{-s}, provided the constants $A_s(g)$ and $B_s(g)$ (defined below) are strictly positive. This implies that if $A_s(g)$ and $B_s(g)$ are strictly positive, then the GWFT is a frame in $H^s(\mathbb{R})$ and $H^{-s}(\mathbb{R})$.

$$A_s(g)\left\|\langle\partial_x\rangle^{\pm s}f(x)\right\|_{L^2} \leq \left\|\langle\partial_x\rangle^{\pm s}F^*Ff(x)\right\|_{L^2} \leq B_s(g)\left\|\langle\partial_x\rangle^{\pm s}f(x)\right\|_{L^2}$$

We must first construct some auxiliary functions. Define:

$$m(\hat{g};k_0) = \inf_{x\in\mathbb{R}}\sum_{b\in\mathbb{Z}}\left|\hat{g}(k+bk_0)\right|^2 \tag{3.9a}$$

$$M(\hat{g};k_0) = \sup_{x\in\mathbb{R}}\sum_{b\in\mathbb{Z}}\left|\hat{g}(k+bk_0)\right|^2 \tag{3.9b}$$

Define, for $s \geq 0$:

$$\beta_s^{\pm}(k') = \sup_k\left[\langle k\rangle^{\mp s}\langle k+k'\rangle^{\pm s}\sum_{b\in\mathbb{Z}}\left|\hat{g}(k+bk_0)\right|\left|\hat{g}(k+bk_0+k')\right|\right]$$

$$A_s(g) = \frac{2\pi}{x_0}\left[m(\hat{g};k_0) - \sum_{a\neq 0}\left(\beta_s^+(2\pi a/x_0)\beta_s^-(-2\pi a/x_0)\right)^{1/2}\right] \tag{3.10a}$$

$$B_s(g) = \frac{2\pi}{x_0}\left[m(\hat{g};k_0) + \sum_{a\neq 0}\left(\beta_s^+(2\pi a/x_0)\beta_s^-(-2\pi a/x_0)\right)^{1/2}\right] \tag{3.10b}$$

Corollary 3.6 *In N dimensions, we find that*

$$\mathbf{H}_{-}^{s}(g)\left\|f(\vec{x})\right\|_{H^{\pm s}} \leq \left\|F^{*}Ff(\vec{x})\right\|_{H^{\pm s}} \leq \mathbf{H}_{+}^{s}(g)\left\|f(\vec{x})\right\|_{H^{\pm s}}$$

where

$$\mathbf{H}_{+}^{s}(g) = NB_{0}(g)^{N-1}B_{s}(g) \tag{3.11a}$$

$$\mathbf{H}_{-}^{s}(g) = NA_{0}(g)^{N-1}A_{s}(g) \tag{3.11b}$$

Thus, in $H^{s}(\mathbb{R}^{N})$ and $H^{-s}(\mathbb{R}^{N})$, the WFT is a frame with frame bounds $\mathbf{H}_{-}^{s}(g)$ and $\mathbf{H}_{+}^{s}(g)$, provided they are both positive.

Proof. We want to compute upper and lower bounds on:

$$\left\|F^{*}Fg(\vec{x})\right\|_{H^{s}} = \sum_{j=1}^{N}\left\|(1+(i\partial_{x_{j}})^{s})F^{*}Fg(\vec{x})\right\|_{L^{2}}$$

To the j'th term of the sum, we apply theorem 3.5 in the $j'th$ direction. This pulls out a factor of $A_{s}(g)$. In the directions $1\ldots j-1$ and $j+1\ldots N$, we do the same thing, which pulls out a factor of $A_{0}(g)$ (since there are no derivatives in that direction). We then add up over $j=1\ldots N$. Thus we obtain the lower bound. The upper bound is done identically. □

Remark 3.7 As one can see from table 1, even for a frame which is oversampled only by $\mathbf{M}=4$, the WFT is a reasonably tight frame even in H^{3}, where it differs from being tight by less than 10 percent. In practice, for filtering outgoing waves, we will often want a higher oversampling rate to ensure good decay of the dual window, so we expect this will not usually pose a problem.

In fact, we believe this bound is suboptimal, and conjecture that the WFT is a frame in any Sobolev space. But we do not know how to prove it, although the result can probably be tightened using the Zak transform.

s	A_s	B_s	B_s/A_s
0	3.853	4.147	1.076
1	3.852	4.148	1.077
2	3.849	4.151	1.079
3	3.836	4.164	1.086
4	3.787	4.213	1.112
5	3.600	4.400	1.222
6	2.865	5.135	1.793

Table 1: Frame Bounds, as a function of s, for a particular GWFT frame. The parameters are $\sigma=1$, $x_{0}=1$, $k_{0}=\pi/2$. For $s=7$, the estimates break down. This table is taken from [11], where it is table VI-A.

We make another observation, about the Sobolev norms of framelets.

Definition 3.8 *We denote the per-framelet energy by:*

$$(\mathcal{M}^s_{(\vec{a},\vec{b})})^2 = \sum_{k=1}^{N} \left\| \partial^s_{x_j} \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|^2_{L^2(\mathbb{R}^N)} \tag{3.12}$$

Also, $\mathcal{M}^0_{(\vec{a},\vec{b})} = 1$.

Note that $\mathcal{M}^0_{(\vec{a},\vec{b})} = 1$. *We have the relation* $\left\| \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|^2_{H^s} = (\mathcal{M}^0_{(\vec{a},\vec{b})})^2 + (\mathcal{M}^s_{(\vec{a},\vec{b})})^2 = 1 + (\mathcal{M}^s_{(\vec{a},\vec{b})})^2$.

Proposition 3.9 *The framelet energy is bounded by:*

$$\mathcal{M}^s_{(\vec{a},\vec{b})} \leq \mathbf{f}_s \left(\sum_{k=1}^{N} (2\sigma)^{-s} (\exp_s(\sqrt{2\sigma}\vec{b}_k k_0))^2 \right)^{1/2} \tag{3.13}$$

$$\mathbf{f}_s = \frac{s!}{\sqrt{2\pi}} \left(\int_0^{2\pi} e^{-2\cos(\tau)} d\tau \right)^{1/2} \tag{3.14}$$

The function $\exp_s(z)$ *is defined by:*

$$\exp_s(z) = \sum_{j=0}^{s} \frac{z^j}{j!} \tag{3.15}$$

Thus, $(\mathcal{M}^s_{(\vec{a},\vec{b})})^2 \leq (\mathbf{f}_s/s!) \left| \vec{b}k_0 \right|^s_s + O\left(\left| \vec{b}k_0 \right|^{s-1}_s \right)$ *as* $\left| \vec{b}k_0 \right| \to \infty$.

Proof. We begin by computing in 1 dimension. We neglect the space translations, which will not effect the mass.

$$\begin{aligned} \partial^s_x e^{ibk_0 x} e^{-x^2/2\sigma^2} &= \sum_{j=0}^{s} \binom{s}{j} (ibk_0)^j e^{ibk_0 x} \partial^{s-j}_x e^{-x^2/2\sigma^2} \\ &= e^{ibk_0 x} \sum_{j=0}^{s} \binom{s}{j} (ibk_0)^j (-2\sigma)^{-(s-j)/2} H_{s-j}(x/\sqrt{2}\sigma) e^{-x^2/2\sigma^2} \end{aligned} \tag{3.16}$$

We use the contour integral representation of $H_n(z)$ to write:

$$\begin{aligned} (3.16) = e^{ibk_0 x} &\sum_{j=0}^{s} \binom{s}{j} (ibk_0)^j (-2\sigma)^{-(s-j)/2} (s-j)! \\ &\times \int_{|z|=1} e^{-(x/\sqrt{2}\sigma - z)^2} z^{-(s-j)-1} \frac{dz}{2\pi i z} \\ = e^{ibk_0 x} s! (-2\sigma)^{-s/2} &\int_{|z|=1} \exp_s(-\sqrt{2\sigma} bk_0 z) e^{-(x/\sqrt{2}\sigma - z)^2} z^{-(s-1)} \frac{dz}{2\pi i z} \end{aligned} \tag{3.17}$$

We multiply this by it's complex conjugate, and integrate with respect to x:

$$\int \Big[(s!)^2 (2\sigma)^{-s} \int_{|z|=1} \int_{|t|=1} \exp_s(-\sqrt{2\sigma} b k_0 z) \exp_s(-\sqrt{2\sigma} b k_0 t)$$
$$e^{-(x/\sqrt{2}\sigma - z)^2} e^{-(x/\sqrt{2}\sigma - t)^2} z^{-(s-1)} \frac{dz}{2\pi i z} t^{-(s-1)} \frac{dt}{2\pi i t} \Big] dx$$
$$= \int \Big[(s!)^2 (2\sigma)^{-s} \int_{|z|=1} \int_{|t|=1} \exp_s(-\sqrt{2\sigma} b k_0 z) \exp_s(-\sqrt{2\sigma} b k_0 t)$$
$$e^{-(x/\sigma - (t+z))^2} e^{-2tz} z^{-(s-1)} \frac{dz}{2\pi i z} t^{-(s-1)} \frac{dt}{2\pi i t} \Big] dx$$
$$= \int_{|z|=1} \int_{|t|=1} \left(\int e^{-(x/\sigma - (t+z))^2} dx \right)$$
$$(s!)^2 (2\sigma)^{-s} \exp_s(-\sqrt{2\sigma} b k_0 z) \exp_s(-\sqrt{2\sigma} b k_0 t) e^{-2tz} z^{-(s-1)} \frac{dz}{2\pi i z} t^{-(s-1)} \frac{dt}{2\pi i t} \tag{3.18}$$

The integral in x is independent of the values of t and z. Thus:

$$(3.18) = \left(\int e^{-x^2/\sigma^2} dx \right) (s!)^2 (2\sigma)^{-s} \int_{|z|=1} \int_{|t|=1}$$
$$\exp_s(-\sqrt{2\sigma} b k_0 z) \exp_s(-\sqrt{2\sigma} b k_0 t) e^{-2tz} z^{-(s-1)} \frac{dz}{2\pi i z} t^{-(s-1)} \frac{dt}{2\pi i t} \tag{3.19}$$

We bound the integral by the $L^1 - L^\infty$ duality, to obtain:

$$|(3.19)| = \int (\partial_x^s e^{ibk_0 x} e^{-x^2/2\sigma^2})(\partial_x^s e^{-ibk_0 x} e^{-x^2/2\sigma^2}) dx$$
$$\leq \left\| \exp_s(-\sqrt{2\sigma} b k_0 z) \exp_s(-\sqrt{2\sigma} b k_0 t) \right\|_{L^\infty(ds/2\pi i s, dt/2\pi i t)}$$
$$\times \left\| e^{-2tz} z^{-(s-1)} t^{-s-1} \right\|_{L^1(ds/2\pi i s, dt/2\pi i t)}$$
$$\leq (s!)^2 (2\sigma)^{-s} (\exp_s(\sqrt{2}\sigma b k_0))^2 \left((2\pi)^{-1} \int_0^{2\pi} e^{-2cos(\theta)} d\theta \right) \tag{3.20}$$

We moved from the second line to the third by computing:

$$\int_{|z|=1} \int_{|t|=1} |e^{-2tz} z^{-s-1} t^{-s-1}| \frac{dt}{2\pi t} \frac{dz}{2\pi t}$$
$$= (2\pi)^{-2} \int_0^{2\pi} \int_0^{2\pi} e^{-2\cos(\theta - \phi)} d\theta d\phi = (2\pi)^{-2} \int_0^{2\pi} \int_0^{2\pi} e^{-2\cos(\tau)} d\tau d\beta$$
$$= (2\pi)^{-1} \int_0^{2\pi} e^{-2\cos(\tau)} d\tau$$

To finish, we compute:

$$
\begin{aligned}
(\mathcal{M}^s_{(\vec{a},\vec{b})})^2 &= \sum_{k=1}^N \left\| \partial^s_{x_j} \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|^2_{L^2(\mathbb{R}^N)} \\
&= \sum_{k=1}^N \int_{\mathbb{R}^N} \left| \partial^s_{x_j} \pi^{-N/4} \sigma^{-N/2} e^{ik_0 \vec{b}\cdot\vec{x}} e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2} \right|^2 d\vec{x} \\
&\leq \sum_{k=1}^N (s!)^2 (2\sigma)^{-s} \left((2\pi)^{-1} \int_0^{2\pi} e^{-2\cos(\tau)} d\tau \right) (\exp_s(\sqrt{2}\sigma \vec{b}_k k_0))^2 \qquad (3.21)
\end{aligned}
$$

This is what we wanted to prove. □

In this subsection, we describe some properties of the WFT frame that we use at various points.

3.2 Dual Window

We now characterize the dual window. Recall that the dual window is the unique function such that

$$
f(\vec{x}) = \sum_{(\vec{a},\vec{b})\in\mathbb{Z}^N\times\mathbb{Z}^N} \left\langle f(x) | e^{ik_0\vec{b}\cdot\vec{x}} \tilde{g}(\vec{x}-\vec{a}x_0) \right\rangle \pi^{-N/4} \sigma^{-N/2} e^{ik_0\vec{b}\cdot\vec{x}} e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2}
$$

for $f(\vec{x}) \in L^2(\mathbb{R}^N)$.

We show that the dual window is exponentially localized in position and momentum, and calculate the constants explicitly (this is theorem 3.11). Our results only apply when $\mathbf{M} \in 2\mathbb{N}$, but this is merely because the algebra becomes simple in this case. It appears highly likely that similar results will hold for $\mathbf{M}$ not an even integer.

Our result implies that as $\mathbf{M} \to \infty$, the exponential decay rate of $\tilde{g}(x)$ grows without bound. This is to be expected, since the dual window is converging to a Gaussian in this case.

The fact that $\tilde{g}(x)$ decays exponentially is also argued in [12] but the precise dependence of the constants on x_0, k_0, σ is not pinned down there (and the argument there does not use the Zak transform).

We state first a technical lemma.

Lemma 3.10 *Let $\mathbf{M} \in 2\mathbb{N}$. Then $S(x_0, \mathbf{M}, \vec{t}, \vec{s})$ reduces to:*

$$
S(x_0, \mathbf{M}, \vec{t}, \vec{s}) = \left(\frac{\mathbf{M}x_0}{\sqrt{\pi}}\right)^N \left(\sum_{\vec{l}\in\mathbb{Z}^N} \exp\left(-x_0^2[(\vec{s}-\vec{l})^2]\right) \right) \prod_{j=1}^N \theta_3(2\pi\mathbf{M}\vec{t}_j | i x_0^2 \mathbf{M}^2/4\pi) \qquad (3.22)
$$

Proof. Consider the sum in (3.6). We can compute:

$$\sum_{\vec{r}\in\{0,\ldots\mathbf{M}-1\}^N}\left|\sum_{\vec{l}\in\mathbb{Z}^N}\exp\left(2\pi i\vec{l}\cdot(\vec{t}-\vec{r}/\mathbf{M})\right)\exp\left(\frac{-x_0^2}{2}(\vec{s}-\vec{l})^2\right)\right|^2 =$$

$$= \sum_{\vec{r}\in\{0,\ldots\mathbf{M}-1\}^N}\left[\sum_{\vec{l}\in\mathbb{Z}^N}\exp\left(2\pi i\vec{l}\cdot(\vec{t}-\vec{r}/\mathbf{M})\right)\exp\left(\frac{-x_0^2}{2}(\vec{s}-\vec{l})^2\right)\right]\times$$

$$\left[\sum_{\vec{n}\in\mathbb{Z}^N}\exp\left(-2\pi i\vec{n}\cdot(\vec{t}-\vec{r}/\mathbf{M})\right)\exp\left(\frac{-x_0^2}{2}(\vec{s}-\vec{n})^2\right)\right]$$

$$= \sum_{\vec{r}\in\{0,\ldots\mathbf{M}-1\}^N}\sum_{\vec{l}\in\mathbb{Z}^N}\sum_{\vec{n}\in\mathbb{Z}^N}\exp\left(2\pi i(\vec{l}-\vec{n})\cdot(\vec{t}-\vec{r}/\mathbf{M})\right)\times$$

$$\exp\left(\frac{-x_0^2}{2}((\vec{s}-\vec{l})^2+(\vec{s}-\vec{n})^2)\right) \quad (3.23)$$

For simplicity, in this calculation, $\vec{v}^2 = \sum_{j=1}^N \vec{v}_j^2$. Note that we do not take absolute values or complex conjugates anywhere, and thus our result is analytic.

By passing the sum over $\vec{r}$ inside the other two sums, and noting the following:

$$\sum_{\vec{r}\in\{0,\ldots\mathbf{M}-1\}^N}\exp\left(-2\pi i(\vec{l}-\vec{n})\cdot(\vec{r}/\mathbf{M})\right) = \begin{cases} 0, (\vec{l}-\vec{n}) \notin (\mathbf{M}\mathbb{Z})^N \\ \mathbf{M}^N, (\vec{l}-\vec{n}) \in (\mathbf{M}\mathbb{Z})^N \end{cases}$$

We can then set $\vec{n} = \vec{l} + \mathbf{M}\vec{k}$. We then find:

$$(3.23) = \sum_{\vec{l}\in\mathbb{Z}^N}\sum_{\vec{n}\in\mathbb{Z}^N}\sum_{\vec{r}\in\{0,\ldots\mathbf{M}-1\}^N}$$

$$\exp\left(2\pi i(\vec{l}-\vec{n})\cdot(\vec{t}-\vec{r}/\mathbf{M})\right)\exp\left(\frac{-x_0^2}{2}((\vec{s}-\vec{l})^2+(\vec{s}-\vec{n})^2)\right) =$$

$$\mathbf{M}^N\sum_{\vec{l}\in\mathbb{Z}^N}\sum_{\vec{k}\in\mathbb{Z}^N}$$

$$\exp\left(2\pi i(\mathbf{M}\vec{k})\cdot(\vec{t}-\vec{r}/\mathbf{M})\right)\exp\left(\frac{-x_0^2}{2}((\vec{s}-\vec{l})^2+(\vec{s}-\vec{l}-\mathbf{M}\vec{k})^2)\right) =$$

$$\mathbf{M}^N\sum_{\vec{k}\in\mathbb{Z}^N}\exp\left(2\pi i\mathbf{M}\vec{k}\cdot\vec{t}\right)\sum_{\vec{l}\in\mathbb{Z}^N}\exp\left(-x_0^2[(\vec{s}-\vec{l}-\mathbf{M}\vec{k}/2)^2+\mathbf{M}^2\vec{k}^2/4]\right) \quad (3.24)$$

This is true whether $\mathbf{M}$ is odd or even.

Now if $\mathbf{M}$ is even, then $\mathbf{M}/2$ is an integer. Therefore:

$$\sum_{\vec{l}\in\mathbb{Z}^N} \exp\left(-x_0^2[(\vec{s}-\vec{l}-\mathbf{M}\vec{k}/2)^2+\mathbf{M}^2\vec{k}^2/4]\right) =$$

$$\exp(-x_0^2\mathbf{M}^2\vec{k}^2/4)\sum_{\vec{l}\in\mathbb{Z}^N}\exp\left(-x_0^2[(\vec{s}-\vec{l})^2]\right)$$

This follows since the latter sum is merely an integer translate (in $\vec{l}$) of the former. But since the sum is taken over all $\mathbb{Z}^N$, integer translates do not matter.

Then we can simplify (3.24) even further to:

(3.24)

$$= \mathbf{M}^N\left(\sum_{\vec{l}\in\mathbb{Z}^N}\exp(-x_0^2[(\vec{s}-\vec{l})^2])\right)\sum_{\vec{k}\in\mathbb{Z}^N}\exp(2\pi i\mathbf{M}\vec{k}\cdot\vec{t})\exp(-x_0^2\mathbf{M}^2\vec{k}^2/4)$$

$$= \mathbf{M}^N\left(\sum_{\vec{l}\in\mathbb{Z}^N}\exp\left(-x_0^2(\vec{s}-\vec{l})^2\right)\right)\prod_{j=1}^N\theta_3(2\pi\mathbf{M}\vec{t}_j|ix_0^2\mathbf{M}^2\vec{k}^2/4\pi)$$

We now multiply by $(x_0/\sqrt{\pi})^N$ to recover $S(x_0,\mathbf{M},t,s)$, thus proving (3.22). □

Theorem 3.11 *Let $x_0k_0 = 2\pi/\mathbf{M}$ for $\mathbf{M}\in 2\mathbb{N}$. Let $\tilde{g}(\vec{x})$ be the dual window to the GWFT. Then $\tilde{g}(\vec{x})$ satisfies the following bounds:*

$$\|\tilde{g}(\vec{x})\|_{L^\infty} \leqslant \left(\frac{x_0}{\sigma}\right)^N A_F^{-1}\sum_{\vec{n}\in\mathbb{Z}^N}\exp\left(-\frac{x_0^2|\vec{n}|^2}{\sigma^2}\right) = \left(\frac{x_0}{\sigma}\right)^N A_F^{-1}\|\phi\|_{L^\infty(\vec{t},\vec{s})} \tag{3.25}$$

Letting $\vec{\alpha}=(\alpha_1,...\alpha_N)$ be a multi-index, we find that:

$$\left|\partial_x^{\vec{\alpha}}\tilde{g}(\vec{x})\right| \leq \mathbf{g}(x_0,k_0,N,\vec{\alpha})e^{-\mathbf{r}(x_0,k_0)|\vec{x}|_1} \tag{3.26}$$

When s is a scalar, we will let $\mathbf{g}(x_0,k_0,N,s)=\mathbf{g}(x_0,k_0,N,(s,0,..,0))$.

The decay rate $\mathbf{r}(x_0,k_0)$ is given by:

$$\mathbf{r}(x_0,k_0) = x_0\mathbf{M}/8\pi\sigma \tag{3.27}$$

The constant $\mathbf{g}(x_0,k_0,N,s)$ is defined below. We must first define the following auxiliary functions:

$$\phi(\vec{t},\vec{s}) = [\mathcal{Z}e^{-x^2}](\vec{t},\vec{s}) = \left(\frac{x_0}{\sigma}\right)^{N/2}\sum_{\vec{l}\in\mathbb{Z}^N}e^{2\pi i(\vec{t}\cdot\vec{l})}\exp(-x_0^2|\vec{s}-\vec{l}|_{l^2}^2/\sigma^2) \tag{3.28}$$

$$F(x_0,\mathbf{M},t,x) = \frac{\phi(t-i\gamma,x/x_0)}{\mathbf{M}x_0\pi^{-1/2}\left(\sum_{l\in\mathbb{Z}}e^{-(x-lx_0)^2/\sigma^2}\right)\theta_3(2\pi\mathbf{M}t|ix_0^2\mathbf{M}^2/4\pi\sigma^2)} \tag{3.29}$$

$$G(x_0,\mathbf{M},t,x) = \frac{\phi(t-i\gamma, x/x_0)}{\left(\sum_{l\in\mathbb{Z}} e^{-(x-lx_0)^2/\sigma^2}\right)\theta_{3,z}(2\pi\mathbf{M}t_j|ix_0^2\mathbf{M}^2/4\pi\sigma^2)} \tag{3.30}$$

Here, $\theta_3(z|\tau)$ is one of Jacobi's theta functions (described in the appendix). The notation $\theta_{3,z}$ signifies $\theta_{3,z}(z_0|\tau) = \partial_z\theta_3(z|\tau)|_{z=z_0}$.

We can now define the constant term:

$$\mathbf{g}(x_0,k_0,N,\vec{\alpha}) = \prod_{j=1}^{N}\left(x_0^{1/2}\sigma^{-1/2}e^{x_0^2\mathbf{M}/8\sigma^2}\left\|\partial_x^{\vec{\alpha}_j}F(x_0,\mathbf{M},t,x)\right\|_{L^\infty}\right.$$
$$\left.+\frac{\sigma^{1/2}}{2\mathbf{M}^2x_0^{1/2}\pi^{1/2}}\lfloor 2\pi\mathbf{M}-1/2\rfloor\left\|\partial_x^{\vec{\alpha}_j}G(x_0,\mathbf{M},t,x)\right\|_{L^\infty}\right) \tag{3.31}$$

Proof. In this theorem, we mainly do calculations on the dual window. We perform the calculations in 1 dimension, and then note that:

$$\tilde{g}(\vec{x}) = \prod_{j=1}^{N}\tilde{g}_{1D}(\vec{x}_j)$$

In one dimension, we find that (dropping the $1D$ subscript) the dual window can be computed (recalling that $\phi(t,s) = \mathcal{Z}e^{-x^2/2}$:

$$\tilde{g}(x) = \mathcal{Z}^{-1}\mathcal{Z}(F^*F)^{-1}e^{-x^2/2} = \mathcal{Z}^{-1}S(x_0,\mathbf{M},t,s)^{-1}\phi(t,s)$$
$$= x_0^{1/2}\int_0^1 \frac{e^{-i2\pi t\lfloor x/x_0\rfloor}\phi(t,x/x_0)}{S(x_0,\mathbf{M},t,x/x_0)}dt \tag{3.32}$$

We also assume $\sigma = 1$, for simplicity. To do the calculation when $\sigma \neq 1$, we merely scale the result.

Bound in L^∞

To bound $\tilde{g}(x)$ in L^∞, we need only bound the integral. Note that $S(x_0,\mathbf{M},t,x/x_0)^{-1}$ is bounded by A_F^{-1} (by theorem 3.4). Thus, we obtain the L^∞ bound:

$$\|\tilde{g}(x)\|_{L^\infty} \leq x_0^{1/2}A_F^{-1}\|\phi(t,s)\|_{L^\infty([0,1]^2,dtds)}$$

Shifting the Integration Contour

Here we work in 1 space dimension. We then observe that the $\tilde{g}(\vec{x}) = \prod_{j=1}^{N}\tilde{g}_{1d}(\vec{x}_j)$.

To determine the decay of the dual window, we move the contour of integration in (3.32) up from $[0,1]$ to $[0,1]\pm i\gamma$ (depending on the sign of x, for simplicity we suppose $x>0$). The constant is chosen to be $\gamma = ix_0^2\mathbf{M}/8\pi^2$, due to the fact that $\theta_3(z|\tau)$ obeys a recurrence relation with this period (see (3.5)).

The endpoints do not contribute to the integral, since $S(x_0,\mathbf{M},t,s)$ and $\phi(t,s)$ are 1-periodic in t. Thus, the integral in (3.32) becomes:

$$e^{-2\pi\gamma\lfloor x/x_0\rfloor}x_0^{1/2}\int_0^1 \frac{e^{-i2\pi t\lfloor x/x_0\rfloor}\phi(t-i\gamma,x/x_0)}{S(x_0,\mathbf{M},t-i\gamma,x/x_0)}dt + \text{Residues} \tag{3.33}$$

Using (3.22) in one dimension, we find that:

$$S(x_0, \mathbf{M}, t, s) = \mathbf{M} x_0 \pi^{-1/2} \left(\sum_{l \in \mathbb{Z}} e^{-x_0^2 (s-l)^2} \right) \theta_3(2\pi \mathbf{M} t | i x_0^2 \mathbf{M}^2 / 4\pi) \qquad (3.34)$$

We now need to find the zeros of $S(x_0, \mathbf{M}, t, s)$ in the region $0 \leq \Re t \leq 1$, $0 \leq \Im t \leq \gamma$.

The product formula (3.4) for the function $\theta_3(z|\tau)$ implies that $\theta_3(z|\tau) = 0$ only when $(2n-1)i\pi\tau \pm 2\pi i z = -\pi i + 2\pi n i$ for some $n \in \mathbb{Z}$, and all zero's at these points are of first order.

Using this and (3.34), we find that the relevant zeros of $S(x_0, \mathbf{M}, t, s)$ occur at $2\pi \mathbf{M} t = 1/2 + j - i x_0^2 \mathbf{M}^2 / 8\pi$, with $t \in [0,1]$. These are

$$t_j = (j + 1/2)/2\pi \mathbf{M} + i x_0^2 \mathbf{M} / 16\pi^2$$

with $j = 0 \ldots \lfloor 2\pi \mathbf{M} - 1/2 \rfloor$.

The residue term therefore takes the form:

$$\text{Residues} = x_0^{1/2} e^{-(x_0^2 \mathbf{M}/16\pi) \lfloor x/x_0 \rfloor} \times \sum_{j=0}^{\lfloor 2\pi \mathbf{M} - 1/2 \rfloor} \frac{e^{-i2\pi t_j \lfloor x/x_0 \rfloor} \phi(t_j, x/x_0)}{\mathbf{M} x_0 \pi^{-1/2} \left(\sum_{l \in \mathbb{Z}} e^{-(x - l x_0)^2} \right) 2\pi \mathbf{M} \theta_{3,z}(2\pi \mathbf{M} t_j | i x_0^2 \mathbf{M}^2 / 4\pi)} \qquad (3.35)$$

Here, $\theta_{3,z}(z_0|\tau) = \partial_z \theta_3(z|\tau)|_{z=z_0}$.

We combine these two results, and note that $\theta_3(z+\tau|\tau) = e^{-i\pi(\tau - 2z)} \theta_3(z, \tau)$ to obtain the following expression for $\tilde{g}(x)$:

$$\tilde{g}(x) = e^{-(x_0^2 \mathbf{M}/8\pi) \lfloor x/x_0 \rfloor} x_0^{1/2} e^{x_0^2 \mathbf{M}/8} \int_0^1 \frac{e^{-i2\pi t \lfloor x/x_0 \rfloor} \phi(t - i\gamma, x/x_0)}{S(x_0, \mathbf{M}, t, x/x_0) e^{i2\pi t}} dt + \frac{\pi^{-1/2} x_0^{-1/2} e^{-(x_0^2 \mathbf{M}/16\pi) \lfloor x/x_0 \rfloor}}{2\mathbf{M}^2 \left(\sum_{l \in \mathbb{Z}} e^{-(x - l x_0)^2} \right)} \sum_{j=0}^{\lfloor 2\pi \mathbf{M} - 1/2 \rfloor} \frac{e^{-i2\pi \Re t_j \lfloor x/x_0 \rfloor} \phi(t_j, x/x_0)}{\theta_{3,z}(2\pi \mathbf{M} t_j | i x_0^2 \mathbf{M}^2 / 4\pi)} \qquad (3.36)$$

Calculation of Derivatives

Let us define the following two functions:

$$F(x_0, \mathbf{M}, t, x) = \frac{\phi(t - i\gamma, x/x_0)}{S(x_0, \mathbf{M}, t, x/x_0)} = \frac{\phi(t - i\gamma, x/x_0)}{\mathbf{M} x_0 \pi^{-1/2} \left(\sum_{l \in \mathbb{Z}} e^{-(x - l x_0)^2} \right) \theta_3(2\pi \mathbf{M} t | i x_0^2 \mathbf{M}^2 / 4\pi)}$$

$$G(x_0, \mathbf{M}, t, x) = \frac{\phi(t - i\gamma, x/x_0)}{\left(\sum_{l \in \mathbb{Z}} e^{-(x - l x_0)^2} \right) \theta_{3,z}(2\pi \mathbf{M} t_j | i x_0^2 \mathbf{M}^2 / 4\pi)}$$

Then we can rewrite (3.36) as follows:

$$\tilde{g}(x) = e^{-(x_0^2\mathbf{M}/8\pi)\lfloor x/x_0\rfloor} x_0^{1/2} e^{x_0^2\mathbf{M}/8} \int_0^1 e^{-i2\pi t\lfloor x/x_0\rfloor} F(x_0,\mathbf{M},t,x)dt$$
$$+ e^{-(x_0^2\mathbf{M}/16\pi)\lfloor x/x_0\rfloor} \frac{\pi^{-1/2}x_0^{-1/2}}{2\mathbf{M}^2} \sum_{j=0}^{\lfloor 2\pi\mathbf{M}-1/2\rfloor} G(x_0,\mathbf{M},t,x) \quad (3.37)$$

Calculation of the Decay Rate

Taking (3.37) as a starting point, we can now calculate the decay rate of $\tilde{g}(x)$. We use the simple fact that:

$$e^{-\alpha\lfloor x/x_0\rfloor} \leq e^{\alpha}e^{-\alpha x/x_0} \quad (3.38)$$

The decay rate can be computed simply enough, taking absolute values of (3.37) and using (3.38):

$$|\partial_x^n \tilde{g}(x)| \leq e^{-(x_0\mathbf{M}/8\pi)x} \Bigg(x_0^{1/2} e^{x_0^2\mathbf{M}/8} \|\partial_x^n F(x_0,\mathbf{M},t,x)\|_{L^\infty}$$
$$+ \frac{\pi^{-1/2}x_0^{-1/2}}{2\mathbf{M}^2} \lfloor 2\pi\mathbf{M}-1/2\rfloor \|\partial_x^n G(x_0,\mathbf{M},t,x)\|_{L^\infty} \Bigg)$$

This is what we wanted to prove. To obtain the result in N dimensions, we take products. To obtain the result when $\sigma \neq 1$, we scale. □

Corollary 3.12 *If we interchange $\vec{x}$ and $\vec{k}$, x_0 and k_0, and σ with σ^{-1} everywhere in the above theorem, then the conclusion still holds.*

Proof. The Fourier transform of the WFT is still a WFT. The Fourier transform of the window function $e^{-|\vec{x}|^2/2}$ is $e^{-|\vec{k}|^2/2}$. Therefore the same result holds with $\vec{x}$ and $\vec{k}$ interchanged. □

3.3 Computation of the WFT Coefficients: A Practical Algorithm

Now that we have discussed the dual window, we present here an algorithm for computing it (taken from [12]). We also present the algorithm for computing the framelet coefficients.

The algorithm is basically nothing more than scanning the dual window over the function, and Fourier transforming at each point $\vec{a}x_0$ for $\vec{a} \in \mathbb{Z}^N$. However, due to the spatial decay of $\tilde{g}(\vec{x})$ (c.f. theorem 3.11), we can truncate the domain to a small box surrounding $\vec{a}x_0$.

Algorithm 3.1 *Calculation of Windowed Fourier Transforms*

```
def wft_coefficients(grid, arange, brange):
   NxN_grid wft_coefficients
   for a in arange:
      xbuff = multiply(exp(-(x-a*xs)^2 / (2*sigma^2)), grid)
      kbuff = FFT(xbuff)
      wft_coefficients[a][:] = kbuff
   return wft_coefficients
```

3.4 Phase Space Localization

The WFT allow us to define a concrete realization of phase space. From here onward, we will consider $\mathbb{Z}^N \times \mathbb{Z}^N$ to be a discrete realization of phase space. The vector $(\vec{a}, \vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N$ will represent the point at $\vec{a}x_0$ in position, and $\vec{b}k_0$ in momentum.

With this in mind, we can now construct phase space localization operators very simply.

Definition 3.13 *For a set $F \in \mathbb{Z}^N \times \mathbb{Z}^N$, we define the phase space localization operator:*

$$\mathcal{P}_F \psi(x) = \sum_{(\vec{a},\vec{b}) \in F} \psi_{(\vec{a},\vec{b})} \phi_{(\vec{a},\vec{b})}(\vec{x}) \tag{3.39}$$

Intuitively, one expects that phase space localization based on the WFT will correspond to the usual phase space localization based on position and momentum projections. Of course, the correspondence is fuzzy, and we do make small errors (which we quantify).

Also, for convenience of notation, here and later, we name the sets of high frequency framelets and low frequency framelets.

Definition 3.14 *For $K \in \mathbb{R}^+$, we define the set of high frequency and low frequency framelets, respectively:*

$$\mathrm{HF}(K) = \left\{ (\vec{a}, \vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N : k_0 |\vec{b}|_\infty > K \right\} \tag{3.40a}$$

$$\mathrm{LF}(K) = \left\{ (\vec{a}, \vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N : k_0 |\vec{b}|_\infty \leq K \right\} \tag{3.40b}$$

First, we show a result concerning high pass filters, namely that a high pass filter constructed from the WFT is very similar to a high pass filter constructed from the Fourier transform.

Remark 3.15 We remark at this time that we do not believe our estimates are optimal. We have taken a number of shortcuts in the proofs of the various theorems in this section. We conjecture that these results can be improved significantly by a more careful analysis.

Theorem 3.16 *Let $P^0_{B_{K'};k_0}(\vec{k})$ be a projection operator onto the set $[-(K - \mathbf{k}^s(\epsilon)), K - \mathbf{k}^s(\epsilon)]^N$. Then:*

$$\begin{aligned}&\left\|\mathcal{P}_{\mathrm{HF}(K)} f(x)\right\|_{H^s}\\ &\quad \leq \mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}) \left\|(1 - P^0_{B_{K'};k_0}(\vec{k}))\hat{f}(\vec{k})\right\|_{H^s} + \epsilon \left\|f(x)\right\|_{H^s} \end{aligned} \tag{3.41}$$

The constant $\mathbf{k}^s(\epsilon)$ is defined by:

$$\begin{aligned}\mathbf{k}^s(\epsilon) = \inf_{M\in\mathbb{N}} \Bigg\{ & Mk_0 : \sqrt{\mathbf{h}^-_s}\,\mathbf{g}(k_0, x_0, N, s)\\ & \left[(1+\mathbf{J}_d)(x_0/2\pi)^{-N}(\mathbf{m}_{c,s}(\sigma,N) + \mathbf{m}'_{c,s}(\sigma,N)) + ((2+\mathbf{J}_d)(x_0/2\pi)^{-N})\right]\\ & \times \mathbf{J}_s \left(1 + k_0^s \sum_{i=1}^{N}\left(\vec{z}_i \frac{d}{d\vec{z}_i}\right)^s\right) \mathbf{a}_{M,N}(\vec{z})\Bigg|_{\vec{z}_j = e^{-\mathbf{r}(k_0,x_0)k_0}} \leq \epsilon \Bigg\}\\ & = O(|\ln \epsilon|)\end{aligned} \tag{3.42}$$

with the generating function $\mathbf{a}_{M,s}(\vec{z})$ defined below, in lemma 3.17.

Before proceeding with the proof, we state a technical lemma which we use.

Lemma 3.17 *We have the following bound for the discrete convolution:*

$$\begin{aligned}&\sum_{\vec{a}\in\mathbb{Z}^N} \langle \vec{a}2\pi/x_0\rangle^s e^{-\sigma^2(\vec{a}2\pi/x_0 - \vec{z})^2}\\ &\qquad \leq (1+\mathbf{J}_d)(x_0/2\pi)^{-N}(\mathbf{m}_{c,s}(\sigma,N) + \mathbf{m}'_{c,s}(\sigma,N))\\ &\qquad\qquad + ((2+\mathbf{J}_d)(x_0/2\pi)^{-N})\langle\vec{z}\rangle^s = O(\langle\vec{z}\rangle^s)\end{aligned} \tag{3.43a}$$

$$\begin{aligned}&\sup_{\left|\vec{k}\right|_\infty < k_0} \sum_{|\vec{k}-\vec{b}k_0|_\infty \geq M} \langle \vec{b}k_0 - \vec{k}\rangle^s e^{-\mathbf{r}(k_0,x_0)\left|\vec{b}k_0 - \vec{k}\right|_1}\\ &\qquad \leq \mathbf{J}_s \left(1 + k_0^s \sum_{i=1}^{N}\left(\vec{z}_i \frac{d}{d\vec{z}_i}\right)^s\right) \mathbf{a}_{M,s}(\vec{z})\Bigg|_{\vec{z}_j = e^{-\mathbf{r}(k_0,x_0)k_0}}\\ &\qquad = O(M^s e^{-\mathbf{r}(k_0,x_0)M})\end{aligned} \tag{3.43b}$$

The generating function $\mathbf{a}_{M,N}(\vec{z})$ is defined as:

$$\mathbf{a}_{M,N}(\vec{z}) = \left(\prod_{j=1}^{N} \frac{1}{1-\vec{z}_j}\right)\left[\sum_{1\leq j\leq N}^{N} \vec{z}_j^M \left(1 + \sum_{j<i\leq N} \vec{z}_i^M\right)\right] \tag{3.44}$$

Proof of Theorem 3.16. We proceed in three steps.

Setup

We begin by decomposing $f(x)$ into high and low frequencies, and applying the high pass filter:

$$\begin{aligned}\left\|\mathcal{P}_{\mathrm{HF}(K)} f(x)\right\|_{H^s} \\ = \left\|\mathcal{P}_{\mathrm{HF}(K)} P^0_{B_{K'};0}(\vec{k}) f(x)\right\|_{H^s} + \left\|\mathcal{P}_{\mathrm{HF}(K)} [1 - P^0_{B_{K'};0}(\vec{k})] f(x)\right\|_{H^s}\end{aligned}$$

The first term is bounded by $\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}) \left\|P^0_{B_{K'};0}(\vec{k})\hat{f}(\vec{k})\right\|_{H^s}$, thus it remains to bound the second. Let $h(x) \in H^{-s}$ have norm 1. Then:

$$\begin{aligned}&\left\langle h(x)|\mathcal{P}_{\mathrm{HF}(K)}[1 - P^0_{B_{K'};0}(\vec{k})] f(x)\right\rangle \\ &= \sum_{(\vec{a},\vec{b})\in \mathrm{HF}(K)} \left\langle h(x)|\phi_{(\vec{a},\vec{b})}(\vec{x})\right\rangle \left\langle \tilde{\phi}_{(\vec{a},\vec{b})}(\vec{x})|[1 - P^0_{B_{K'};0}(\vec{k})] f(x)\right\rangle \\ &= \sum_{\vec{a}\in\mathbb{Z}^N} \sum_{k_0|\vec{b}|_\infty > K} \int\int \hat{h}(\vec{k})^* \hat{\phi}_{(\vec{a},\vec{b})}(\vec{k}) \hat{\tilde{\phi}}_{(\vec{a},\vec{b})}(\vec{k'})^* [1 - P^0_{B_{K'};0}(\vec{k'})]\hat{f}(\vec{k'}) d\vec{k'} d\vec{k} \\ &= \int\int \left(\hat{h}(\vec{k})^*[1 - P^0_{B_{K'};0}(\vec{k}+\vec{z})]\hat{f}(\vec{k}+\vec{z})\right)\left(\sum_{\vec{a}\in\mathbb{Z}^N} e^{i\vec{a}x_0\cdot\vec{z}}\right) \\ &\qquad \times \left(\sum_{k_0|\vec{b}|_\infty > K} \hat{\tilde{g}}(\vec{k}+\vec{z}-\vec{b}k_0)e^{-\sigma^2(\vec{k}-\vec{b}k_0)^2}\right) d\vec{z}d\vec{k} \qquad (3.45)\end{aligned}$$

Between lines 3 and 4 we used the change of variables, $\vec{k'} = \vec{k} + \vec{z}$. We use here the fact that:

$$\sum_{\vec{a}\in\mathbb{Z}^N} e^{i\vec{a}x_0\cdot\vec{z}} = \sum_{\vec{a}\in\mathbb{Z}^N} \delta(\vec{z} - \vec{a}2\pi/x_0)$$

Substituting this into (3.45) allows us to do the $\vec{z}$ integral relatively simply. We obtain:

$$
\begin{aligned}
|(3.45)|^2 = \Bigg| \int \hat{h}(\vec{k})^* \sum_{\vec{a}\in\mathbb{Z}^N} \sum_{k_0|\vec{b}|_\infty > K} \Big(& \hat{\hat{g}}(\vec{k}+\vec{a}2\pi/x_0 - \vec{b}k_0) e^{-\sigma^2(\vec{k}-\vec{b}k_0)^2} \\
& \times [1 - P^0_{B_{K'};0}(\vec{k}+\vec{a}2\pi/x_0)]\hat{f}(\vec{k}+\vec{a}2\pi/x_0)\Big) d\vec{k} \Bigg|^2 \\
& \leq \left\| \langle \vec{k}\rangle^{-s} \hat{h}(\vec{k}) \right\|^2_{L^2} \int \Bigg| [1 - P^0_{B_{K'};0}(\vec{k})]\hat{f}(\vec{k}) \\
\times \sum_{\vec{a}\in\mathbb{Z}^N} \sum_{k_0|\vec{b}|_\infty > K} & \hat{\hat{g}}(\vec{k}-\vec{b}k_0) \langle \vec{k} - \vec{a}2\pi/x_0\rangle^s e^{-\sigma^2(\vec{k}-\vec{a}2\pi/x_0-\vec{b}k_0)^2} \Bigg|^2 d\vec{k} \\
& \leq \mathbf{h}_s^- \, \| h(x)\|^2_{H^{-s}} \, \|f(x)\|^2_{L^2} \\
\times \sup_{|\vec{k}|_\infty \leq K - \mathbf{k}^s(\epsilon)} \Bigg| \sum_{\vec{a}\in\mathbb{Z}^N} \sum_{k_0|\vec{b}|_\infty > K} & \hat{\hat{g}}(\vec{k}-\vec{b}k_0)\langle \vec{k}-\vec{a}2\pi/x_0\rangle^s e^{-\sigma^2(\vec{k}-\vec{a}2\pi/x_0-\vec{b}k_0)^2} \Bigg|^2
\end{aligned} \tag{3.46}
$$

Thus it remains to bound the sup term in the last equation.

Bounds on the Sum

We consider this term, dropping the $|\cdot|^2$ since everything underneath is positive. We obtain:

$$
\begin{aligned}
& \sup_{|\vec{k}|_\infty \leq K - \mathbf{k}^s(\epsilon)} \sum_{\vec{a}\in\mathbb{Z}^N} \sum_{k_0|\vec{b}|_\infty > K} \hat{\hat{g}}(\vec{k}-\vec{b}k_0)\langle \vec{k}-\vec{a}2\pi/x_0\rangle^s e^{-\sigma^2(\vec{k}-\vec{a}2\pi/x_0-\vec{b}k_0)^2} \\
& = \sup_{|\vec{k}|_\infty \leq K - \mathbf{k}^s(\epsilon)} \sum_{k_0|\vec{b}|_\infty > K} \hat{\hat{g}}(\vec{k}-\vec{b}k_0) \sum_{\vec{a}\in\mathbb{Z}^N} \langle \vec{k}-\vec{a}2\pi/x_0\rangle^s e^{-\sigma^2(\vec{k}-\vec{a}2\pi/x_0-\vec{b}k_0)^2}
\end{aligned} \tag{3.47}
$$

Thus we find, after applying theorem 3.11 in order to bound the $\hat{\hat{g}}(\,\cdot\,)$ terms:

$$
\begin{aligned}
(3.47) \leq \sup_{|\vec{k}|_\infty \leq K - \mathbf{k}^s(\epsilon)} \mathbf{g}(k_0, x_0, N, s) & \sum_{k_0|\vec{b}|_\infty > K} e^{-\mathbf{r}(k_0,x_0)|\vec{b}k_0 - \vec{k}|_1} \\
& \times \sum_{\vec{a}\in\mathbb{Z}^N} \langle \vec{k}-\vec{a}2\pi/x_0\rangle^s e^{-\sigma^2(\vec{k}-\vec{a}2\pi/x_0-\vec{b}k_0)^2}
\end{aligned} \tag{3.48}
$$

We bound the sum over $\vec{a}$ term using lemma 3.17 (stated just after this proof), in particular (3.43a). This yields:

$$
\begin{aligned}
(3.48) \leq \mathbf{g}(k_0, x_0, N, s)(1+\mathbf{J}_d)(x_0/2\pi)^{-N}(\mathbf{m}_{c,s}(\sigma,N)+\mathbf{m}'_{c,s}(\sigma,N)) \\
\times \sup_{|\vec{k}|_\infty < K-\mathbf{k}^s(\epsilon)} \sum_{k_0|\vec{b}|_\infty > K} e^{-\mathbf{r}(k_0,x_0)|\vec{b}k_0-\vec{k}|_1} \\
+ \mathbf{g}(k_0, x_0, N, s)((2+\mathbf{J}_d)(x_0/2\pi)^{-N}) \\
\times \sup_{|\vec{k}|_\infty < K-\mathbf{k}^s(\epsilon)} \sum_{k_0|\vec{b}|_\infty > K} \langle \vec{b}k_0 - \vec{k}\rangle^s e^{-\mathbf{r}(k_0,x_0)|\vec{b}k_0-\vec{k}|_1}
\end{aligned} \tag{3.49}
$$

We observe now that for $|\vec{k}|_\infty \leq K - \mathbf{k}^s(\epsilon)$, we find that $|\vec{k}-\vec{b}k_0|_\infty \geq \mathbf{k}^s(\epsilon)$ if $k_0|\vec{b}|_\infty \geq K$. Thus, we can continue:

$$
\begin{aligned}
(3.49) \leq \mathbf{g}(k_0, x_0, N, s)(1+\mathbf{J}_d)(x_0/2\pi)^{-N}(\mathbf{m}_{c,s}(\sigma,N)+\mathbf{m}'_{c,s}(\sigma,N)) \\
\times \sup_{|\vec{k}|_\infty < K-\mathbf{k}^s(\epsilon)} \sum_{|\vec{k}-\vec{b}k_0|_\infty \geq \mathbf{k}^s(\epsilon)} e^{-\mathbf{r}(k_0,x_0)|\vec{b}k_0-\vec{k}|_1} \\
+ \mathbf{g}(k_0, x_0, N, s)((2+\mathbf{J}_d)(x_0/2\pi)^{-N}) \\
\times \sup_{|\vec{k}|_\infty < K-\mathbf{k}^s(\epsilon)} \sum_{|\vec{k}-\vec{b}k_0|_\infty \geq \mathbf{k}^s(\epsilon)} \langle \vec{b}k_0 - \vec{k}\rangle^s e^{-\mathbf{r}(k_0,x_0)|\vec{b}k_0-\vec{k}|_1} \\
\leq \mathbf{g}(k_0, x_0, N, s)\Big[(1+\mathbf{J}_d)(x_0/2\pi)^{-N}(\mathbf{m}_{c,s}(\sigma,N)+\mathbf{m}'_{c,s}(\sigma,N)) \\
+ ((2+\mathbf{J}_d)(x_0/2\pi)^{-N})\Big] \\
\times \sup_{|\vec{k}|_\infty < k_0} \sum_{|\vec{k}-\vec{b}k_0|_\infty \geq \mathbf{k}^s(\epsilon)} \langle \vec{b}k_0 - \vec{k}\rangle^s e^{-\mathbf{r}(k_0,x_0)|\vec{b}k_0-\vec{k}|_1}
\end{aligned} \tag{3.50}
$$

To get from the first inequality to the second, we used the fact that $\langle \vec{b}k_0 - \vec{k}\rangle^s \geq 1$ to combine the sums[5]. Then we used the fact that the sum is invariant under translations on the lattice $k_0\mathbb{Z}^N$ to reduce the domain of the sup.

We bound this (applying 3.17, in particular (3.43b)) as follows:

$$
\begin{aligned}
(3.50) \leq \mathbf{g}(k_0, x_0, N, s)\Big[(1+\mathbf{J}_d)(x_0/2\pi)^{-N}(\mathbf{m}_{c,s}(\sigma,N)+\mathbf{m}'_{c,s}(\sigma,N)) \\
+ ((2+\mathbf{J}_d)(x_0/2\pi)^{-N})\Big] \\
\times \mathbf{J}_s \left(1 + k_0^s \sum_{i=1}^N \left(\vec{z}_i \frac{d}{d\vec{z}_i}\right)^s\right) \mathbf{a}_{\mathbf{k}^s(\epsilon),s}(\vec{z})\Bigg|_{\vec{z}_j = e^{-\mathbf{r}(k_0,x_0)k_0}}
\end{aligned} \tag{3.51}
$$

We note that the bound in (3.51) is $O(\mathbf{k}^s(\epsilon)^2 e^{-\mathbf{r}(k_0,x_0)\mathbf{k}^s(\epsilon)})$.

Conclusion

[5] This is a suboptimal result, but differs from the best result based on this proof strategy only logarithmically.

We now finish the argument. We observe that (by (3.45) and (3.46)):

$$\left|\left\langle h(x)|\mathcal{P}_{\mathrm{HF}(K)}[1-P^0_{B_{K'};0}(\vec{k})]f(x)\right\rangle\right|^2 \\ \leq \mathbf{h}_s^- \left\|h(x)\right\|^2_{H^{-s}} \left\|f(x)\right\|^2_{L^2} \left|(3.51)\right|^2 \quad (3.52)$$

for any $h(x)$ having norm 1 in H^{-s}. Thus:

$$\left\|\mathcal{P}_{\mathrm{HF}(K)}[1-P^0_{B_{K'};0}(\vec{k})]f(x)\right\|_{H^s} \leq \sqrt{\mathbf{h}_s^-}\left\|f(x)\right\|_{H^s}\left|(3.51)\right|$$

$$= \Bigg(\sqrt{\mathbf{h}_s^-}\,\mathbf{g}(k_0,x_0,N,s)\Big[(1+\mathbf{J}_d)(x_0/2\pi)^{-N}(\mathbf{m}_{c,s}(\sigma,N)+\mathbf{m}'_{c,s}(\sigma,N)) \\ + ((2+\mathbf{J}_d)(x_0/2\pi)^{-N})\Big] \\ \times \mathbf{J}_s\left(1+k_0^s\sum_{i=1}^{N}\left(\vec{z}_i\frac{d}{d\vec{z}_i}\right)^s\right)\mathbf{a}_{\mathbf{k}^s(\epsilon),s}(\vec{z})\Bigg|_{\vec{z}_j=e^{-\mathbf{r}(k_0,x_0)k_0}}\Bigg)\left\|f(x)\right\|_{H^s} \\ = O(\mathbf{k}^s(\epsilon)^2 e^{-\mathbf{r}(k_0,x_0)\mathbf{k}^s(\epsilon)})\left\|f(x)\right\|_{H^s}$$

But $\mathbf{k}^s(\epsilon)$ is defined precisely so that this is less than $\epsilon\left\|f(x)\right\|_{H^s}$. Hence we are finished. □

Proof of lemma 3.17. Divide and conquer.

Equation (3.43a)

We interpret this as a Riemann sum, approximating an integral, and calculate.

$$\sum_{\vec{a}\in\mathbb{Z}^N}\langle\vec{a}2\pi/x_0\rangle^s e^{-\sigma^2(\vec{a}2\pi/x_0-\vec{z})^2} \\ \leq (x_0/2\pi)^{-N}\left(\int_{\mathbb{R}^N}\langle\vec{a}\rangle^s e^{-\sigma^2(\vec{a}-\vec{z})^2}+\left|\nabla\langle\vec{a}\rangle^s e^{-\sigma^2(\vec{a}-\vec{z})^2}\right|_1 d\vec{a}\right) \\ \leq (x_0/2\pi)^{-N}\int_{\mathbb{R}^N}\langle\vec{a}\rangle^s e^{-\sigma^2(\vec{a}-\vec{z})^2}d\vec{a}+(x_0/2\pi)^{-N}\int_{\mathbb{R}^N}\left|\nabla\langle\vec{a}\rangle^s\right|e^{-\sigma^2(\vec{a}-\vec{z})^2}d\vec{a} \\ + \int_{\mathbb{R}^N}\langle\vec{a}\rangle^s\left|\nabla e^{-\sigma^2(\vec{a}-\vec{z})^2}\right|d\vec{a} \\ \leq (1+\mathbf{J}_d)(x_0/2\pi)^{-N}\int_{\mathbb{R}^N}\langle\vec{a}\rangle^s e^{-\sigma^2(\vec{a}-\vec{z})^2}d\vec{a} \\ + (x_0/2\pi)^{-N}\int_{\mathbb{R}^N}\langle\vec{a}\rangle^s\left|\nabla e^{-\sigma^2(\vec{a}-\vec{z})^2}\right|d\vec{a} \\ \leq (1+\mathbf{J}_d)(x_0/2\pi)^{-N}(\mathbf{m}_{c,s}(\sigma,N)+\mathbf{m}'_{c,s}(\sigma,N))+((2+\mathbf{J}_d)(x_0/2\pi)^{-N})\langle\vec{z}\rangle^s$$

Equation (3.43b)

First, we consider the sum over $\vec{b}_j \geq 0$ only, and pull out a factor of 2^N:

$$\sum_{|\vec{k}-\vec{b}k_0|_\infty \geq M} \langle \vec{b}k_0 - \vec{k}\rangle^s e^{-\mathbf{r}(k_0,x_0)\left|\vec{b}k_0-\vec{k}\right|_1}$$
$$\leq 2^N \sum_{\substack{|\vec{k}-\vec{b}k_0|_\infty \geq M \\ \vec{b}_j \geq 0}} \langle \vec{b}k_0 - \vec{k}\rangle^s e^{-\mathbf{r}(k_0,x_0)\left|\vec{b}k_0-\vec{k}\right|_1}$$
$$\leq 2^N \sum_{\substack{|\vec{b}k_0|_\infty \geq M-k_0 \\ \vec{b}_j \geq 0}} \mathbf{J}_s(1+|\vec{b}k_0|_s^s) e^{-\mathbf{r}(k_0,x_0)\left|\vec{b}k_0\right|_1} \tag{3.53}$$

The last line follows because $|\vec{k}|_\infty \leq k_0$. We will now represent the sum by a generating function, analytic jointly in the variable $\vec{z}$. We will evaluate the generating function at $\vec{z}_j = e^{-\mathbf{r}(k_0,x_0)k_0}$ to obtain the bound.

Note that:

$$\sum_{\substack{\left|\vec{b}\right|_\infty > M \\ \vec{b}_j \geq 0}} \vec{z}^{\vec{b}} = \sum_{\vec{b}_j \geq 0} \vec{z}^{\vec{b}} - \sum_{\substack{\left|\vec{b}\right|_\infty \leq M \\ \vec{b}_j > 0}} \vec{z}^{\vec{b}} = \prod_{j=1}^N \frac{1}{1-\vec{z}_j} - \prod_{j=1}^N \left(\frac{1-\vec{z}_j^M}{1-\vec{z}_j}\right)$$
$$= \left(\prod_{j=1}^N \frac{1}{1-\vec{z}_j}\right) \left[\sum_{1\leq j \leq N} \vec{z}_j^M \left(1 + \sum_{j<i\leq N} \vec{z}_i^M\right)\right] = \mathbf{a}_{M,s}(\vec{z})$$

Then observe that multiplying under the sum by $\vec{k}_i^s$ is equivalent to applying the operator $\vec{z}_i \frac{d}{d\vec{z}_i}$ to the generating function. Thus:

$$\sum_{\substack{\left|\vec{b}\right|_\infty > K \\ \vec{b}_j \geq 0}} \langle \vec{b}k_0\rangle^s e^{-\mathbf{r}(k_0,x_0)\left|\vec{b}k_0\right|_1} \leq \sum_{\substack{\left|\vec{b}\right|_\infty > K \\ \vec{b}_j \geq 0}} \mathbf{J}_s \left(1 + k_0^s \sum_{i=1}^N \vec{b}_i^s\right)) e^{-\mathbf{r}(k_0,x_0)\left|\vec{b}k_0\right|_1}$$
$$= \mathbf{J}_s \left(1 + k_0^s \sum_{i=1}^N \left(\vec{z}_i \frac{d}{d\vec{z}_i}\right)^s\right) \mathbf{a}_{M,s}(\vec{z}) \Big|_{\vec{z}_j = e^{-\mathbf{r}(k_0,x_0)k_0}}$$
$$= O(M^s e^{-\mathbf{r}(k_0,x_0)M})$$

Thus we obtain the bound we seek. □

Remark 3.18 Later on, we will make certain demands on the framelet coefficients of the wavefunction $\psi(\vec{x},t)$. One assumption will demand that $\left\|\mathcal{P}_{\mathrm{HF}(K)} f(x)\right\|_{H^s}$ be small. The assumption is formulated in that way merely for technical simplicity. Theorem 3.16 will allow us to use the simpler statement that $\left\|P^0_{\left|\vec{k}\right|_\infty > K; k_0}(\vec{k}) f(x)\right\|_{H^s}$ to verify this assumption.

We now state a theorem regarding the phase space localization of the Gaussian WFT. The theorem says that if function $f(x)$ is small outside the box $[-X,X]^N \times [-K,K]^N$ (in phase space), then $f_{(\vec{a},\vec{b})}$ are small outside a somewhat larger box

$$[-X - \mathbf{X}^s(\epsilon,K), X + \mathbf{X}^s(\epsilon,K)] \times [-K - \mathbf{K}^s(\epsilon,K), K + \mathbf{K}^s(\epsilon,K)]$$

(with $\mathbf{X}^s(\epsilon,K)$ and $\mathbf{K}^s(\epsilon,K)$ given below).

This result is an extension of theorem 3.5.2 from [12]. We extend that result to N dimensions, and an arbitrary Sobolev space, while also pinning down the constants precisely. However, we use the gaussian WFT frame specifically (with even integer oversampling), while the aforementioned result works with an arbitrary window.

Theorem 3.19 *Let $B_X = [-X,X]^N$, $B_K = [-K,K]^N$ for $X, K < \infty$. Then letting $X' = X - \mathbf{X}^s_\square(\epsilon,K,X)$, $K' = K - \mathbf{K}^s_\square(\epsilon,K)$, we find that:*

$$\begin{aligned} &\left\| f(x) - \mathcal{P}_{B_{X'} \times B_{K'}} f(x) \right\|_{H^s} \leq \mathbf{H}^s_+(\tilde{g}(\vec{x})) \mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}) \\ &\times \left(\left\| (1 - P^s_{B_X;x_0}(\vec{x})) f(\vec{x}) \right\|_{H^s} + \left\| (1 - P^0_{B_K;k_0}(\vec{k})) f(\vec{x}) \right\|_{H^s} + \epsilon \left\| f \right\|_{H^s} \right) \end{aligned} \tag{3.54}$$

The constants are given by:

$$\begin{aligned} \mathbf{X}^s_\square(\epsilon,K,X) = \inf \Bigg\{ & t \in \mathbb{R}^+ : \\ & e^{-\mathbf{r}(x_0,k_0)t} \sum_{j=0}^{\infty} 2N(2j + 2\lceil (X + t/x_0) \rceil + 1)^{N-1} e^{-\mathbf{r}(x_0,k_0)j} \\ & \leq (\epsilon/2) \times \Bigg[\mathbf{g}(x_0,k_0,N,0) 2^{(N+2)/2} (X + x_0)^{(N-1)/2} \\ & \times \sum_{|\vec{b}|_\infty \leq K'/k_0} \left(1 + \mathbf{f}^2_s \left(\sum_{k=1}^{N} (2\sigma)^{-s} (\exp_s(\sqrt{2\sigma}\vec{b}_k k_0))^2 \right) \right)^{1/2} \Bigg]^{-1} \Bigg\} \end{aligned}$$

$$\mathbf{K}^s_\square(\epsilon,K) = \mathbf{k}^s(\epsilon/2) \tag{3.55a}$$

Proof.

Setup

To begin, we separate this into two separate problems:

$$\begin{aligned}\left\|f(x)-\mathcal{P}_{B_{X'}\times B_{K'}}\right\|_{H^s_b} &= \left\|(\mathcal{P}_{\mathrm{HF}(K')}+\mathcal{P}_{\mathrm{LF}(K')\cap B^C_{X'}})f(x)\right\|_{H^s_b}\\ &\leq \left\|\mathcal{P}_{\mathrm{HF}(K')}f(x)\right\|_{H^s_b}+\left\|\mathcal{P}_{\mathrm{LF}(K')\cap B^C_{X'}}f(x)\right\|_{H^s_b}\\ &\leq \left\|\mathcal{P}_{\mathrm{HF}(K')}f(x)\right\|_{H^s_b}\\ +\left\|\mathcal{P}_{\mathrm{LF}(K')\cap B^C_{X'}}(1-P^s_{B_X;x_0}(\vec{x}))f(x)\right\|_{H^s_b} & \left\|\mathcal{P}_{\mathrm{LF}(K')\cap B^C_{X'}}P^s_{B_X;x_0}(\vec{x})f(x)\right\|_{H^s_b}\end{aligned}$$

We apply theorem 3.16 to $\left\|\mathcal{P}_{\mathrm{HF}(K')}f(x)\right\|_{H^s_b}$, and bound

$$\begin{aligned}&\left\|\mathcal{P}_{\mathrm{LF}(K')\cap B^C_{X'}}(1-P^s_{B_X;x_0}(\vec{x}))f(x)\right\|_{H^s_b}\\ &\qquad\leq \mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})\left\|(1-P^s_{B_X;x_0}(\vec{x}))f(x)\right\|_{H^s_b},\end{aligned}$$

obtaining:

$$\begin{aligned}&\left\|f(x)-\mathcal{P}_{B_{X'}\times B_{K'}}\right\|_{H^s_b}\\ &\quad\leq \mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})\left\|(1-P^0_{B_K;k_0}(\vec{k}))\hat{f}(\vec{k})\right\|_{H^s}+(\epsilon/2)\left\|f(x)\right\|_{H^s}\\ &\qquad+\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})\left\|(1-P^s_{B_X;x_0}(\vec{x}))f(x)\right\|_{H^s_b}\\ &\qquad\qquad+\left\|\mathcal{P}_{\mathrm{LF}(K')\cap B^C_{X'}}f(x)\right\|_{H^s_b}\end{aligned}$$

Thus, to complete the proof, we must bound the last term by $(\epsilon/2)\left\|f(x)\right\|_{H^s_b}$. We write:

$$\begin{aligned}&\mathcal{P}_{\mathrm{LF}(K')\cap B^C_{X'}}P^s_{B_X;x_0}(\vec{x})f(x)\\ &\quad=\sum_{|\vec{a}|_\infty>X'/x_0}\ \sum_{|\vec{b}|_\infty\leq K'/k_0}\left\langle\tilde{\phi}_{(\vec{a},\vec{b})}(\vec{x})|P^s_{B_X;x_0}(\vec{x})f(x)\right\rangle\phi_{(\vec{a},\vec{b})}(\vec{x})\\ &=\sum_{|\vec{a}|_\infty>X'/x_0}\ \sum_{|\vec{b}|_\infty\leq K'/k_0}\phi_{(\vec{a},\vec{b})}(\vec{x})\int_{\mathbb{R}^N}e^{-i\vec{b}k_0\cdot\vec{x}}\tilde{g}(\vec{x}-\vec{a}x_0)^*P^s_{B_X;x_0}(\vec{x})f(\vec{x})d\vec{x}\end{aligned}\tag{3.56}$$

We will construct first a bound on the integral term, as a function of $\vec{a},\vec{b}$, and then return to (3.56) to complete the proof.

Bounds per framelet

For $\vec{b}$ small, we do the following:

$$\begin{aligned}&\left|\int_{\mathbb{R}^N}e^{-i\vec{b}k_0\cdot\vec{x}}\tilde{g}(\vec{x}-\vec{a}x_0)^*P^s_{B_X;x_0}(\vec{x})f(\vec{x})d\vec{x}\right|\\ &\qquad\leq\int_{\mathbb{R}^N}\mathbf{g}(x_0,k_0,N,0)\left|e^{-\mathbf{r}(x_0,k_0)|\vec{x}-\vec{a}x_0|_1}P^s_{B_X;x_0}(\vec{x})f(\vec{x})\right|d\vec{x}\end{aligned}\tag{3.57}$$

Observe that $D = [-(X+x_0),(X+x_0)]^N$ contains the support of $P^s_{B_X;x_0}(\vec{x})$, and apply Cauchy-Schwartz to obtain:

$$|(3.57)| \leq \mathbf{g}(x_0,k_0,N,0)\left\| P^0_{D;0}(\vec{x})e^{-\mathbf{r}(x_0,k_0)|\vec{x}-\vec{a}x_0|_1}\right\|_{L^2}\|f(\vec{x})\|_{L^2} \tag{3.58}$$

We now wish to bound $\left\| P^0_{D;0}(\vec{x})e^{-\mathbf{r}(x_0,k_0)|\vec{x}-\vec{a}x_0|_1}\right\|_{L^2}$.

We assume, without loss of generality, that $\vec{a}_j \geq 0$ for $j = 1..N$. We also observe that $|\vec{a}x_0|_\infty \geq (X+x_0)$, and let l be the (possibly not unique) dimension in $|\vec{a}_l x_0| - |\vec{x}_l|$ is maximized. Then:

$$\begin{aligned}
\left\| P^0_{D;0}(\vec{x})e^{-\mathbf{r}(x_0,k_0)|\vec{x}-\vec{a}x_0|_1}\right\|_{L^2} &= \left(\int_{[-(X+x_0),X+x_0]^N} e^{-2\mathbf{r}(x_0,k_0)|\vec{x}-\vec{a}x_0|_1}d\vec{x}\right)^{1/2} \\
&\leq \left(2^N\int_{[0,X+x_0]^N} e^{-2\mathbf{r}(x_0,k_0)|\vec{x}-\vec{a}x_0|_1}d\vec{x}\right)^{1/2} \\
&\leq \left(2^N\int_{[0,X+x_0]^N} e^{-2\mathbf{r}(x_0,k_0)|\vec{x}-\vec{a}x_0|_\infty}d\vec{x}\right)^{1/2} \\
&\leq 2^{N/2}\left(\int_{[0,X+x_0]}\int_{[0,X+x_0]^{N-1}} e^{-2\mathbf{r}(x_0,k_0)(\vec{a}_l-\vec{x}_l)}d\vec{x}_\perp d\vec{x}_l\right)^{1/2} \\
&= 2^{N/2}(X+x_0)^{(N-1)/2}\left(e^{-\mathbf{r}(x_0,k_0)(\vec{a}_l-(X+x_0))} - e^{-\mathbf{r}(x_0,k_0)\vec{a}_l}\right) \\
&\leq 2^{(N+2)/2}(X+x_0)^{(N-1)/2}e^{-\mathbf{r}(x_0,k_0)|\vec{a}|_\infty}(1+e^{\mathbf{r}(x_0,k_0)(X+x_0)})
\end{aligned} \tag{3.59}$$

Noting that $(1+e^{\mathbf{r}(x_0,k_0)(X+x_0)}) \leq 2e^{\mathbf{r}(x_0,k_0)(x+x_0)}$, we find:

$$\begin{aligned}
&\left|\int_{\mathbb{R}^N} e^{-i\vec{b}k_0\cdot\vec{x}}\tilde{g}(\vec{x}-\vec{a}x_0)^* P^s_{B_X;x_0}(\vec{x})f(\vec{x})d\vec{x}\right| \\
&\qquad \leq (\mathbf{g}(x_0,k_0,N,0)2^{(N+4)/2}) \\
&\qquad \times \|f(\vec{x})\|_{L^2}(X+x_0)^{(N-1)/2}e^{-\mathbf{r}(x_0,k_0)|\vec{a}|_\infty}e^{\mathbf{r}(x_0,k_0)(X+x_0)}
\end{aligned} \tag{3.60}$$

Conclusion

We now return to (3.56).

$$
\begin{aligned}
\|(3.56)\|_{H^s} \leq & \sum_{|\vec{a}|_\infty > X'/x_0} \sum_{|\vec{b}|_\infty \leq K'/k_0} \\
& \left\|\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{H^s} \left|\int_{\mathbb{R}^N} e^{-i\vec{b}k_0\cdot\vec{x}}\tilde{g}(\vec{x}-\vec{a}x_0)^* P^s_{B_X;x_0}(\vec{x}) f(\vec{x}) d\vec{x}\right| \\
\leq & \sum_{|\vec{a}|_\infty > X'/x_0} \sum_{|\vec{b}|_\infty \leq K'/k_0} \left[\left(1+\mathbf{f}_s^2\left(\sum_{k=1}^N (2\sigma)^{-s}(\exp_s(\sqrt{2\sigma}\vec{b}_k k_0))^2\right)\right)^{1/2}\right. \\
& \times \|f(\vec{x})\|_{L^2}\, \mathbf{g}(x_0,k_0,N,0) 2^{(N+2)/2} \\
& \left.\times (X+x_0)^{(N-1)/2} e^{-\mathbf{r}(x_0,k_0)|\vec{a}|_\infty} e^{\mathbf{r}(x_0,k_0)(X+x_0)}\right] \qquad (3.61)
\end{aligned}
$$

To get from the second line to the third line, we applied proposition 3.9 to bound $\left\|\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{H^s}$ and (3.60) to bound the integral term in the second line.

We now do the sum over $\vec{b}$ first, pulling out the terms that depend only on $\vec{b}$:

$$
\begin{aligned}
(3.61) \leq & \left(\sum_{|\vec{b}|_\infty \leq K'/k_0} \left(1+\mathbf{f}_s^2\left(\sum_{k=1}^N (2\sigma)^{-s}(\exp_s(\sqrt{2\sigma}\vec{b}_k k_0))^2\right)\right)^{1/2}\right) \\
& \times \|f(\vec{x})\|_{L^2}\, \mathbf{g}(x_0,k_0,N,0) 2^{(N+2)/2} (X+x_0)^{(N-1)/2} \\
& \times \left(e^{\mathbf{r}(x_0,k_0)(X+x_0)} \sum_{|\vec{a}|_\infty > X'/x_0} e^{-\mathbf{r}(x_0,k_0)|\vec{a}|_\infty}\right) \qquad (3.62)
\end{aligned}
$$

We observe that for a given integer j, the number of integer lattice pts $\vec{a}$ with $|\vec{a}|_\infty = j$ is bounded by $2N(2j+1)^{N-1}$. We also note that $X' = X + \mathbf{X}^s_\Box(\epsilon, K, X)$, to find:

$$
\begin{aligned}
& e^{\mathbf{r}(x_0,k_0)(X+x_0)} \sum_{|\vec{a}|_\infty > X'/x_0} e^{-\mathbf{r}(x_0,k_0)|\vec{a}|_\infty} \\
& = e^{\mathbf{r}(x_0,k_0)(X+x_0)} \sum_{j > (X+\mathbf{X}^s_\Box(\epsilon,K,X))/x_0} 2N(2j+1)^{N-1} e^{-\mathbf{r}(x_0,k_0)j} \\
& = e^{\mathbf{r}(x_0,k_0)(X+x_0)} e^{-\mathbf{r}(x_0,k_0)\lceil (X+\mathbf{X}^s_\Box(\epsilon,K,X))/x_0\rceil x_0} \\
& \times \sum_{j=0}^\infty 2N(2j+2\lceil (X+\mathbf{X}^s_\Box(\epsilon,K,X))/x_0\rceil+1)^{N-1} e^{-\mathbf{r}(x_0,k_0)j} \\
\leq & e^{-\mathbf{r}(x_0,k_0)\mathbf{X}^s_\Box(\epsilon,K,X)} \sum_{j=0}^\infty 2N(2j+2\lceil (X+\mathbf{X}^s_\Box(\epsilon,K,X))/x_0\rceil+1)^{N-1} e^{-\mathbf{r}(x_0,k_0)j}
\end{aligned}
$$

By the definition of X', we find that:

$$e^{-\mathbf{r}(x_0,k_0)\mathbf{X}^s_\Box(\epsilon,K,X)}$$
$$\times \sum_{j=0}^{\infty} 2N(2j+2\lceil (X+\mathbf{X}^s_\Box(\epsilon,K,X))/x_0\rceil +1)^{N-1} e^{-\mathbf{r}(x_0,k_0)j}$$
$$\leq (\epsilon/2) \times \left[\mathbf{g}(x_0,k_0,N,0) 2^{(N+2)/2} (X+x_0)^{(N-1)/2} \right.$$
$$\left. \times \sum_{|\vec{b}|_\infty \leq K'/k_0} \left(1+\mathbf{f}_s^2\left(\sum_{k=1}^{N} (2\sigma)^{-s} (\exp_s(\sqrt{2\sigma}\vec{b}_k k_0))^2\right)\right)^{1/2}\right]^{-1}$$

and therefore

$$(3.62) \leq (\epsilon/2) \left\| f(x) \right\|_{L^2} \tag{3.63}$$

Thus, we observe that:

$$\left\| \mathcal{P}_{\mathrm{LF}(K')\cap B^C_{X'}} P^s_{B_X;x_0}(\vec{x}) f(x) \right\|_{H^s} = \|(3.56)\|_{H^s} \leq (3.61) \leq (3.62) \leq (3.63)$$
$$\leq (\epsilon/2) \left\| f(x) \right\|_{L^2} \leq (\epsilon/2) \left\| f(x) \right\|_{H^s}$$

This is what we wanted to prove (recalling the discussion just before (3.56)). □

Remark 3.20 One can tune this estimate more carefully, if necessary. For any $\theta \in (0,1)$, the following choices of $\mathbf{X}^s_\Box(\epsilon,K,X)$ and $\mathbf{K}^s_\Box(\epsilon,K)X$ are also valid:

$$\mathbf{X}^s_\Box(\epsilon,K,X) = \inf \left\{ t \in \mathbb{R}^+ : \right.$$
$$e^{-\mathbf{r}(x_0,k_0)t} \sum_{j=0}^{\infty} 2N(2j+2\lceil (X+t/x_0\rceil +1)^{N-1} e^{-\mathbf{r}(x_0,k_0)j}$$
$$\leq \epsilon\theta \left[\mathbf{g}(x_0,k_0,N,0) 2^{(N+2)/2} (X+x_0)^{(N-1)/2} \right.$$
$$\left. \left. \times \sum_{|\vec{b}|_\infty \leq K'/k_0} \left(1+\mathbf{f}_s^2\left(\sum_{k=1}^{N} (2\sigma)^{-s} (\exp_s(\sqrt{2\sigma}\vec{b}_k k_0))^2\right)\right)^{1/2}\right]^{-1} \right\}$$
$$\mathbf{K}^s_\Box(\epsilon,K) = \mathbf{k}^s(\epsilon(1-\theta)) \tag{3.64a}$$

We now state a slightly technical corollary that we will use.

Corollary 3.21 *Let $f(x) \in H^s$. Let $B_{X'}$, $B_{K'}$ be as in theorem 3.19. Then:*

$$\left\| \mathcal{P}_{B_{X'}\times B_{K'}\setminus \mathrm{HF}(K)} f(x) \right\|_{H^s} \leq \mathbf{H}^s_+(\tilde{g}(\vec{x})) \mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})$$
$$\times (\|(1-P_X(\vec{x}))f(\vec{x})\|_{H^s} + \epsilon) + \left\| \mathcal{P}_{\mathrm{HF}(K)} f(x) \right\|_{H^s} \tag{3.65}$$

Proof. Repeat the proof of Theorem 3.19. However, instead of bounding $\left\|\mathcal{P}_{\mathrm{HF}(K)}f(x)\right\|_{H^s}$ using theorem 3.16 to bound this term, we simply leave it as it is. □

4 Time Evolution of Gaussian Framelets

In this section we study the behavior of Gaussian framelets under the free flow, $e^{i(1/2)\Delta t}$. This is quite explicit, because we can write $e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})$ in closed form:

$$\begin{aligned} e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x}) &= e^{i(1/2)\Delta t}\pi^{-N/4}\sigma^{-N/2}e^{ik_0\vec{b}\cdot\vec{x}}e^{-|\vec{x}-\vec{a}x_0|_2^2/2\sigma^2} \\ &= \frac{\exp\left(i\vec{b}k_0\cdot(\vec{x}-\vec{b}k_0t-\vec{a}x_0)\right)}{\pi^{N/4}\sigma^{N/2}(1+it/\sigma^2)^{N/2}}\exp\left(\frac{-|\vec{x}-\vec{b}k_0t-\vec{a}x_0|_2^2}{2\sigma^2(1+it/\sigma^2)}\right) \end{aligned} \tag{4.1}$$

This allows us to compute precisely most of our framelet functions (error, relevance, etc).

We begin with a general result, which allows us to control the error associated with approximating Fourier multipliers on $\mathbb{R}^N$ by restricting them to a box. This result is sufficiently general to allow for the use of certain kinds of low pass filters (in frequency) on the box, although we do not use it in this generality.

Theorem 4.1 *Let $S(i\nabla)\varphi(\vec{x})$ satisfy the hypothesis of the Poisson summation formula, that is $|S(i\nabla)\varphi(x)| \leq C\langle x\rangle^{N+\epsilon}$ and $\left|S(i\vec{k})\hat{\varphi}(k)\right| \leq C\langle k\rangle^{N+\epsilon}$. Let $S(\vec{k})$, $S_b(\vec{k})$ be continuous bounded Fourier multiplication operators which are equal for $\vec{k} \in B$ (where B is some closed set).*

Then:

$$\begin{aligned} &\left\| S(i\nabla)\varphi(\vec{x}) - \sum_{\vec{k}\in B} e^{i\pi\vec{k}\cdot\vec{x}/L}S_b(\pi\vec{k}/L)\hat{\varphi}(\pi\vec{k}/L)\right\|_{H_b^s} \\ &\leq \|S(i\nabla)\varphi(\vec{x}+2L\vec{n})\|_{H^s(([-L,L]^N)^C)} + \left\|\hat{\varphi}(\vec{k})\right\|_{H^s(B^C)} \sup_{\vec{k}\in B^C}\left|S(\vec{k})-S_b(\vec{k})\right| \end{aligned} \tag{4.2}$$

Remark 4.2 We only use this theorem with $S(i\nabla) = S_b(i\nabla)$; thus, the last term in (4.2) is zero for our purposes . The more general version might be useful when studying the effects of low pass filters on numerical schemes. For many years (since, e.g. [30]), low pass filters have been applied to numerical schemes in order to preserve numerical stability. This result might be useful in proving error bounds for such schemes.

Proof. The Poisson summation formula states that:

$$\sum_{n\in\mathbb{Z}^d} f(\vec{x}+n2L) = \sum_{k\in\mathbb{Z}^d} e^{i\pi\vec{k}\cdot\vec{x}/L}\hat{f}(\pi k/L) \tag{4.3}$$

We let $\hat{f}(\vec{k}) = S(\vec{k})\hat{\varphi}(\vec{k})$. Then, by rearranging (4.3), we find:

$$S(i\nabla)\varphi(\vec{x}) - \sum_{\vec{k}\in\mathbb{Z}^N} e^{i\pi\vec{k}\cdot\vec{x}/L} S(\pi\vec{k}/L)\hat{\varphi}(\pi\vec{k}/L) = -\sum_{\substack{\vec{n}\in\mathbb{Z}^N\\ \vec{n}\neq 0}} S(i\nabla)\varphi(\vec{x}+2L\vec{n}) \quad (4.4)$$

Now, we observe that $S(\vec{k})$ and $S_b(\vec{k})$ are equal on B. We add and subtract

$$\sum_{\pi\vec{k}/L\in\mathbb{Z}^N} e^{i\pi\vec{k}\cdot\vec{x}/L}(S_b(\pi\vec{k}/L) - S(\pi\vec{k}/L))\hat{\varphi}(\pi\vec{k}/L)$$

to both sides of (4.4), to obtain:

$$\begin{aligned} &S(i\nabla)\varphi(\vec{x}) - \sum_{\vec{k}\in\mathbb{Z}^N} e^{i\pi\vec{k}\cdot\vec{x}/L} S_b(\pi\vec{k}/L)\hat{\varphi}(\pi\vec{k}/L) \\ &= -\sum_{\substack{\vec{n}\in\mathbb{Z}^N\\ \vec{n}\neq 0}} S(i\nabla)\varphi(\vec{x}+2L\vec{n}) + \sum_{\pi\vec{k}/L\in\mathbb{Z}^N} e^{i\pi\vec{k}\cdot\vec{x}/L}(S_b(\pi\vec{k}/L) - S(\pi\vec{k}/L))\hat{\varphi}(\pi\vec{k}/L) \end{aligned}$$

We again apply (4.3), and observe that:

$$\begin{aligned} &\sum_{\pi\vec{k}/L\in\mathbb{Z}^N} e^{i\pi\vec{k}\cdot\vec{x}/L}(S_b(\pi\vec{k}/L) - S(\pi\vec{k}/L))\hat{\varphi}(\pi\vec{k}/L) \\ &\qquad = \sum_{\vec{n}\in\mathbb{Z}^N} (S_b(i\nabla) - S(i\nabla))\varphi(\vec{x}+2L\vec{n}) \end{aligned}$$

We now take norms and apply the triangle inequality. We find that:

$$\sum_{\substack{\vec{n}\in\mathbb{Z}^N\\ \vec{n}\neq 0}} \|S(i\nabla)\varphi(\vec{x}+2L\vec{n})\|_{H_b^s} = \|S(i\nabla)\varphi(\vec{x}+2L\vec{n})\|_{H^s(([-L,L]^N)^C)}$$

and that:

$$\begin{aligned} \sum_{\vec{n}\in\mathbb{Z}^N} \|(S_b(i\nabla) - S(i\nabla))\varphi(\vec{x}+2L\vec{n})\|_{H_b^s} &= \|(S_b(i\nabla) - S(i\nabla))\varphi(\vec{x}+2L\vec{n})\|_{H^s} \\ &\leq \left\|\hat{\varphi}(\vec{k})\right\|_{H^s(B^C)} \sup_{\vec{k}\in B^C} \left|S(\vec{k}) - S_b(\vec{k})\right| \end{aligned}$$

We put everything together to obtain the result we seek. □

4.1 Error and Relevance functionals

Using theorem 4.1 and equation (4.1), we can compute per-framelet error bounds in $L^2(\mathbb{R})$. Before we continue, we define a function we will use a number of times.

Definition 4.3 *We define the Hermite Error Function, for x, k real and $s > 0$ to be:*

$$\mathrm{Herf}^s(x,k) = \frac{2}{\sqrt{\pi}} \int_0^x \left(\partial_w^s e^{iwk} e^{-w^2/2}\right) \left(\partial_w^s e^{-iwk} e^{-w^2/2}\right) dw \tag{4.5}$$

Note that $\mathrm{Herf}^0(x,k) = \mathrm{erf}(x)$. *We also define* $\mathrm{Herfi}^s(x,k)$ *to be the inverse function of* $\mathrm{Herf}^s(\,\cdot\,,k)$.

Remark 4.4 We observe that to leading order in k (as k becomes large), that

$$\mathrm{Herf}^s(x,k) = |k|^{2s}\,\mathrm{erf}(x) + O(|k|^{2s-1})$$

In $L^2 = H^0$, $\mathrm{Herf}^s(x,k) = \mathrm{erf}(x)$.In higher Sobolev spaces, they can be determined by a symbolic computation utility, e.g. Maple.

We will use the Herf^s function when we need to compute the L^2 norm of derivatives of gaussians.

Proposition 4.5 *In H^s, we can compute the framelet functionals:*

$$\begin{aligned}
\mathcal{R}^s_{(\vec{a},\vec{b})}(t)^2 &= \mathcal{R}^0_{(\vec{a},\vec{b})}(t)^2 + 2^{-N}(\sigma^{-1}(1+t^2/\sigma^4)^{1/2})^{2s} \\
&\times \sum_{j=1}^{N} \Bigg(\Bigg[\mathrm{Herf}^s\left(\frac{L_{\mathrm{int}} + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}}, \vec{b}_j k_0 (\sigma^{-1}(1+t^2/\sigma^4)^{-1/2}\right) \\
&\quad - \mathrm{Herf}^s\left(\frac{-L_{\mathrm{int}} + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}}, \vec{b}_j k_0 (\sigma^{-1}(1+t^2/\sigma^4)^{-1/2})\right) \Bigg] \\
&\times \prod_{\substack{k=1\\k\neq j}}^{N} \left[\mathrm{erf}\left(\frac{L_{\mathrm{int}} + \vec{b}_k k_0 t + \vec{a}_k x_0}{\sigma\sqrt{1+t^2/\sigma^4}}\right) - \mathrm{erf}\left(\frac{-L_{\mathrm{int}} + \vec{b}_k k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}}\right) \right] \Bigg)
\end{aligned} \tag{4.6a}$$

$$\begin{aligned}
\mathcal{E}^s_{(\vec{a},\vec{b})}(t)^2 &= \mathcal{E}^0_{(\vec{a},\vec{b})}(t)^2 + (\mathcal{M}^s_{(\vec{a},\vec{b})})^2 - 2^{-N}(\sigma^{-1}(1+t^2/\sigma^4)^{1/2})^{2s} \\
&\times \sum_{j=1}^{N} \Bigg(\Bigg[\mathrm{Herf}^s\left(\frac{L_{\mathrm{buff}} + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}}, \vec{b}_j k_0 (\sigma^{-1}(1+t^2/\sigma^4)^{-1/2}\right) \\
&\quad - \mathrm{Herf}^s\left(\frac{-L_{\mathrm{buff}} + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}}, \vec{b}_j k_0 (\sigma^{-1}(1+t^2/\sigma^4)^{-1/2}\right) \Bigg] \\
&\times \prod_{\substack{k=1\\k\neq j}}^{N} \left[\mathrm{erf}\left(\frac{L_{\mathrm{buff}} + \vec{b}_k k_0 t + \vec{a}_k x_0}{\sigma\sqrt{1+t^2/\sigma^4}}\right) - \mathrm{erf}\left(\frac{-L_{\mathrm{buff}} + \vec{b}_k k_0 t + \vec{a}_k x_0}{\sigma\sqrt{1+t^2/\sigma^4}}\right) \right] \Bigg)
\end{aligned} \tag{4.6b}$$

Proof. By theorem 4.1, to calculate $\mathcal{E}^s_{(\vec{a},\vec{b})}(t)$, we need only compute the mass outside the box $B = [-(L_{\text{int}}+w), (L_{\text{int}}+w)]^N$. We observe that $\left\|\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{H^s} = 1 + \mathcal{M}^s_{(\vec{a},\vec{b})}$, so therefore:

$$\left\|e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{H^s(\mathbb{R}^N\setminus[-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N)} = 1 + \mathcal{M}^s_{(\vec{a},\vec{b})} - \left\|e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{H^s([-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N)}$$

We need to compute

$$\left\|\partial^s_{x_j} e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{L^2([-L_{\text{int}},L_{\text{int}}]^N)}$$

for $j = 1 \dots N$, and also for $s = 0$. We compute as follows:

$$\begin{aligned}
&\left\|\partial^s_{x_j} e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|^2_{L^2([-L_{\text{int}},L_{\text{int}}]^N)} \\
&= \int_{[-L_{\text{int}},L_{\text{int}}]^N} \left| \partial^s_{x_j} \frac{\exp\left(i\vec{b}k_0 \cdot (\vec{x} - \vec{b}k_0 t - \vec{a}x_0)\right)}{\pi^{N/4}\sigma^{N/2}(1+it/\sigma^2)^{N/2}} \exp\left(\frac{-|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{2\sigma^2(1+it/\sigma^2)}\right)\right|^2 d\vec{x} \\
&= \frac{1}{\pi^{N/2}\sigma^N\sqrt{1+t^2/\sigma^4}} \int_{[-L_{\text{int}},L_{\text{int}}]^N} \left| \partial^s_{x_j} e^{i\vec{b}k_0\cdot\vec{x}} \exp\left(\frac{-\left|\vec{x} - \vec{b}k_0 t - \vec{a}x_0\right|^2}{2\sigma^2(1+it\sigma^2)}\right)\right|^2 d\vec{x}
\end{aligned} \tag{4.7}$$

We change variables to $\vec{y}_j = \sigma^{-1}(1+t^2/\sigma^4)^{-1/2}(\vec{x}_j - \vec{b}_j k_0 t - \vec{a}_j x_0)$, then $\sigma\sqrt{1+t^2/\sigma^4}d\vec{y}_j = d\vec{x}_j$.

$$\begin{aligned}
(4.7) = &\left[\prod_{\substack{1\leq k\leq N \\ k\neq j}} \int_{(-L_{\text{int}}+\vec{b}_j k_0 t + \vec{a}_j x_0)/\sigma\sqrt{1+t^2/\sigma^4}}^{(L_{\text{int}}+\vec{b}_j k_0 t + \vec{a}_j x_0)/\sigma\sqrt{1+t^2/\sigma^4}} e^{-\vec{y}_j^2} d\vec{y}_j\right] \\
&\left[\int_{\sigma^{-1}(1+t^2/\sigma^4)^{-1/2}(-L_{\text{int}}-\vec{b}k_0 t - \vec{a}x_0)}^{\sigma^{-1}(1+t^2/\sigma^4)^{-1/2}(L_{\text{int}}-\vec{b}k_0 t - \vec{a}x_0)}\right. \\
&\left.\left|(\sigma^{-1}(1+t^2/\sigma^4)^{-s/2})\partial^s_{y_j} e^{i\vec{b}_j k_0 \sigma^{+1}(1+t^2/\sigma^4)^{1/2}\vec{y}_j} e^{-y_j^2/2}\right|^2 dx_j\right]
\end{aligned} \tag{4.8}$$

Evaluating the integrals yields:

$$
\begin{aligned}
(4.8) = {} & (\sigma^{-1}(1+t^2/\sigma^4)^{1/2})^{2s} \\
& \times \left(\mathrm{Herf}^s \left(\frac{L_{\mathrm{int}} + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}}, \vec{b}_j k_0 (\sigma^{-1}(1+t^2/\sigma^4)^{-1/2}) \right) \right. \\
& \left. - \mathrm{Herf}^s \left(\frac{L_{\mathrm{int}} + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}}, \vec{b}_j k_0 (\sigma^{-1}(1+t^2/\sigma^4)^{-1/2}) \right) \right) \\
2^{-N} & \prod_{\substack{1\le i\le N \\ i\neq j}} \left[\mathrm{erf}\left(\frac{L_{\mathrm{int}} + \vec{b}_i k_0 t + \vec{a}_i x_0}{\sigma\sqrt{1+t^2/\sigma^4}} \right) - \mathrm{erf}\left(\frac{-L_{\mathrm{int}} + \vec{b}_i k_0 t + \vec{a}_i x_0}{\sigma\sqrt{1+t^2/\sigma^4}} \right) \right]
\end{aligned}
\tag{4.9}
$$

We add this up for $j = 1..N$ (since we take derivatives in each component of $\vec{x}$) and add a term with $s = 0$. This yields the result we seek. A similar computation allows us to compute $\mathcal{E}^s_{(\vec{a},\vec{b})}(t)$. □

Remark 4.6 For the specific cases of L^2 and H^1, we include simpler formulas. We single out these cases because they are sufficient to encompass most simulations of practical interest.

In L^2, we obtain:

$$
\begin{aligned}
\mathcal{E}^0_{(\vec{a},\vec{b})}(t) = 1 - 2^{-N/2} \prod_{j=1}^{N} & \left[\mathrm{erf}\left(\frac{(L+w) + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}} \right) - \right. \\
& \left. \mathrm{erf}\left(\frac{-(L+w) + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}} \right) \right]^{1/2}
\end{aligned}
\tag{4.10a}
$$

$$
\begin{aligned}
& \mathcal{R}^0_{(\vec{a},\vec{b})}(t) \\
& \quad = 2^{-N/2} \prod_{j=1}^{N} \left[\mathrm{erf}\left(\frac{L + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}} \right) - \mathrm{erf}\left(\frac{-L + \vec{b}_j k_0 t + \vec{a}_j x_0}{\sigma\sqrt{1+t^2/\sigma^4}} \right) \right]^{1/2}
\end{aligned}
\tag{4.10b}
$$

In $H^1(\mathbb{R})$, we find that $\mathcal{R}^1_{(\vec{a},\vec{b})}(t)$ is given by:

$$\begin{aligned}
\left|\mathcal{R}^1_{(\vec{a},\vec{b})}(t)\right|^2 &= \left|\mathcal{R}^0_{(\vec{a},\vec{b})}(t)\right|^2 \\
&\quad + 2^{-N}\sum_{k=1}^{N}\Bigg\{\Bigg(\frac{(2bk_0t-2L_{\text{int}}-2ax_0)}{8\sqrt{\pi(1+t^2)}} \\
&\quad \times\left[e^{-(L_{\text{int}}+\vec{a}_kx_0+\vec{b}_kk_0t)^2/(1+t^2)}-e^{-(L_{\text{int}}-\vec{a}_kx_0-\vec{b}_kk_0t)^2/(1+t^2)}\right] \\
&\quad + 8^{-1}\left(1+2b^2k_0^2\right)\left[\operatorname{erf}\left(\frac{Lb+ax_0+bk_0t}{\sqrt{1+t^2}}\right)+\operatorname{erf}\left(\frac{Lb-ax_0-bk_0t}{\sqrt{1+t^2}}\right)\right]\Bigg) \\
&\quad \times\prod_{j=1,j\neq k}^{N}\left[\operatorname{erf}\left(\frac{L_{\text{int}}+\vec{b}_jk_0t+\vec{a}_jx_0}{\sigma\sqrt{1+t^2/\sigma^4}}\right)-\operatorname{erf}\left(\frac{-L_{\text{int}}+\vec{b}_jk_0t+\vec{a}_jx_0}{\sigma\sqrt{1+t^2/\sigma^4}}\right)\right]\Bigg\}
\end{aligned} \tag{4.11a}$$

$$\begin{aligned}
\left|\mathcal{E}^1_{(\vec{a},\vec{b})}(t)\right|^2 &= \left|\mathcal{E}^0_{(\vec{a},\vec{b})}(t)\right|^2 + (\mathcal{M}^s_{(\vec{a},\vec{b})})^2 \\
&\quad - 2^{-N}\sum_{k=1}^{N}\Bigg\{\Bigg(\frac{(2bk_0t-2(L_{\text{int}}+w)-2ax_0)}{8\sqrt{\pi(1+t^2)}} \\
&\quad \times\left[e^{-((L_{\text{int}}+w)+\vec{a}_kx_0+\vec{b}_kk_0t)^2/(1+t^2)}-e^{-((L_{\text{int}}+w)-\vec{a}_kx_0-\vec{b}_kk_0t)^2/(1+t^2)}\right] \\
&\quad + 8^{-1}\left(1+2b^2k_0^2\right)\Bigg[\operatorname{erf}\left(\frac{(L_{\text{int}}+w)+ax_0+bk_0t}{\sqrt{1+t^2}}\right) \\
&\quad + \operatorname{erf}\left(\frac{(L_{\text{int}}+w)-ax_0-bk_0t}{\sqrt{1+t^2}}\right)\Bigg]\Bigg) \\
&\quad \times\prod_{j=1,j\neq k}^{N}\Bigg[\operatorname{erf}\left(\frac{(L_{\text{int}}+w)+\vec{b}_jk_0t+\vec{a}_jx_0}{\sigma\sqrt{1+t^2/\sigma^4}}\right) \\
&\quad - \operatorname{erf}\left(\frac{-(L_{\text{int}}+w)+\vec{b}_jk_0t+\vec{a}_jx_0}{\sigma\sqrt{1+t^2/\sigma^4}}\right)\Bigg]\Bigg\}
\end{aligned} \tag{4.11b}$$

These formulas were found by a Maple computation. Similar formulas not involving Herf^s can be found for $s \geq 2$ by maple as well, but there is no need to list them here.

4.2 Bounding Boxes

We now introduce the bounding box, which we use to pinpoint the location of each framelet after it is propagated under the free flow, $e^{i(1/2)\Delta t}$. Intuitively, we are treating each framelet as a classical particle which has a finite radius which varies with time.

Definition 4.7 *The collection of sets* $\{\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)\}$ *(indexed by* $(\vec{a},\vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N$*,* $\epsilon \in \mathbb{R}^+$*,* $t \in \mathbb{R}$*) is a family of bounding boxes if:*

$$\left\| e^{i(1/2)\Delta t} \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H^s(\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)^C)} \leq \varepsilon \tag{4.12}$$

In particular, if $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)$ *is a collection of balls having radii which do not vary with* $\vec{a}$*, we let* $\mathbf{W}^s(\vec{b},\epsilon,t)$ *denote the radius.*

We also let $\mathbf{w}_i^s(\vec{b},\epsilon)$*,* $\mathbf{w}_v^s(\vec{b},\epsilon)$ *denote the initial radius and the rate of dispersion, respectively, so that:*

$$\mathbf{W}^s(\vec{b},\epsilon,t) \leq \mathbf{w}_i^s(\vec{b},\epsilon) + \mathbf{w}_v^s(\vec{b},\epsilon)t \tag{4.13a}$$

$$\lim_{t\to\infty} \frac{\mathbf{W}^s(\vec{b},\epsilon,t)}{\mathbf{w}_v^s(\vec{b},\epsilon)t} = 1 \tag{4.13b}$$

Remark 4.8 We only prove that the numbers $\mathbf{w}_i^s(\vec{b},\epsilon)$, $\mathbf{w}_v^s(\vec{b},\epsilon)$ satisfying (4.13) exist for $s = 0, 1$ (c.f. proposition 4.12). However, we believe it is intuitively clear that they will exist for any $s \in \mathbb{N}$, and that they could be found by doing calculations similar to those used in the proof of proposition 4.12.

We now state a pair of Lemmas which demonstrate the usefulness of bounding boxes. This results show that to determine whether a given framelet is in BAD or NECC, it suffices to track it's bounding box. They are each formulated in somewhat technical terms. But the basic idea is this: if the distance between the classical center of mass of the framelet and the interior box is greater than the spreading of the framelet, the framelet is not relevant. Similarly, if the distance between the classical center of mass and the exterior of the computational boxx is less than the spreading of the framelet, the framelet is not bad.

Lemma 4.9 *Fix* $T > 0$*. Then the following two implications hold:*

a. Suppose, for $t \in [0,T]$*, that* $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t) \cap [-L_{\mathrm{int}}, L_{\mathrm{int}}]^N = \emptyset$ *(or* $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t) \cap [-L_{\mathrm{int}}, L_{\mathrm{int}}]^N$ *has measure* 0*). Then* $(\vec{a},\vec{b}) \notin \mathrm{NECC}(\epsilon,s,T)$*.*

b. Suppose, for $t \in [0,T]$*, that* $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t) \subset [-(L_{\mathrm{int}}+w),(L_{\mathrm{int}}+w)]^N$ *(or* $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t) \cap ([-(L_{\mathrm{int}}+w),(L_{\mathrm{int}}+w)]^N)^C$ *has measure* 0*). Then* $(\vec{a},\vec{b}) \notin \mathrm{BAD}(\epsilon,s,T)$*.*

Proof.

a. If $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t) \cap [-L_{\mathrm{int}}, L_{\mathrm{int}}]^N = \emptyset$ (after possibly ignoring a set of measure 0), then $[-L_{\mathrm{int}}, L_{\mathrm{int}}]^N \subset \mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)^C$. Therefore:

$$\mathcal{R}^s_{(\vec{a},\vec{b})}(t) = \left\| e^{i(1/2)\Delta t} \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H^s([-L_{\mathrm{int}},L_{\mathrm{int}}]^N)} \leq \left\| e^{i(1/2)\Delta t} \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H^s(\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)^C)} \leq \epsilon$$

where the last step follows by the definition of $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)$. Thus, $\mathcal{R}^s_{(\vec{a},\vec{b})}(t) \leq \epsilon$ for $t \in [0,T]$ and $(\vec{a},\vec{b}) \notin \mathrm{NECC}(\epsilon,s,T)$.

b. If $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t) \subset [-(L_{\mathrm{int}}+w),(L_{\mathrm{int}}+w)]^N$, then $([-(L_{\mathrm{int}}+w),(L_{\mathrm{int}}+w)]^N)^C \subset \mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)^C$. By theorem 4.1, we find that:

$$\mathcal{E}^s_{(\vec{a},\vec{b})}(t) \leq \left\| e^{i(1/2)\Delta t} \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H^s(([-(L_{\mathrm{int}}+w),(L_{\mathrm{int}}+w)]^N)^C)} \leq \left\| e^{i(1/2)\Delta t} \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H^s(\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)^C)} \leq \epsilon$$

Again, the last step follows by the definition of $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)$. Thus $(\vec{a},\vec{b}) \notin \mathrm{BAD}(\epsilon,s,T)$.

□

Lemma 4.10 *Fix $T > 0$. Then the following two implications hold.*

a. Suppose, for $t \in [0,T]$, that $d(\vec{a}x_0 + \vec{b}k_0 t, [-L_{\mathrm{int}}, L_{\mathrm{int}}]^N) \geq \mathbf{w}^s_i(\vec{b},\epsilon) + \mathbf{w}^s_v(\vec{b},\epsilon)t$. Then $(\vec{a},\vec{b}) \notin \mathrm{NECC}(\epsilon,s,T)$.

b. Suppose, for $t \in [0,T]$, that $|\vec{a}x_0 + \vec{b}k_0 t|_\infty \leq \mathbf{w}^s_i(\vec{b},\epsilon) + \mathbf{w}^s_v(\vec{b},\epsilon)t$. Then $(\vec{a},\vec{b}) \notin \mathrm{BAD}(\epsilon,s,T)$.

Proof.

a. If $d(\vec{a}x_0 + \vec{b}k_0 t, [-L_{\mathrm{int}}, L_{\mathrm{int}}]^N) \geq \mathbf{w}^s_i(\vec{b},\epsilon) + \mathbf{w}^s_v(\vec{b},\epsilon)t$, then

$$\mathrm{interior}\{\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)\} \cap [-L_{\mathrm{int}}, L_{\mathrm{int}}]^N = \emptyset$$

Since the boundary of $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)$ has measure 0, we find that $(\vec{a},\vec{b})$ satisfies lemma 4.9, part (a).

b. The same idea applis, except now:

$$\mathrm{interior}\{\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t)\} \cap ([-(L_{\mathrm{int}}+w),(L_{\mathrm{int}}+w)]^N)^C = \emptyset$$

This, combined with lemma 4.9, part (b) yields the result we seek.

□

We now calculate precisely a bounding box in the spaces L^2 and H^1. We recall first the complementary incomplete Gamma function, and define it's partial inverse.

Definition 4.11 *The complementary incomplete Gamma function, $\Gamma(a,x)$ is defined by:*

$$\Gamma(a,x) = \int_x^\infty e^{-t} t^{a-1} dt \tag{4.14}$$

It has the asymptotic behavior:

$$\Gamma(a,x) \sim x^{a-1} e^{-x} \sum_{j=0}^{\infty} \frac{(a-1)(a-2)\ldots(a-j)}{x^j} \tag{4.15}$$

Moreover, if $n \geq a-1$, we find that:

$$\left| \Gamma(a,x) - x^{a-1} e^{-x} \sum_{j=0}^{n} \frac{(a-1)(a-2)\ldots(a-j)}{x^j} \right| \leq x^{a-1} e^{-x} \frac{(a-1)(a-2)\ldots(a-(n+1))}{x^{n+1}} \tag{4.16}$$

We define the partial inverse of the complementary incomplete Gamma function, $\Gamma^{-1}(a,x)$ to be the inverse of the function $\mathbb{R}^+ \ni x \mapsto \Gamma(a,x)$ for fixed a, so that $\Gamma(a, \Gamma^{-1}(a,x)) = x$.

Note that because $\Gamma(a,x)$ is monotone decreasing in x for a real, $\Gamma^{-1}(a,\epsilon)$ is monotonically increasing as $\epsilon \to 0$. The rate of increase is slower than ϵ^{-t} for any $t > 0$.

Proposition 4.12 *The following family forms a collection of bounding boxes:*

$$\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon,t) = B_{\mathbf{W}^s(\vec{b},\epsilon,t)}(\vec{a}x_0 + \vec{b}k_0 t) \tag{4.17}$$

For $s = 0,1$, $\mathbf{W}^s(\vec{b},\epsilon,t)$ is given by:

$$\mathbf{W}^0(\vec{b},\epsilon,t) = \sqrt{\sigma^2 + t^2/\sigma^2}(\Gamma^{-1}(N/2, 2\epsilon^2 \pi^{N/2} / \left|S^{N-1}\right|))^{1/2} \tag{4.18a}$$

$$\mathbf{W}^1(\vec{b},\epsilon,t) = \sqrt{\sigma^2 + t^2/\sigma^2} \max \left\{ \left[\Gamma^{-1} \left(N/2, \frac{\epsilon^2 \pi^N / 2}{2\left|S^{N-1}\right|(1 + |\vec{b}k_0|_2^2)} \right) \right]^{1/2}, \left[\Gamma^{-1} \left((N+2)/2, \frac{\epsilon^2 \sigma^2 \pi^{N/2}}{2\left|S^{N-1}\right|} \right) \right]^{1/2} \right\} \tag{4.18b}$$

Here, $\left|S^{N-1}\right|$ is the angular measure of the unit ball. We also find that:

$$\mathbf{w}_i^0(\vec{b},\epsilon) = \sigma(\Gamma^{-1}(N/2, 2\epsilon^2 \pi^{N/2} / \left|S^{N-1}\right|))^{1/2}$$

$$\mathbf{w}_v^0(\vec{b},\epsilon) = \sigma^{-1}(\Gamma^{-1}(N/2, 2\epsilon^2\pi^{N/2}/\left|S^{N-1}\right|))^{1/2} \tag{4.19a}$$

$$\mathbf{w}_i^1(\vec{b},\epsilon) = \sigma \max\left\{ \left[\Gamma^{-1}\left(N/2, \frac{\epsilon^2\pi^N/2}{2\left|S^{N-1}\right|(1+|\vec{b}k_0|_2^2)}\right)\right]^{1/2}, \left[\Gamma^{-1}\left((N+2)/2, \frac{\epsilon^2\sigma^2\pi^{N/2}}{2\left|S^{N-1}\right|}\right)\right]^{1/2} \right\}$$

$$\mathbf{w}_v^1(\vec{b},\epsilon) = \sigma^{-1} \max\left\{ \left[\Gamma^{-1}\left(N/2, \frac{\epsilon^2\pi^N/2}{2\left|S^{N-1}\right|(1+|\vec{b}k_0|_2^2)}\right)\right]^{1/2}, \left[\Gamma^{-1}\left((N+2)/2, \frac{\epsilon^2\sigma^2\pi^{N/2}}{2\left|S^{N-1}\right|}\right)\right]^{1/2} \right\} \tag{4.19b}$$

Proof. A straightforward computation, similar to the previous results. The main difference is that we work in spherical, rather than rectangular coordinates. To begin, change variables to $\vec{z}(t) = (\vec{x} - \vec{b}k_0t - \vec{a}x_0)/\sqrt{\sigma^2 + t^2/\sigma^2}$. We note that $d\vec{x} = (\sigma^2 + t^2/\sigma^2)^{N/2}d\vec{z}$. In this new coordinate system, we find that:

$$\left|e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right|^2 = \pi^{-N/2}(\sigma^2 + t^2/\sigma^2)^{-N/2}e^{-z^2} \tag{4.20}$$

Thus:

$$\int \left|e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right|^2 d\vec{x} = \int \left| \frac{\exp\left(i\vec{b}k_0\cdot(\vec{x} - \vec{b}k_0t - \vec{a}x_0)\right)}{\pi^{N/4}\sigma^{N/2}(1+it/\sigma^2)^{N/2}} \exp\left(\frac{-|\vec{x} - \vec{b}k_0t - \vec{a}x_0|_2^2}{2\sigma^2(1+it/\sigma^2)}\right)\right|^2 d\vec{x} = \int \pi^{-N/2}e^{-|\vec{z}|_2^2}d\vec{z} \tag{4.21}$$

Note that the domain of integration also needs to be altered, but we suppressed this to simplify (4.21).

Bounding Boxes in L^2

We switch to polar coordinates about the center of mass of the framelet, $\vec{z} = r\vec{\Omega}$, where $\Omega \in S^{N-1}$.

Thus, if we integrate outside a ball of radius R around the point $\vec{z}(t)$, we obtain:

$$\int_{S^{N-1}}\int_R^\infty \pi^{-N/2}e^{-r^2}r^{N-1}drd\vec{\Omega} = \pi^{-N/2}\left|S^{N-1}\right|\int_{R^2}^\infty u^{(N-1)/2}e^{-u}\frac{du}{2\sqrt{u}} = (1/2)\pi^{-N/2}\left|S^{N-1}\right|\int_{R^2}^\infty u^{N/2-1}e^{-u}du = (1/2)\pi^{-N/2}\left|S^{N-1}\right|\Gamma(N/2,R^2) \tag{4.22}$$

where $\Gamma(a,x)$ is the incomplete Gamma function (c.f. [1]).

Therefore, if $R = (\Gamma^{-1}(N/2, 2\epsilon^2\pi^{N/2}/\left|S^{N-1}\right|))^{1/2}$, then we find that (4.22) $\leq \epsilon^2$. Backtracking, this implies that in the $\vec{z}(t)$ coordinate system, the bounding box is a ball of radius $(\Gamma^{-1}(N/2, 2\epsilon^2\pi^{N/2}/\left|S^{N-1}\right|))^{1/2}$. In the $\vec{x}$ coordinate system, this implies that the bounding box is a ball of radius $\sqrt{\sigma^2 + t^2/\sigma^2}(\Gamma^{-1}(N/2, 2\epsilon^2\pi^{N/2}/\left|S^{N-1}\right|))^{1/2}$ around the point $\vec{a}x_0 + \vec{b}k_0 t$.

Bounding Boxes in H^1

The main difference between L^2 and H^1 is that in H^1, we need to compute:

$$\int \left|e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right|^2 + \sum_{j=1}^{N}\left|\partial_{x_j} e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right|^2 d\vec{x}$$

We begin by computing $\partial_{x_j} e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})$.

$$\begin{aligned}\partial_{x_j} \frac{\exp\left(i\vec{b}k_0 \cdot (\vec{x} - \vec{b}k_0 t - \vec{a}x_0)\right)}{\pi^{N/4}\sigma^{N/2}(1+it/\sigma^2)^{N/2}} \exp\left(\frac{-|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{2\sigma^2(1+it/\sigma^2)}\right) \\ = \left(i\vec{b}_j k_0 - \frac{|\vec{x}_j - \vec{b}_j k_0 t - \vec{a}_j x_0|}{\sigma^2(1+it/\sigma^2)}\right) \\ \times \frac{\exp\left(i\vec{b}k_0 \cdot (\vec{x} - \vec{b}k_0 t - \vec{a}x_0)\right)}{\pi^{N/4}\sigma^{N/2}(1+it/\sigma^2)^{N/2}} \exp\left(\frac{-|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{2\sigma^2(1+it/\sigma^2)}\right)\end{aligned} \tag{4.23}$$

We take the absolute square of this, to obtain:

$$\begin{aligned}\left(|\vec{b}_j k_0|^2 + \frac{|\vec{x}_j - \vec{b}_j k_0 t - \vec{a}_j x_0|^2}{\sigma^4(1+t^2/\sigma^4)} + \text{antisymmetric terms}\right) \\ \times \pi^{-N/2}(\sigma^2 + t^2/\sigma^2)^{-N} \exp\left(\frac{|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{\sigma^2(1+t^2/\sigma^4)}\right)\end{aligned} \tag{4.24}$$

The antisymmetric terms are antisymmetric about the point $\vec{x} = \vec{a}_j x_0 + \vec{b}_j k_0 t$. Thus, upon integration in $\vec{x}$, these terms will vanish.

We then add this up for $j = 1 \dots N$, and add a constant term. This implies that:

$$
\begin{aligned}
&\pi^{-N/2}(\sigma^2 + t^2/\sigma^2)^{-N} \exp\left(\frac{|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{\sigma^2(1 + t^2/\sigma^4)}\right) \\
&\quad + \sum_{j=1}^{N} \left(|\vec{b}_j k_0|^2 + \frac{|\vec{x}_j - \vec{b}_j k_0 t - \vec{a}_j x_0|^2}{\sigma^4(1 + t^2/\sigma^4)} + \text{antisymmetric terms}\right) \\
&\qquad \times \pi^{-N/2}(\sigma^2 + t^2/\sigma^2)^{-N} \exp\left(\frac{|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{\sigma^2(1 + t^2/\sigma^4)}\right) \\
&\quad = \pi^{-N/2}(\sigma^2 + t^2/\sigma^2)^{-N}(1 + |\vec{b}k_0|_2^2) \exp\left(\frac{|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{\sigma^2(1 + t^2/\sigma^4)}\right) \\
&\qquad + \frac{|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{\sigma^4(1 + t^2/\sigma^4)} \exp\left(\frac{|\vec{x} - \vec{b}k_0 t - \vec{a}x_0|_2^2}{\sigma^2(1 + t^2/\sigma^4)}\right) \qquad (4.25)
\end{aligned}
$$

Switching to the $\vec{z}$ coordinate system yields:

$$
\begin{aligned}
(4.25) = {} & \pi^{-N/2}(\sigma^2 + t^2/\sigma^2)^{-N}(1 + |\vec{b}k_0|_2^2)e^{-|\vec{z}|_2^2} \\
& + \pi^{-N/2}(\sigma^2 + t^2/\sigma^2)^{-N}\sigma^{-2}|\vec{z}|_2^2 e^{-|\vec{z}|_2^2} \qquad (4.26)
\end{aligned}
$$

Switching again to polar coordinates and integrating out the angular part yields:

$$
\begin{aligned}
&\int_R^\infty (4.26) d\vec{z} \\
&= \pi^{-N/2}\left|S^{N-1}\right| \left((1 + |\vec{b}k_0|_2^2)\int_R^\infty e^{-r^2} r^{N-1} dr + \sigma^{-2}\int_R^\infty r^2 e^{-r^2} r^{N-1} dr\right) \\
&= (1/2)\pi^{-N/2}\left|S^{N-1}\right| \left((1 + |\vec{b}k_0|_2^2)\Gamma(N/2, R^2) + \sigma^{-2}\Gamma(N/2 + 1, R^2)\right) \qquad (4.27)
\end{aligned}
$$

If R^2 satisfies

$$
\begin{aligned}
R^2 \geq \max\Bigg\{ & \Gamma^{-1}\left(N/2, \frac{\epsilon^2 \pi^N/2}{2\left|S^{N-1}\right|(1 + |\vec{b}k_0|_2^2)}\right), \\
& \Gamma^{-1}\left((N+2)/2, \frac{\epsilon^2\sigma^2\pi^{N/2}}{2\left|S^{N-1}\right|}\right)\Bigg\} \qquad (4.28)
\end{aligned}
$$

then:

$$
\begin{aligned}
(1/2)\pi^{-N/2}\left|S^{N-1}\right|(1 + |\vec{b}k_0|_2^2)\Gamma(N/2, R^2) &\leq \epsilon^2/2 \\
(1/2)\pi^{-N/2}\left|S^{N-1}\right|\Gamma(N/2 + 1, R^2)\sigma^{-2} &\leq \epsilon^2/2
\end{aligned}
$$

and thus $(4.27) \leq \epsilon^2$.

Switching from polar coordinates to $\vec{z}$ coordinates implies that the bounding box consists of $B_R(0)^C$ with R satisfying (4.28). Changing coordinates once more to $\vec{x}$ yields the result we seek.

To obtain (4.19), we simply observe that $\sqrt{\sigma^2 + t^2/\sigma^2} \leq \sigma + t/\sigma$ for $t > 0$, and apply this to (4.18). □

Similar computations can be done in H^s for $s > 1$, but we neglect to do them here.

We now state one more result, which we will use later.

Proposition 4.13 *Let $s = 0, 1$. Then:*

$$\sup_{\vec{b} \in \mathrm{LF}(K)} \mathbf{W}^\epsilon(\vec{b}, 0, t) = \sqrt{\sigma^2 + t^2/\sigma^2}(\Gamma^{-1}(N/2, 2\epsilon^2 \pi^{N/2} / \left|S^{N-1}\right|))^{1/2} \quad (4.29a)$$

$$\sup_{\vec{b} \in \mathrm{LF}(K)} \mathbf{W}^\epsilon(\vec{b}, 1, t) = \sqrt{\sigma^2 + t^2/\sigma^2}$$

$$\times \max \left\{ \left[\Gamma^{-1}\left(N/2, \frac{\epsilon^2 \pi^N/2}{2\left|S^{N-1}\right|(1+NK^2)}\right)\right]^{1/2}, \left[\Gamma^{-1}\left((N+2)/2, \frac{\epsilon^2 \sigma^2 \pi^{N/2}}{2\left|S^{N-1}\right|}\right)\right]^{1/2} \right\} \quad (4.29b)$$

Note the result is independent of K for $s = 0$.

Proof. If $s = 0$, $\mathbf{W}^\epsilon(\vec{b}, 0, t)$ does not vary with $\vec{b}$. This proves (4.29a).

We now prove (4.29b). This follows simply because if $t < t'$, $\Gamma^{-1}(a, t) \geq \Gamma^{-1}(a, t')$ for any $a \in \mathbb{R}^+$. Applying this to (4.18b), we find that the sup on the left side of (4.29b) is maximized when $|\vec{b}k_0|_2$ is maximized. This occurs when $\vec{b}_j k_0 = \lfloor K \rfloor$. Thus, $|\vec{b}k_0|_2 \leq \sqrt{N}K$, and we obtain the bound we seek. □

5 Algorithm, Assumptions, and error bounds

In this section, we prove the accuracy of our method, subject to some assumptions on the equation.

We do not prove a complete error bound. Let $\psi(\vec{x}, t)$ be the solution to (1.1) on $\mathbb{R}^N$ and let $\Psi(\vec{x}, t)$ be the approximate solution generated by our algorithm (defined on $[-L_{\mathrm{comp}}, L_{\mathrm{comp}}]^N$).

To obtain complete control on the error (letting $\Psi_d(\vec{x}, t)$ be the discretized version of $\Psi(\vec{x}, t)$), we need to control:

$$\|\psi(\vec{x}, t) - \Psi_d(\vec{x}, t)\|_{H_b^s} \leq \|\psi(\vec{x}, t) - \Psi(\vec{x}, t)\|_{H_b^s} + \|\Psi(\vec{x}, t) - \Psi_d(\vec{x}, t)\|_{H_b^s}$$

We only prove a bound on the first term, $\|\psi(\vec{x}, t) - \psi_b(\vec{x}, t)\|_{H_b^s}$.

Bounds on the second term depend crucially on many details of the implementation. That is, they will vary depending on whether one chooses a finite element, finite difference or spectral method. They will vary with the timestep, space discretization and also floating point (or other roundoff) error. We assume this is known and is also sufficiently small as to be negligable.

Our goal, is to reduce the error caused by $\|\psi(\vec{x},t) - \Psi(\vec{x},t)\|_{H^s_b}$ to the same order of magnitude as the discretization error, $\|\Psi(\vec{x},t) - \Psi_d(\vec{x},t)\|_{H^s_b}$.

5.1 Assumptions

Let us assume we wish to solve (1.1) on a time interval $[0, T_{\max}]$ with error ε measured in a Sobolev space $H^s([-L_{\text{int}}, L_{\text{int}}]^N)$. We now state our assumptions.

Assumption 1 *We assume the solution to* (1.1) *exists and is unique on* $\mathbb{R}^N$ *for* $t \in [0, T_{\max}]$. *We denote by* $\mathcal{U}(t)$ *the propagator on* $\mathbb{R}^N$.

In particular, we assume that there exists a function $\mathbf{L}(t)$ *and a large number* M *such that for all* $\psi_0(x)$ *with* $\|\psi_0(x)\|_{H^s} \leq M$*:*

$$\|\mathcal{U}(t)\psi_0(x) - \mathcal{U}(t)\psi_1(x)\|_{\mathcal{L}(H^s,H^s)} \leq \mathbf{L}(t) \|\psi_0(x) - \psi_1(x)\|_{H^s} \tag{5.1}$$

Assumption 2 *There exists a maximal momentum* $k_{\max} = k_{\max}(\psi_0)$ *in the following sense. For all* $t \in [0, T_{\max}]$, $\delta_{\max} > 0$, *we can compute a* $k_{\max}(\delta_{\max})$ *such that:*

$$\sup_{t\in[0,T_{\max}]} \left\|\mathcal{P}_{\text{HF}(k_{\max})}\psi(\vec{x},t)\right\| < \delta_{\max} \tag{5.2}$$

Assumption 3 *The nonlinearity is Lipschitz in* H^s. *That is, there exists a constant* $\mathbf{G}$ *such that for* $u, v \in H^s$*:*

$$\|g(t,\vec{x},u)u - g(t,\vec{x},v)v\|_{H^s} \leq \mathbf{G} \|u - v\|_{H^s} \tag{5.3}$$

Although many common nonlinearities are not Lipschitz, they are typically locally Lipschitz, c.f. [8, section 3.2]. Therefore most nonlinearities of interest can be modified appropriately to satisfy these assumptions.

Assumption 4 *The nonlinearity* $g(t,\vec{x},\psi)\psi$ *is well localized in phase space. That is, for any* $\delta_{\text{NL}} > 0$, *there exist constants* $L_{\text{NL}} = L_{\text{NL}}(\delta_{\text{NL}})$ *and* $k_{\max,\text{NL}} = k_{\max,\text{NL}}(\delta_{\text{NL}})$ *(uniform on* $t \in [0,T]$*) such that:*

$$\|\mathcal{P}_{\text{NL}^C}\, g(t,\vec{x},\psi(\vec{x},t))\psi(\vec{x},t)\|_{H^s} < \delta_{\text{NL}} \|\psi(\vec{x},t)\|_{H^s} \tag{5.4a}$$

$$\text{NL} = \{(\vec{a},\vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N : |\vec{a}|_\infty \leq L_{\text{NL}}(\delta_{\text{NL}}) \text{ and } \left|\vec{b}\right|_\infty \leq k_{\max,\text{NL}}(\delta_{\text{NL}})\} \tag{5.4b}$$

Assumption 5 *We assume that for each* $\delta_{\rm F} > 0$*, we can find an* $\epsilon = \epsilon(\delta_{\rm F})$*,* $L_F = L_F(\delta_{\rm F})$*, so that the following implication holds:*

Let $F \subseteq \mathbb{Z}^N \times \mathbb{Z}^N$ *be a set for which,*

$$\forall (\vec{a}, \vec{b}) \in F \sup_{t \in [0, T_{\max}]} \left\| e^{i(1/2)\Delta t} \phi_{(\vec{a},\vec{b})}(\vec{t}) \right\|_{H^s(-[L_F, L_F]^N)} < \varepsilon.$$

Then $\mathcal{P}_F \psi$ *propagates essentially freely, in the following sense:*

$$\sup_{t \in [0, T_{\max}]} \left\| \mathcal{U}(t|\psi_0) \mathcal{P}_F \psi(x) - e^{i(1/2)\Delta t} \mathcal{P}_F \psi(x) \right\|_{H^s_b} \leq \delta_{\rm F} \left\| \mathcal{P}_F \psi(x) \right\|_{H^s_b} \tag{5.5a}$$

$$\sup_{t \in [0, T_{\max}]} \left\| \mathcal{U}(t|\psi_0) \mathcal{P}_{F^C} \psi_0(x) - \mathcal{U}(t|\mathcal{P}_{F^C} \psi_0) \mathcal{P}_{F^C} \psi_0(x) \right\|_{H^s_b} \leq \mathbf{L}_{\rm ext}(t) \left\| \mathcal{P}_F \psi(x) \right\|_{H^s_b} \tag{5.5b}$$

The function $\mathbf{L}_{\rm ext}(t)$ *must satisfy* $\mathbf{L}_{\rm ext}(0) = 0$ *and* $\sup_{t \in [0, T_{\max}]} \mathbf{L}_{\rm ext}(t) = \delta_{\rm F}$.

Remark 5.1 This proposition says that outside of a certain box in phase space, the problem is essentially linear, and therefore the free propagator is sufficiently accurate. This assumption will be the most difficult assumption to verify in the nonlinear case.

We note that we can, in principle, use $\mathbf{L}(t)$ as a bound on $\mathbf{L}_{\rm ext}(t)$. However, this is far from optimal. $\mathbf{L}_{\rm ext}(t)$ should be small for relatively long times, while $\mathbf{L}(t)$ may not be. In the linear case, as an example, measuring error in $H^0 = L^2$, $\mathbf{L}(t) = 1$ and $\mathbf{L}_{\rm ext}(t) = 0$ (identically).

Assumption 6 *We assume that mass does not pile up on tangential, slow waves or returning waves in the following sense. We assume there exists a* $k_{\min} = k_{\min}(\delta_{\min})$*,* $L_{\min} = L_{\min}(\delta_{\min})$ *such that:*

$$\sup_{t \in [0, T_{\max}]} \left\| \mathcal{P}_S \psi(\vec{x}, t) \right\|_{H^s_b} < \delta_{\min} \tag{5.6}$$

with S *a set satisfying:*

$$\forall (\vec{a}, \vec{b}) \in S, !(\exists j, |\vec{a}_j x_0| \geq L_{\min} \text{ and } \vec{b}_j k_0 (\vec{a}_j / |\vec{a}_j|) > k_{\min}) \text{ and } |\vec{a} x_0|_\infty \geq L_{\min} \tag{5.7}$$

Essentially, what assumption 6 is saying is that most of the waves outside the box $[-L_{\min}, L_{\min}]^N$ are moving faster than some small velocity $k_{\min}$, and are moving outward (away from $[-L_{\min}, L_{\min}]^N$).

5.1.1 Remarks on the assumptions

It is simple to observe that Gronwall's lemma combined with assumption 3 implies assumption 1 with $\mathbf{L}(t) = \mathbf{G}e^{\mathbf{G}t}$. However, if better estimates are available, they should be used, since the error estimates we give will be given in terms of $\mathbf{L}(t)$.

Although we state our assumptions in terms of WFT coefficients, they are actually just rephrased versions of more standard assumptions. We provide here some sufficient conditions for verifying the more technical assumptions.

Proposition 5.2 (Sufficient conditions for Assumption 2) *Suppose that there exists a maximal momentum $k_{\max} = k_{\max}(\psi_0)$ in the following sense. For all $t \in [0, T_{\max}]$, $\delta_{\max} > 0$, we can compute a $k_{\max}(\delta_{\max})$ such that:*

$$\left\| P^0_{[-K',K']^N;0}(k)\psi(\vec{x},t) \right\|_{H^s} < \delta_{\max}/(2\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})) \tag{5.8}$$

with $K' = k_{\max} - \mathbf{k}^s(K)$. Then assumption 2 holds.

Proof. Merely apply theorem 3.16. □

Proposition 5.3 (Sufficient conditions for Assumption 4) *Suppose that tThe nonlinearity $g(t, \vec{x}, \psi)\psi$ is well localized in phase space in the traditional sense. That is, for any $\delta_{\mathrm{NL}} > 0$, there exist constants $L'_{\mathrm{NL}} = L'_{\mathrm{NL}}(\delta_{\mathrm{NL}})$ and $k'_{\max,\mathrm{NL}} = k'_{\max,\mathrm{NL}}(\delta_{\mathrm{NL}})$ (uniform on $t \in [0,T]$) such that:*

$$\left\| P^s_{[-k'_{\max,\mathrm{NL}},k'_{\max,\mathrm{NL}}]^N;k_0}(\vec{x}) g(t,\vec{x},\psi(\vec{x},t))\psi(\vec{x},t) \right\|_{H^s} < \frac{\delta_{\mathrm{NL}} \left\|\psi(\vec{x},t)\right\|_{H^s}}{(4\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}))} \tag{5.9a}$$

$$\left\| P^s_{[-L'_{\mathrm{NL}},L'_{\mathrm{NL}}]^N;x_0}(\vec{x}) g(t,\vec{x},\psi(\vec{x},t))\psi(\vec{x},t) \right\|_{H^s} < \frac{\delta_{\mathrm{NL}} \left\|\psi(\vec{x},t)\right\|_{H^s}}{(4\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}))} \tag{5.9b}$$

The constants L'_{NL} and $k'_{\max,\mathrm{NL}}$ are related to those in assumption 4 by the relations

$$L'_{\mathrm{NL}} = L_{\mathrm{NL}} - \mathbf{X}^s_\square(\delta_{\mathrm{NL}}/4\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}), k_{\max,\mathrm{NL}}, L_{\mathrm{NL}}) \tag{5.10}$$

$$k'_{\max,\mathrm{NL}} = k_{\max,\mathrm{NL}} - \mathbf{K}^s_\square(\delta_{\mathrm{NL}}/4\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}), k_{\max,\mathrm{NL}}) \tag{5.11}$$

Then assumption 4 holds.

Proof. Merely apply theorem 3.19. □

We now discuss assumption 5. This assumption says that framelets which are propagated out of the box under the free flow are also propagated outwards under the full flow. We show that this can be verified by an Enss type condition[6].

Proposition 5.4 (Sufficient condition for Assumption 5) *Let F be as in assumption 5. Assume the right side of* (5.12) *is bounded, for all $\psi(x)$ with $\|\psi(x)\|_{H^s} \leq M$ (the same M as in assumption 1).*

Assume further that $g(t, \vec{x}, \psi(\vec{x}, t))\psi(\vec{x}, t)$ is a real valued potential (possible time dependent), that is

$$g(t, \vec{x}, \psi(\vec{x}, t))\psi(\vec{x}, t) = V(\vec{x}, t)\psi(\vec{x}, t).$$

Then $\mathbf{L}_{\text{ext}}(t) = 0$ and δ_{F} is bounded:

$$\delta_{\text{F}} \leq \int_0^{T_{\max}} \left\| e^{i(1/2)\Delta(t-t')} V(\vec{x}, t)\mathcal{U}(t')\mathcal{P}_F\psi(x) \right\|_{H_b^s} dt' \tag{5.12}$$

Supposing additionally that δ_{F} can be made arbitrarily small by increasing L_F, then assumption 5 holds.

Proof. The fact that $\mathbf{L}_{\text{ext}}(t) = 0$ follows because the propagators $\mathcal{U}(t)$ and $\mathcal{U}_b(t)$ do not vary depending on the initial condition. That is to say:

$$\mathcal{U}(t|\psi_0) = \mathcal{U}(t|\mathcal{P}_{F^C}) = \mathcal{U}(t)$$

Now let us construct the bound on δ_{F}. Let $u(x, 0) = \mathcal{P}_F\psi(\vec{x}, t)$. Let $u(\vec{x}, t)$ solve:

$$i\partial_t u(\vec{x}, t) = -(1/2)\Delta u(\vec{x}, t) + g(t, \vec{x}, \mathcal{U}(s)\psi(x))u(x, s)$$

Then setting up Duhamel's equation, we find:

$$u(\vec{x}, t) = e^{i(1/2)\Delta t}u(x, 0) + i\int_0^t Uf(t-s)g(t, \vec{x}, \mathcal{U}(s)\psi(x))u(x, s)$$

Subtracting $e^{i(1/2)\Delta t}u(x, 0)$ from both sides and taking norms proves (5.12). □

Note that assumption 5 is strictly weaker than the conditions given in propsition 5.4. The reason for his is as follows. Proposition 5.4 requires that the free flow and the full flow are almost the same on framelets which don't interact with the nonlinearity. Assumption 5 requires only that they are equal inside the box. Assumption 5 will be satisfied even if the free flow and full flow diverge from each other completely, provided the divergence remains outside the box.

Assumption 6 is two statements. First, it assumes that the mass of the solution below some velocity $k_{\min}$ is small. Second, it assumes that the solution stays on the "propagation set", that is the solution remains restricted to trajectories where $\vec{x} \parallel \vec{k}$. This assumption is really just a rephrasing of standard propagation estimates into the language of framelets.

A stronger assumption than assumption 6 would be the following:

[6]The Enss condition is a common method used to prove asymptotic completeness and other such results in scattering theory. See, e.g. chapter 5 (in particular 5.3) from [9] for details on this method.

Proposition 5.5 (Sufficient condition for Assumption 6) *Let* $\mathrm{PS}(L, k_{\min})$ *(the propagation set) be defined by:*

$$\mathrm{PS}(L, k_{\min}) = \{(\vec{a}, \vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N : |\vec{b}k_0|_2 > 2\sqrt{N} k_{\min}, \\ |\vec{b}k_0 - (|\vec{a}|_2^{-1}\vec{a}) \cdot \vec{b}k_0|_2 \leq |\vec{b}k_0|_2/(4\sqrt{N})\}$$

Suppose that for any $\delta_{\min}$*,* $\exists k_{\min}, L_{\min}$ *so that if* S *is a set satisfying*

$$S \cap \mathrm{PS}(L_{\min}, k_{\min}) = \emptyset \quad (5.13a)$$
$$S \subseteq \{(\vec{a}, \vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N : |\vec{a}x_0|_2 \geq L_{\min}\}, \quad (5.13b)$$

then:

$$\sup_{t \in [0, T_{\max}]} \|\mathcal{P}_S \psi(\vec{x}, t)\|_{H_b^s} < \delta_{\min} \quad (5.14)$$

Then assumption 6 holds.

Proof. We must show that any set S satisfying (5.7) also satisfies (5.13). This will show that the conditions of proposition 5.5 imply assumption 6.

Toward that end, let S be such a set. Since for any $(\vec{a}, \vec{b}) \in S$, $|\vec{a}x_0|_\infty \geq L_{\min}$, we find that (5.13b) is satisfied. We must now show that:

$$\forall (\vec{a}, \vec{b}) \in S, !(\exists j, |\vec{a}_j x_0| \geq L_{\min} \,\mathrm{and}\, \vec{b}_j k_0 (\vec{a}_j / |\vec{a}_j|) > k_{\min})$$

Equivalently:

$$\forall (\vec{a}, \vec{b}) \in S, \forall j, |\vec{a}_j x_0| \leq L_{\min} \,\mathrm{or}\, \vec{b}_j k_0 (\vec{a}_j / |\vec{a}_j|) \leq k_{\min}$$

Now fix $(\vec{a}, \vec{b}) \in S$. We must show that $(\vec{a}, \vec{b}) \notin \mathrm{PS}(L_{\min}, k_{\min})$. We proceed by contradiction.

Suppose $(\vec{a}, \vec{b}) \in \mathrm{PS}(L_{\min}, k_{\min}) \cap S$. Define $\vec{z} = |\vec{a}|_2^{-1} \vec{a} \cdot \vec{b}k_0$. Then:

$$|\vec{z}|_2 \geq |\vec{b}k_0|_2 - |\vec{b}k_0 - \vec{z}|_2 \geq |\vec{b}k_0|_2 - |\vec{b}k_0|_2/(4\sqrt{N}) \quad (5.15)$$

Since $\vec{z}$ is a vector in the direction of $\vec{a}$, we find that $\exists j \in 1 \ldots N$ so that $|\vec{z}_j| \geq |\vec{z}|_2/\sqrt{N}$, and in addition, for this same j, $|\vec{a}_j x_0| \geq |\vec{a}x_0|_2/\sqrt{N}$. If j is chosen to be the component for which $|\vec{a}_j|$ is largest, then in addition $|\vec{a}_j x_0| \geq L_{\min}$.

This implies that:

$$|\vec{z}_j| \geq |\vec{b}k_0|_2/\sqrt{N} - |\vec{b}k_0|_2/(4\sqrt{N})$$
$$|\vec{a}_j x_0| \geq L_{\min}$$

In addition, the signs of $\vec{a}_j$ and $\vec{z}_j$ are the same. Now, observe that:

$$|\vec{b}_j k_0 - \vec{z}_j| \leq |\vec{b}k_0 - \vec{z}|_2 \leq |\vec{b}k_0|_2/(4\sqrt{N})$$

so:

$$|\vec{b}_j k_0| \geq |\vec{z}_j| - |\vec{b}k_0|_2/(4\sqrt{N}) \geq |\vec{b}k_0|_2/\sqrt{N} - 2[|\vec{b}k_0|_2/(4\sqrt{N})]$$
$$\geq |\vec{b}k_0|_2/(2\sqrt{N}) > k_{\min}$$

But this contradicts (5.7), and also (5.15). Therefore there does not exist $(\vec{a}, \vec{b}) \in \mathrm{PS}(L_{\min}, k_{\min}) \cap S$, and we are done. □

Remark 5.6 Without using framelets, statements such as those assumed in proposition 5.5 are common if we ignore low frequencies. The following estimate holds when $g(t, \vec{x}, \psi(x,t))\psi(x,t) = 0$ (in which case $C = \|\vec{x}\psi(x,t)\|_{L^2}$), and also for the case when $g(t, \vec{x}, \psi(\vec{x},t))\psi(\vec{x},t) = |\psi(\vec{x},t)|^{\alpha}\, \psi(\vec{x},t)$ (for certain α[7], [8, proposition 7.3.4]):

$$\sup_{t \in [0,\infty]} \|(\vec{x} + it\nabla)\psi(\vec{x},t)\|_{L^2} \leq C \tag{5.16}$$

We now make a heuristic argument suggesting that this estimate implies the conditions of proposition 5.5. Suppose we have, for some large time, a gaussian at a position $\vec{a}x_0$ (far from the origin, say L units) where $\left|\vec{a}x_0 - \vec{b}k_0 t\right| \geq L/2$ (where $L/2$ is chosen simply for concreteness). Then supposing $|\vec{b}k_0|_2 \gg 0$:

$$(\vec{x} + it\nabla)\phi_{(\vec{a},\vec{b})}(\vec{x}) \approx (\vec{a}x_0 - it\vec{b}k_0)\phi_{(\vec{a},\vec{b})}(\vec{x})$$

But then:

$$\left\|(\vec{x} + it\nabla)\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{L^2} \geq (L/2)$$

Therefore, if $\psi(x,t) = \psi_{(\vec{a},\vec{b})}(t)\phi_{(\vec{a},\vec{b})}(\vec{x}) + \text{rest}$, then either $\left|\psi_{(\vec{a},\vec{b})}\right| \leq 2C/L$ or else $\psi(x,t)$ will violate (5.16).

5.2 The Algorithm

We now describe how to construct the approximate solution, $\Psi(\vec{x},t)$. First, we assume that the various parameters we have described satisfy the constraints given in section 5.2.1.

The precise mathematical definition of $\Psi(\vec{x},t)$ is as follows:

$$\Psi(x, nT_{\text{step}} + t') = \mathcal{U}_b(t')\mathcal{P}_{\text{NECC}\cap\text{BB}}\Psi(\vec{x}, nT_{\text{step}}) \tag{5.17a}$$

$$\Psi(x, (n+1)T_{\text{step}}) = \mathcal{U}_b(T_{\text{step}})\mathcal{P}_{\text{NECC}\cap\text{BB}}\Psi(\vec{x}, nT_{\text{step}}) \tag{5.17b}$$

$$\Psi(x, 0) = \mathcal{P}_{\text{NECC}\cap\text{BB}}\psi(\vec{x}, 0) \tag{5.17c}$$

Here, $0 < t' \leq T_{\text{step}}$ and $n \in \mathbb{N}$. Note that $\Psi(\vec{x},t)$ is not continuous in t at $t = nT_{\text{step}}$, due to the filtering.

The critically important part of the algorithm is satisfying the constraints we have described. This ensures that the framelets which we delete from the solution are, in fact, outgoing framelets.

[7] In particular $\alpha \geq (2 - N + \sqrt{N^2 + 12N + 4})/(2N)$.

5.2.1 Choosing the Parameters

There are a number of constraitns on the parameters which need to be satisfied in order for the algorithm to work. One constraint demands that outside the interior box, waves must move freely. That is:

$$L_{\mathrm{int}} \geq L_F \tag{5.18}$$

This result is needed to prove Theorem 5.10.

Theorem 5.12 imposes a number of conditions on the parameters, nearly all of which are there in order to make sure certain sets of framelets stay inside the box for time T_{step}.

$$\begin{aligned}
\forall \vec{b} \in \mathrm{HF}(k_{\min}), |\vec{b}k_0|_\infty &\geq \mathbf{w}_v^s(\vec{b},\epsilon) && (5.19\mathrm{a})\\
w &\geq 3 \sup_{\vec{b}\in\mathrm{LF}(k_{\max})} \mathbf{w}_i^s(\vec{b},\epsilon) && (5.19\mathrm{b})\\
T_{\mathrm{step}} &\leq \frac{w}{3(k_{\max} + \mathbf{w}_v^s(\vec{b},\epsilon))} && (5.19\mathrm{c})\\
L_{\mathrm{int}} &\leq L_{\min} && (5.19\mathrm{d})\\
T_{\mathrm{step}} &\leq \inf_{|\vec{b}k_0|_2 \leq k_{\max,\mathrm{NL}}} \frac{L_{\mathrm{int}} + w/2 - L_{\mathrm{NL}}}{k_{\max,\mathrm{NL}} + \mathbf{w}_v^s(\vec{b},\epsilon)} && (5.19\mathrm{e})\\
L_{\mathrm{NL}} &\leq L_{\mathrm{int}} && (5.19\mathrm{f})\\
\sup_{|\vec{b}k_0|_2 \leq k_{\max,\mathrm{NL}}} \mathbf{w}_i^s(\vec{b},\epsilon) &\leq w/2 && (5.19\mathrm{g})\\
L_{\mathrm{int}} + w/3 &\leq L_{\min} && (5.19\mathrm{h})
\end{aligned}$$

This list of constraints is deceptively short. In addition to these constraints, one also needs to determine the relation between, e.g. $\delta_{\min}$ and $L_{\min}$, and the various other parameters described in the assumptions. These are model dependent, and can not be treated at this level of generality.

5.3 Statement and Proof of the Error Bound

We make some demands on the parameters ($L_{\mathrm{int}}, T_{\mathrm{step}}$, etc), which are summarized in section 5.2.1.

We will first compute the error between NT_{step} and $(N+1)T_{\mathrm{step}}$.

Definition 5.7 *We define the auxiliary functions:*

$$\widehat{\mathcal{E}}(t) = A_F^{-1} \left(\sum_{(\vec{a},\vec{b})\in \mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \left| \mathcal{E}^s_{(\vec{a},\vec{b})}(t) \right|^2 \right)^{1/2} \tag{5.20a}$$

$$\widehat{\mathcal{R}}(t) = A_F^{-1} \left(\sum_{(\vec{a},\vec{b})\in \mathrm{NECC}^C \cap \mathrm{BB}} \left| \mathcal{E}^s_{(\vec{a},\vec{b})}(t) \right|^2 \right)^{1/2} \tag{5.20b}$$

$$\widehat{\mathcal{Q}}(t) = tA_F^{-1}\left(\sum_{(\vec{a},\vec{b})\in \mathrm{NL}} \left|\mathcal{E}^s_{(\vec{a},\vec{b})}(t)\right|^2\right)^{1/2} \tag{5.20c}$$

We now state a simple upper bound on $\widehat{\mathcal{E}}(t)$ and $\widehat{\mathcal{R}}(t)$. In practice, it should not be used. $\widehat{\mathcal{E}}(t)$ and $\widehat{\mathcal{R}}(t)$ are finite sums of known quantities, and thus they should be computed precisely. But it is convenient to demonstrate the order of magnitude of $\widehat{\mathcal{E}}(t)$ and $\widehat{\mathcal{R}}(t)$.

Proposition 5.8 *The following inequalities hold for* $0 \leq t \leq T_{\mathrm{step}}$.

$$\begin{aligned}\sup_{t\in[0,T_{\mathrm{step}}]} &\widehat{\mathcal{E}}(t) \\ &\leq A_F^{-1}(2L_{\mathrm{WFT}}/x_0)^{N/2}(2k_{\max}/k_0)^{N/2} \sup_{(\vec{a},\vec{b})\in \mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \left|\mathcal{E}^s_{(\vec{a},\vec{b})}(t)\right| \\ &\leq \epsilon A_F^{-1}(2L_{\mathrm{WFT}}/x_0)^{N/2}(2k_{\max}/k_0)^{N/2}\end{aligned} \tag{5.21}$$

$$\begin{aligned}\sup_{t\in[0,T_{\max}]} &\widehat{\mathcal{R}}(t) \\ &\leq A_F^{-1}(2L_{\mathrm{WFT}}/x_0)^{N/2}(2k_{\max}/k_0)^{N/2} \sup_{(\vec{a},\vec{b})\in \mathrm{NECC}^C \cap \mathrm{BB}} \left|\mathcal{E}^s_{(\vec{a},\vec{b})}(t)\right| \\ &\leq \epsilon A_F^{-1}(2L_{\mathrm{WFT}}/x_0)^{N/2}(2k_{\max}/k_0)^{N/2}\end{aligned} \tag{5.22}$$

$$\begin{aligned}\sup_{t\in[0,T_{\max}]} &\widehat{\mathcal{Q}}(t) \\ &\leq A_F^{-1}(2L_{\mathrm{NL}}/x_0)^{N/2}(2k_{\max,\mathrm{NL}}/k_0)^{N/2} \sup_{(\vec{a},\vec{b})\in \mathrm{NECC}^C \cap \mathrm{BB}} \left|\mathcal{E}^s_{(\vec{a},\vec{b})}(t)\right| \\ &\leq \epsilon A_F^{-1}(2L_{\mathrm{NL}}/x_0)^{N/2}(2k_{\max,\mathrm{NL}}/k_0)^{N/2}\end{aligned} \tag{5.23}$$

Proof. A simple calculation. Just count the number of elements in the sums. Then observe that for $t \in [0, T_{\mathrm{step}}]$, $\sup_{(\vec{a},\vec{b})\in \mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \left|\mathcal{E}^s_{(\vec{a},\vec{b})}(t)\right| \leq \epsilon$ by the definition of $\mathrm{BAD} = \mathrm{BAD}(\epsilon, s, T_{\mathrm{step}})$ (and similarly for the other equation).

The bound for $\widehat{\mathcal{Q}}(t)$ is proven by similarly, except by counting the number of elements in L_{NL} (a region in phase space of width L_{NL} in position and $k_{\max,\mathrm{NL}}$ in momentum, see assumption 4). □

Remark 5.9 In practice, proposition 5.8 should not be used. Rather, one can calculate $\widehat{\mathcal{E}}(t)$, $\widehat{\mathcal{R}}(t)$ and $\widehat{\mathcal{Q}}(t)$ precisely. This should be done in practice to choose the parameters. However, we provide these crude upper bounds in order to demonstrate the validity of the method, and to provide rough guidelines as to the choices of the parameters.

5.3.1 Local (1 step) Error

We first compute the error we make over short time intervals (time $[0, T_{\text{step}}]$). We will later string together a number of these short time errors, and calculate the global in time error.

Suppose we are given an initial condition $f(x)$, and an initial error $e(x)$ (the error accumulated from previous timesteps).

We want to compute a bound on:

$$\sup_{t\in[0,T_{\text{step}}]} \|\mathcal{U}(t)f(x) - \mathcal{U}_b(t)\mathcal{P}_{\text{NECC}\cap\text{BB}}[f(x)+e(x)]\|_{H^s_b} \tag{5.24}$$

We first add and subtract $\mathcal{U}(t|f(x))\mathcal{P}_{\text{NECC}^C} f(x)$ under the norm, and apply the triangle inequality. Thus, we find:

$$\begin{aligned} \|\mathcal{U}(t)f(x) - \mathcal{U}_b(t)\mathcal{P}_{\text{NECC}\cap\text{BB}}[f(x)+e(x)]\|_{H^s_b} \\ \leq \|\mathcal{U}(t|f)f(x) - \mathcal{U}(t|f)\mathcal{P}_{\text{NECC}}f(x)\|_{H^s_b} \\ + \|\mathcal{U}(t|f)\mathcal{P}_{\text{NECC}}f(x) - \mathcal{U}_b(t)\mathcal{P}_{\text{NECC}\cap\text{BB}}[f(x)+e(x)]\|_{H^s_b} \end{aligned} \tag{5.25}$$

We state our first result.

Theorem 5.10 (Outgoing waves) *Suppose the following constraints are satisfied:*

$$L_F \leq L_{\text{int}} \tag{5.26a}$$

$$\epsilon(\delta_{\text{F}}) \leq \epsilon \tag{5.26b}$$

with $\epsilon(\delta_{\text{F}})$ defined as in assumption 5. Then the following holds:

$$\begin{aligned} \|\mathcal{U}(t|f)f(x) - \mathcal{U}(t|f)\mathcal{P}_{\text{NECC}}f(x)\|_{H^s_b} = \|\mathcal{U}(t|f(x))\mathcal{P}_{\text{NECC}^C}f(x)\|_{H^s_b} \\ \leq \delta_{\text{F}}\,\|\mathcal{P}_{\text{NECC}^C}f(x)\|_{H^s_b} + \widehat{\mathcal{R}}(t)\,\|f(x)\|_{L^2} \\ + \mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}) \times \Big[\widehat{\mathcal{E}}(T_{\text{step}})\,\|f(x)+e(x)\|_{L^2} + \\ (\widehat{\mathcal{Q}}(T_{\text{step}})\mathbf{G} + t\delta_{\text{NL}}) \sup_{t'\in[0,t]} \|\mathcal{U}(t')(f(x)+e(x))\|_{H^s} + \epsilon\Big] + \delta_{\max} \\ \equiv \text{OUT}(t) \end{aligned} \tag{5.27}$$

This is proved in section 7.1 on page 86. Applying this result, yields:

$$\begin{aligned} (5.25) \leq \text{OUT}(t) \\ + \|\mathcal{U}(t|f)\mathcal{P}_{\text{NECC}}f(x) - \mathcal{U}_b(t)\mathcal{P}_{\text{NECC}\cap\text{BB}}[f(x)+e(x)]\|_{H^s_b} \end{aligned} \tag{5.28}$$

We now add and subtract $\mathcal{U}(t|\mathcal{P}_{\text{NECC}}f)\mathcal{P}_{\text{NECC}}f(x)$ inside the norm, to obtain:

$$\begin{aligned} (5.28) \leq \text{OUT}(t) \\ + \|\mathcal{U}(t|f)\mathcal{P}_{\text{NECC}}f(x) - \mathcal{U}(t|\mathcal{P}_{\text{NECC}}f)\mathcal{P}_{\text{NECC}}f(x)\|_{H^s_b} \\ + \|\mathcal{U}(t|\mathcal{P}_{\text{NECC}}f)\mathcal{P}_{\text{NECC}}f(x) - \mathcal{U}_b(t)\mathcal{P}_{\text{NECC}\cap\text{BB}}[f(x)+e(x)]\|_{H^s_b} \end{aligned} \tag{5.29}$$

Observing that $\|\mathcal{U}(t|f)\mathcal{P}_{\mathrm{NECC}}f(x) - \mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}}f)\mathcal{P}_{\mathrm{NECC}}f(x)\|_{H^s_b}$ is bounded by $\mathbf{L}_{\mathrm{ext}}(t)\,\|\mathcal{P}_{\mathrm{NECC}}f(x)\|_{H^s_b}$ (by assumption 5), we find:

$$(5.29) \leq \mathrm{OUT}(t) + \mathbf{L}_{\mathrm{ext}}(t)\,\|\mathcal{P}_{\mathrm{NECC}}f(x)\|_{H^s_b} + \|\mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}}f)\mathcal{P}_{\mathrm{NECC}}f(x) - \mathcal{U}_b(t)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}[f(x)+e(x)]\|_{H^s_b} \quad (5.30)$$

We add and subtract $\mathcal{U}(t)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}f(x)$ next, yielding:

$$(5.30) \leq \mathrm{OUT}(t) + \mathbf{L}_{\mathrm{ext}}(t)\,\|\mathcal{P}_{\mathrm{NECC}}f(x)\|_{H^s_b} + \|\mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}}f)\mathcal{P}_{\mathrm{NECC}}f(x) - \mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}})\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}f(x)\|_{H^s_b} + \|\mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}f)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}f(x) - \mathcal{U}_b(t)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}[f(x)+e(x)]\|_{H^s_b} \quad (5.31)$$

We state another result:

Theorem 5.11 (Residual Waves) *The residual waves satisfy the following estimate:*

$$\|\mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}}f)\mathcal{P}_{\mathrm{NECC}}f(x) - \mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}})\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}f(x)\|_{H^s_b} \leq \mathbf{L}(t)\Bigg(\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})\Big[\widehat{\mathcal{E}}(T_{\mathrm{step}})\,\|f(x)+e(x)\|_{L^2} + (\widehat{\mathcal{Q}}(T_{\mathrm{step}})\mathbf{G} + t\delta_{\mathrm{NL}})\sup_{t'\in[0,t]}\|\mathcal{U}(t')(f(x)+e(x))\|_{H^s} + \epsilon\Big] + \delta_{\min}\Bigg) \equiv \mathrm{RES}(t) \quad (5.32)$$

This is proved in section 7.2 on page 87.

Applying this yields:

$$(5.31) \leq \mathrm{OUT}(t) + \mathbf{L}_{\mathrm{ext}}(t)\,\|\mathcal{P}_{\mathrm{NECC}}f(x)\|_{H^s_b} + \mathrm{RES}(t) + \|\mathcal{U}(t)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}f(x) - \mathcal{U}_b(t)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}[f(x)+e(x)]\|_{H^s_b} \quad (5.33)$$

We now add and subtract $\mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}(f+e))\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}(f(x)+e(x))$, and bound this by $\mathbf{L}(t)\,\|e(x)\|_{H^s_b}$:

$$(5.33) \leq \mathrm{OUT}(t) + \mathbf{L}_{\mathrm{ext}}(t)\,\|\mathcal{P}_{\mathrm{NECC}}f(x)\|_{H^s_b} + \mathrm{RES}(t) + \|e(x)\|_{H^s_b}\,\mathbf{L}(t) + \|\mathcal{U}(t)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}[f(x)+e(x)] - \mathcal{U}_b(t)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}[f(x)+e(x)]\|_{H^s_b} \quad (5.34)$$

Finally, we bound the last term as follows.

Theorem 5.12 (Lingering Waves) *Let the nonlinearity satisfy assumption 3. Let the following conditions on the parameters be satisfied:*

$$\forall \vec{b} \in \mathrm{HF}(k_{\min}), |\vec{b}k_0|_\infty \geq \mathbf{w}_v^s(\vec{b},\epsilon) \tag{5.35a}$$

$$w \geq 3 \sup_{\vec{b}\in \mathrm{LF}(k_{\max})} \mathbf{w}_i^s(\vec{b},\epsilon) \tag{5.35b}$$

$$T_{\text{step}} \leq \frac{w}{3(k_{\max} + \mathbf{w}_v^s(\vec{b},\epsilon))} \tag{5.35c}$$

$$L_{\text{int}} \leq L_{\min} \tag{5.35d}$$

$$T_{\text{step}} \leq \inf_{|\vec{b}k_0|_2 \leq k_{\max,\text{NL}}} \frac{L_{\text{int}} + w/2 - L_{\text{NL}}}{k_{\max,\text{NL}} + \mathbf{w}_v^s(\vec{b},\epsilon)} \tag{5.35e}$$

$$L_{\text{NL}} \leq L_{\text{int}} \tag{5.35f}$$

$$\sup_{|\vec{b}k_0|_2 \leq k_{\max,\text{NL}}} \mathbf{w}_i^s(\vec{b},\epsilon) \leq w/2 \tag{5.35g}$$

$$L_{\text{int}} + w/3 \leq L_{\min} \tag{5.35h}$$

Let $\psi(x,t=0) = \mathcal{P}_{\text{NECC}\,\cap\,\text{BB}}\psi_0(x)$. *Then the following estimate holds:*

$$\|(\mathcal{U}(t) - \mathcal{U}_b(t))\mathcal{P}_{\text{NECC}\,\cap\,\text{BB}}\psi_0(x)\|_{H_b^s} \leq (E(t) + Q(t)) + \mathbf{G}e^{\mathbf{G}t} \star (E(t) + Q(t)) \tag{5.36a}$$

$$\|(\mathcal{U}(t) - \mathcal{U}_b(t))\mathcal{P}_{\text{NECC}\,\cap\,\text{BB}}\psi_0(x)\|_{H_b^s} \leq (E(t) + Q_b(t)) + \mathbf{G}e^{\mathbf{G}t} \star (E(t) + Q_b(t)) \tag{5.36b}$$

The free error and interaction error are given by:

$$E(t) \leq \widehat{\mathcal{E}}(t)\,\|\psi\|_{L^2} + 2\delta_{\min} \tag{5.37a}$$

$$Q(t) \leq (\widehat{\mathcal{Q}}(t)\mathbf{G} + t\delta_{\text{NL}})\,\|\psi\|_{H^s} \tag{5.37b}$$

A similar estimate holds for $Q_b(t)$ *but with* $\psi(\vec{x},t)$ *replaced by* $\psi_b(\vec{x},t)$. *The functions* $\widehat{\mathcal{E}}(t)$ *and* $\widehat{\mathcal{Q}}(t)$ *are defined in 5.7 on page 63.*

This result is proved in section 6. Applying this result shows that:

$$\begin{aligned}(5.34) \leq\ & \mathrm{OUT}(t) + \mathbf{L}_{\text{ext}}(t)\,\|\mathcal{P}_{\text{NECC}}f(x)\|_{H_b^s} + \mathrm{RES}(t) \\ & + \|e(x)\|_{H_b^s}\,\mathbf{L}(t) \\ & + (1 + \mathbf{G}e^{\mathbf{G}t}\star)(\widehat{\mathcal{E}}(t)\,\|\psi\|_{L^2} + 2\delta_{\min} + (\widehat{\mathcal{Q}}(t)\mathbf{G} + t\delta_{\text{NL}})\,\|\psi\|_{H^s})\end{aligned} \tag{5.38}$$

Remark 5.13 This analysis can be extended to encompass discretization errors. Assuming one has control of discretization errors on the box, one can simply include these errors in $e(x)$. We do not do this here, since it is well beyond the scope of this paper.

5.3.2 Global Error

Given the above result on the one timestep error, we now compute the global-in-time error.

At time $t = 0$, we let $f(x) = \psi_0(x)$ and $e(x) = 0$. At time nT_{step} ($n = 1, \ldots, N$), we let $f(x) = \Psi(x, nT_{\text{step}})$ and

$$e(x) = \mathcal{U}(T_{\text{step}})\mathcal{P}_{\text{NECC}\,\cap\,\text{BB}}\Psi(x,(n-1)T_{\text{step}}) - \mathcal{U}_b(T_{\text{step}})\mathcal{P}_{\text{NECC}\,\cap\,\text{BB}}\Psi(x,(n-1)T_{\text{step}})$$

Putting this all together, for $n = 0 \ldots M$, with $M = T_{\max}/T_{\text{step}}$, we find:

$$\begin{aligned} &\|\mathcal{U}(MT_{\text{step}})\psi_0(x) - \Psi(x, MT_{\text{step}})\|_{H_b^s} \\ &\quad \leq \sum_{n=0}^{M} \Bigg(\text{OUT}((M-n)T_{\text{step}}) + \mathbf{L}_{\text{ext}}((M-n)T_{\text{step}})\, \|\mathcal{P}_{\text{NECC}} f(x)\|_{H_b^s} \\ &+ \mathbf{L}((M-n)T_{\text{step}})\,\text{RES}(nT_{\text{step}}) + \mathbf{L}((M-n)T_{\text{step}})\,\text{BoxError}(nT_{\text{step}}) \Bigg) \end{aligned} \tag{5.39}$$

The term $\text{BoxError}(nT_{\text{step}})$ is bounded by (5.36) with $\psi_0(x) = \Psi(x, nT_{\text{step}})$.

Remark 5.14 This result is essentially what one would expect. The term $\text{RES}(nT_{\text{step}})$ represents the main source of error. This is the error caused by waves we cannot filter with our algorithm. The error bound says that at tine nT_{step}, we make an error of size $\text{RES}(nT_{\text{step}})$. After that, the error grows at a rate $\mathbf{L}(t - nT_{\text{step}})$.

$\text{BoxError}(nT_{\text{step}})$ represents the error due to filtering at time nT_{step}, and this also grows at the rate $\mathbf{L}(t - nT_{\text{step}})$ after that.

We now wish to make sense of (5.39). We first substitute everything in order to get a complete picture. We will then rearrange and simplify significantly.

$$
\begin{aligned}
&\|\mathcal{U}(NT_{\text{step}})\psi_0(x) - \Psi(x, NT_{\text{step}})\|_{H_b^s} \\
&\leq \sum_{n=0}^{M} \delta_{\text{F}} \|\mathcal{P}_{\text{NECC}^C}\Psi(x, nT_{\text{step}})\|_{H_b^s} + \widehat{\mathcal{R}}((M-n)T_{\text{step}}) \|\Psi(x, nT_{\text{step}})\|_{L^2} \\
&\qquad + \mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}) \Bigg[\widehat{\mathcal{E}}(T_{\text{step}}) \|\Psi(x, (n-1)T_{\text{step}})\|_{L^2} \\
&\quad + (\widehat{\mathcal{Q}}(T_{\text{step}}) + t\delta_{\text{NL}}) \sup_{t' \in [0,t]} \|\mathcal{U}(t')\Psi(x, (n-1)T_{\text{step}})\|_{H^s} + \epsilon \Bigg] + \delta_{\max} \\
&\qquad + \mathbf{L}_{\text{ext}}((M-n)T_{\text{step}}) \|\mathcal{P}_{\text{NECC}}\Psi(x, nT_{\text{step}})\|_{H^s} \\
&\qquad \mathbf{L}((M-n)T_{\text{step}}) \Bigg(\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}) \\
&\qquad \Bigg[\widehat{\mathcal{E}}(T_{\text{step}}) \|\Psi(x, (n-1)T_{\text{step}})\|_{L^2} \\
&\quad + (\widehat{\mathcal{Q}}(T_{\text{step}}) + t\delta_{\text{NL}}) \sup_{t' \in [0,t]} \|\mathcal{U}(t')\Psi(x, (n-1)T_{\text{step}})\|_{H^s} + \epsilon \Bigg] + \delta_{\min} \Bigg) \\
&\quad \mathbf{L}((M-n)T_{\text{step}})(1 + T_{\text{step}}\mathbf{G}e^{\mathbf{G}T_{\text{step}}}) \Big[\widehat{\mathcal{E}}(T_{\text{step}}) \|\Psi(x, nT_{\text{step}})\|_{L^2} + \delta_{\min} \\
&\qquad + (\widehat{\mathcal{Q}}(T_{\text{step}}) + T_{\text{step}}\delta_{\text{NL}}) \sup_{t \in [0, T_{\text{step}}]} \|\Psi(x, nT_{\text{step}} + t)\|_{L^2} \Big] \qquad (5.40)
\end{aligned}
$$

We now take this and collect all the terms containing

$$
\Big[\widehat{\mathcal{E}}(T_{\text{step}}) \|\Psi(x, nT_{\text{step}})\|_{L^2} + \widehat{\mathcal{Q}}(T_{\text{step}}) \sup_{t \in [0, T_{\text{step}}]} \|\Psi(x, nT_{\text{step}} + t)\|_{L^2} \Big]
$$

as well as $\delta_{\min}$, δ_{F}, $\mathbf{L}_{\text{ext}}(t)$, etc. We also replace the terms $\|\mathcal{P}_F\Psi(\vec{x},t)\|_{L^2}$ by $\sqrt{B_F/A_F}\,\|\Psi(\vec{x},t)\|_{L^2}$ and $\|\mathcal{P}_F\Psi(\vec{x},t)\|_{H^s}$ by $\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2})\,\|\Psi(\vec{x},t)\|_{H^s}$. We thus arrive at our main theorem.

Theorem 5.15 (Global Error Bound) *We have the following bound on the* *error:*

$$\sup_{t\in[0,T_{\max}]} \|\mathcal{U}(t)\psi_0(x) - \Psi(x,t)\|_{H^s_b} \leq (5.40) \leq \sup_{t\in[0,T_{\max}]} \|\Psi(\vec{x},t)\|_{H^s} \Bigg[$$

$$\widehat{\mathcal{E}}(T_{\text{step}}) \left(\left[(1 + T_{\text{step}}\mathbf{G}e^{\mathbf{G}T_{\text{step}}}) + 2\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}) \right] \sum_{n=0}^{M} \mathbf{L}((M-n)T_{\text{step}}) \right)$$

$$+ \left(\sum_{n=0}^{M} \widehat{\mathcal{R}}((M-n)T_{\text{step}}) \right)$$

$$+ \widehat{\mathcal{Q}}(T_{\text{step}}) \Bigg[(2 + T_{\text{step}}\mathbf{G}e^{\mathbf{G}T_{\text{step}}}) \left(\sum_{n=0}^{M} \mathbf{L}((M-n)T_{\text{step}}) \right)$$

$$+ (T_{\max}/T_{\text{step}})\mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2}) \Bigg]$$

$$+ \delta_{\text{NL}} T_{\text{step}} \left(\sum_{n=0}^{M} \widehat{\mathcal{R}}((M-n)T_{\text{step}}) \right) (2 + T_{\text{step}}\mathbf{G}e^{\mathbf{G}T_{\text{step}}})$$

$$+ \delta_{\text{F}}(T_{\max}/T_{\text{step}}) + \left(\sum_{n=0}^{M} \mathbf{L}_{\text{ext}}((M-n)T_{\text{step}}) \right)$$

$$\Bigg]$$

$$+ \delta_{\min}(2 + T_{\text{step}}\mathbf{G}e^{\mathbf{G}T_{\text{step}}}) \left(\sum_{n=0}^{M} \mathbf{L}((M-n)T_{\text{step}}) \right) + \delta_{\max}(T_{\max}/T_{\text{step}}) \tag{5.41}$$

Although the error bound looks complicated, each term has a simple meaning.

The term $\delta_{\text{NL}}(\ldots)$ is similar. This term measures how much of the nonlinearity actually outside the computational domain. In order to accurately compute the effect of the nonlinearity, it must be contained inside the computational domain. Thus, whatever mass exists outside the computational region (namely $[-L_{\text{NL}}, L_{\text{NL}}]^N \times [-k_{\max,\text{NL}}, k_{\max,\text{NL}}]^N$ in phase space) will also cause an error.

The term $\delta_{\text{F}}(T_{\max}/T_{\text{step}})$ measures how much of the solution which we thought was outgoing actually wasn't. That is, we examined each gaussian, and determined that under the free flow, that particular gaussian was leavining the computational domain. But although the flow is nearly free on the boundary, it is possible that some small fraction of the waves we believe are outgoing are returning. That is measured by δ_{F}.

The next piece,

$$\left(\sum_{n=0}^{M} \mathbf{L}_{\text{ext}}((M-n)T_{\text{step}}) \right),$$

is a little bit trickier to describe. This part of the error measures how the nonlinearity changes in response to the small errors made when we filter off the outgoing waves. In the event the "nonlinearity" is linear, this term is identically zero. But in other cases, it may grow rather large with t.

It is best illustrated by an example. Consider the NLS:

$$i\partial_t \psi(x,t) = (-(1/2)\Delta_b + V(x))\psi(x,t) + f(|\psi(x,t)|^2)\psi(x,t)$$

with $V(x)$ an even, real valued potential having two (nonlinear) bound states, and $(|\psi(x,t)|)$ a monotone real-positive function satisfying certain other constraints (see [39]). It is known that this system exhibits ground state selection [39]. That is, if $\psi(x,0)$ is an odd function, then $\psi(x,t)$ remains situated on the odd (excited) bound state for all time. If, however, we replace $\psi(x,0) = \text{odd}(x) + \epsilon\,\text{even}(x)$, then half the mass of $\psi(x,t)$ will radiate off to infinity, while the other half will be trapped in the ground state.

The function $\mathbf{L}_{\text{ext}}(t)$ measures the capacity of the system to behave nonlinearly in response to perturbations, in a manner like that which we just described.

The last term, $\delta_{\max}(T_{\max}/T_{\text{step}})$, is essentially the amount of mass at frequencies higher than $k_{\max}$. Although $k_{\max}$ (as used in assumption 2) is slightly different from the usual definition of $k_{\max}$ (namely $k_{\max} = \pi/\Delta x$, with Δx the lattice spacing in position on the grid), it is a very similar object, namely the largest frequency we can resolve.

Finally, we come to the term containing $k_{\min}(\ldots)$. This term contains waves with frequency sufficiently low so that it is very difficult to tell if they are entering the box or leaving. This is basically due to the fact that for functions localized in the filter region, the Heisenberg uncertainty principle says that we cannot determine whether low frequency waves are incoming or outgoing. In most of our experiments, this was the dominant term in the error.

We now prove a corollary to theorem 5.15, which states that under the assumptions given in section 5.1, we can make the error due to boundary reflections vanish by making certain explicit choices of the parameters.

Corollary 5.16 (Convergence to Zero) *We can choose the parameters T_{step}, L_{int} and w in such a way that for any $\tau > 0$ and $T_{\max} < \infty$,*

$$\sup_{t\in[0,T_{\max}]} \|\mathcal{U}(t)\psi_0(x) - \Psi(x,t)\|_{H_b^s} \leq \tau \tag{5.42}$$

The proof is deferred to the end of this section, after we have discussed the sources of the error.

Proof of Corollary 5.16. We show here how we can make the error bound (5.41) arbitrarily small.

We begin by considering the terms $\delta_{\min}$, $\delta_{\max}$ δ_{NL}, δ_{F} and $\mathbf{L}_{\text{ext}}(t)$ found in the last four lines of (5.41). According to assumptions 6, 2, 4 and 5 (respectively), we can choose the parameters $k_{\min}$, $k_{\max}$, L_{NL}, $k_{\max,\text{NL}}$ and L_F in such a way that $\delta_{\min}$, $\delta_{\max}$ δ_{NL}, δ_{F} and $\mathbf{L}_{\mathrm{ext}}(t)$[8] are all arbitrarily small. Therefore, it is possible to choose these parameters in such a way that:

$$\delta_{\mathrm{NL}} \sup_{t\in[0,T_{\max}]} \|\Psi(\vec{x},t)\|_{H^s} T_{\mathrm{step}} \left(\sum_{n=0}^{M} \widehat{\mathcal{R}}((M-n)T_{\mathrm{step}})\right)(2+T_{\mathrm{step}}\mathbf{G}e^{\mathbf{G}T_{\mathrm{step}}})$$
$$+\,\delta_{\mathrm{F}} \sup_{t\in[0,T_{\max}]} \|\Psi(\vec{x},t)\|_{H^s} (T_{\max}/T_{\mathrm{step}})$$
$$+\left(\sum_{n=0}^{M} \mathbf{L}_{\mathrm{ext}}((M-n)T_{\mathrm{step}})\right) \sup_{t\in[0,T_{\max}]} \|\Psi(\vec{x},t)\|_{H^s}$$
$$+\,\delta_{\min}(2+T_{\mathrm{step}}\mathbf{G}e^{\mathbf{G}T_{\mathrm{step}}})\left(\sum_{n=0}^{M} \mathbf{L}((M-n)T_{\mathrm{step}})\right)+\delta_{\max}(T_{\max}/T_{\mathrm{step}})$$
$$\leq \tau/2 \quad (5.43)$$

The exact manner in which this will be done is highly model dependent. Later on (in remark 5.17) we will discuss briefly the obvious way to make this small, and why this may not be the best way to satisfy (5.43).

We now take $k_{\min}$, $k_{\max}$, L_{NL}, $k_{\max,\mathrm{NL}}$ and L_F to be fixed quantities.

Once these terms are chosen, we must choose L_{int},w satisfying the various constraints. After this is done, Proposition 5.8 provides a bound on $\widehat{\mathcal{E}}(T_{\mathrm{step}})$, $\widehat{\mathcal{R}}(T_{\mathrm{step}})$ and $\widehat{\mathcal{Q}}(T_{\mathrm{step}})$ – in particular each is bounded by $const \times \epsilon$ (with $const$ a function of the various parameters).

More precisely, we do the following. We now need to obtain the following bound:

$$\sup_{t\in[0,T_{\max}]} \|\Psi(\vec{x},t)\|_{H^s} \Bigg[$$
$$\widehat{\mathcal{E}}(T_{\mathrm{step}})\left(\left[(1+T_{\mathrm{step}}\mathbf{G}e^{\mathbf{G}T_{\mathrm{step}}})+2\mathbf{H}_{+}^{s}(\tilde{g}(\vec{x}))\mathbf{H}_{+}^{-s}(e^{-x^2/\sigma^2})\right]\sum_{n=0}^{M}\mathbf{L}((M-n)T_{\mathrm{step}})\right)$$
$$+\left(\sum_{n=0}^{M}\widehat{\mathcal{R}}((M-n)T_{\mathrm{step}})\right)$$
$$+\,\widehat{\mathcal{Q}}(T_{\mathrm{step}})\Bigg[(2+T_{\mathrm{step}}\mathbf{G}e^{\mathbf{G}T_{\mathrm{step}}})\left(\sum_{n=0}^{M}\mathbf{L}((M-n)T_{\mathrm{step}})\right)$$
$$+\,(T_{\max}/T_{\mathrm{step}})\mathbf{H}_{+}^{s}(\tilde{g}(\vec{x}))\mathbf{H}_{+}^{-s}(e^{-x^2/\sigma^2})\Bigg]\Bigg] \leq \tau/2 \quad (5.44)$$

We recall the bounds computed in Proposition 5.8, and substitute them in

[8] Recall that $\sup_{t\in[0,T_{\max}]}\mathbf{L}_{\mathrm{ext}}(t) \leq \delta_{\mathrm{F}}$. In principle, one could simply use this bound. However, in practice, we expect that $\sum_{n=0}^{M}\mathbf{L}_{\mathrm{ext}}((M-n)T_{\mathrm{step}}) \ll M\delta_{\mathrm{F}}$, so this would be an inefficient choice.

to obtain:

$$
\begin{aligned}
(5.44) \leq \sup_{t\in[0,T_{\max}]} \|\Psi(\vec{x},t)\|_{H^s} \Bigg[& \\
& \epsilon A_F^{-1}(2L_{\mathrm{WFT}}/x_0)^{N/2}(2k_{\max}/k_0)^{N/2} \\
\times \Bigg(\Big[(1+T_{\mathrm{step}}\mathbf{G}e^{\mathbf{G}T_{\mathrm{step}}}) + 2\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}) \Big] & \sum_{n=0}^{M} \mathbf{L}((M-n)T_{\mathrm{step}}) \Bigg) \\
& + \epsilon A_F^{-1}(2L_{\mathrm{WFT}}/x_0)^{N/2}(2k_{\max}/k_0)^{N/2}(T_{\max}/T_{\mathrm{step}}) \\
& + \epsilon A_F^{-1}(2L_{\mathrm{NL}}/x_0)^{N/2}(2k_{\max,\mathrm{NL}}/k_0)^{N/2} \\
& \times \Bigg[(2+T_{\mathrm{step}}\mathbf{G}e^{\mathbf{G}T_{\mathrm{step}}}) \left(\sum_{n=0}^{M} \mathbf{L}((M-n)T_{\mathrm{step}}) \right) \\
& + (T_{\max}/T_{\mathrm{step}})\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}) \Bigg] \Bigg]
\end{aligned} \qquad (5.45)
$$

We observe that this is linear in ϵ. Thus, by making the choice:

$$
\begin{aligned}
\epsilon^{-1} = 2\tau^{-1} \sup_{t\in[0,T_{\max}]} \|\Psi(\vec{x},t)\|_{H^s} \Bigg[& \\
& A_F^{-1}(2L_{\mathrm{WFT}}/x_0)^{N/2}(2k_{\max}/k_0)^{N/2} \\
\times \Bigg(\Big[(1+T_{\mathrm{step}}\mathbf{G}e^{\mathbf{G}T_{\mathrm{step}}}) + 2\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}) \Big] & \sum_{n=0}^{M} \mathbf{L}((M-n)T_{\mathrm{step}}) \Bigg) \\
& + A_F^{-1}(2L_{\mathrm{WFT}}/x_0)^{N/2}(2k_{\max}/k_0)^{N/2}(T_{\max}/T_{\mathrm{step}}) \\
& + A_F^{-1}(2L_{\mathrm{NL}}/x_0)^{N/2}(2k_{\max,\mathrm{NL}}/k_0)^{N/2} \\
& \times \Bigg[(2+T_{\mathrm{step}}\mathbf{G}e^{\mathbf{G}T_{\mathrm{step}}}) \left(\sum_{n=0}^{M} \mathbf{L}((M-n)T_{\mathrm{step}}) \right) \\
& + (T_{\max}/T_{\mathrm{step}})\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}) \Bigg] \Bigg]
\end{aligned}
$$

we find that (5.44) $\leq$ (5.45) $\leq \tau/2$. This holds only of $\epsilon \leq \epsilon(\delta_{\mathrm{F}})$, with $\epsilon(\delta_{\mathrm{F}})$ defined in assumption 5.

Thus, by this choice of parameters, we have made the error smaller than τ.
□

Remark 5.17 The obvious way to make (5.43) small is to make the following choices for $k_{\min}$, $k_{\max}$, $L_{\rm NL}$, $k_{\max,\rm NL}$ and L_F:

$$L_{\rm NL} = L_{\rm NL}\left(\frac{\tau}{10\sup_{t\in[0,T_{\max}]}\|\Psi(\vec{x},t)\|_{H^s}} \times \frac{1}{T_{\rm step}\left(\sum_{n=0}^{M}\widehat{\mathcal{R}}((M-n)T_{\rm step})\right)(2+T_{\rm step}\mathbf{G}e^{\mathbf{G}T_{\rm step}})}\right) \tag{5.46a}$$

$$k_{\max,\rm NL} = k_{\max,\rm NL}\left(\frac{\tau}{10\sup_{t\in[0,T_{\max}]}\|\Psi(\vec{x},t)\|_{H^s}} \times \frac{1}{T_{\rm step}\left(\sum_{n=0}^{M}\widehat{\mathcal{R}}((M-n)T_{\rm step})\right)(2+T_{\rm step}\mathbf{G}e^{\mathbf{G}T_{\rm step}})}\right) \tag{5.46b}$$

$$L_F = L_F\left(\frac{\tau T_{\rm step}}{20T_{\max}\sup_{t\in[0,T_{\max}]}\|\Psi(\vec{x},t)\|_{H^s}}\right) \tag{5.46c}$$

$$k_{\min} = k_{\min}\left(\frac{\tau}{10(2+T_{\rm step}\mathbf{G}e^{\mathbf{G}T_{\rm step}})\left(\sum_{n=0}^{M}\mathbf{L}((M-n)T_{\rm step})\right)}\right) \tag{5.46d}$$

$$k_{\max} = k_{\max}\left(\frac{\tau T_{\rm step}}{10T_{\max}}\right) \tag{5.46e}$$

This particular choice ensures that each term on the right hand side of (5.43) is smaller than $\tau/10$. Since there are 5 terms on the right, the whole thing is less than $\tau/2$.

Although obvious and clearly effective, this choice is likely to be inefficient. Supposing one term to be significantly more expensive than the others (e.g. one term being polynomial in τ^{-1}, the rest being logarithmic), it makes more sense to make the expensive term only smaller than, e.g. $(1-\delta)\tau/2$, and make each of the others smaller than $\delta\tau/2$ (with $\delta \ll 1/2$).

Thus, although we illustrate that this can be done with (5.46), we emphasize that the exact method of satisfying (5.43) is strongly dependent on the particular model chosen.

Remark 5.18 To get from (5.44) to (5.45), we made use of the the weak form of proposition 5.8. That is to say, in the bounds on $\widehat{\mathcal{E}}(t)$, $\widehat{\mathcal{R}}(t)$ and $\widehat{\mathcal{Q}}(t)$, we had an intermediate estimate which appeared unwieldy. Nevertheless, the intermediate estimate is far sharper, and is the one that should be used in practice. We used the less sharp estimate simply to demonstrate that $\widehat{\mathcal{E}}(t)$, $\widehat{\mathcal{R}}(t)$ and $\widehat{\mathcal{Q}}(t)$ are quantities which we can make arbitrarily small.

5.4 Comments

5.4.1 Near Optimality of the Estimates

The estimates we give here are crude at some points, and can probably be improved significantly. However, in principle, we believe that a result of the form (5.39) is the best possible result one can hope for with our method, or any other method based on time stepping.

The reason for this is the following. Consider any numerical method based on time integration. Suppose that it makes an error (however small) at times t_0. This error has now been made, and it is highly unlikely that further errors will completely cancel it. Suppose after t_0, we have the ability to propagate further with no error (but we need to take the incorrect result $\Psi(x, t_0)$ as an initial condition). Then $\|\mathcal{U}(t)\psi(x, t_0) - \mathcal{U}(t)\Psi(x, t_0)\|_{H^s_b}$ is only bounded by $\mathbf{L}(t) \|\psi(x, t_0) - \Psi(x, t_0)\|_{H^s}$. Repeating this argument every time an error is made leads to a bound very similar to ours.

5.4.2 No Hierarchy of Boundaries

Unlike the Dirichlet-to-Neumann approach, the TDPSF is not embedded in a hierarchy of increasingly accurate boundary conditions. The reason for this is that we are not attempting to construct the exact solution on the boundary. Rather, we are merely assuming the wave behaves freely and semiclassically on the boundary, and filtering it based on this. Thus, apart from increasing w, we have little recourse to increase the accuracy of this method. So although our method is highly accurate, we can not increase the accuracy without bound while leaving the size of the box fixed.

5.4.3 Bourgain's Phenomenon

One potential difficulty in solving time dependent problems is that a problem which is stable on $\mathbb{R}^N$ may exhibit long time instability on a periodic boxes. Given a box $[-L_{\text{comp}}, L_{\text{comp}}]^N$ with periodic boundaries, Bourgain (c.f. [5]) has proven the existence of a time dependent potential $V(\vec{x}, t)$ which is smooth and well localized in $\vec{x}$ having the property that $\|\mathcal{U}_b(t)\psi_0\|_{H^s_b}$ grows logarithmically in time. This occurs because the time dependent potential essentially plays a quantum mechanical variant of "ping pong".

This suggests that some numerical methods might exhibit this long time instability if one attempt to solve (1.1) on $\mathbb{R}^N$ with such a potential. However, our method prevents this from occurring. We do this by periodically removing all framelets which move faster than $k_{\max}$ (since we filter off waves which are outside of NECC $\cap$ BB, and BB has no framelets with $\vec{b}k_0 \geq k_{\max}$).

5.4.4 Lack of Bounds on $k_{\min}$

Another potential difficulty comes from the fact that in general, one has no bounds on $k_{\min}$. We describe here a situation with a simple linear (time-dependent) potential for which $k_{\min}$ can be arbitrarily small while leaving the potential bounded and smooth in any reasonable norm.

Consider a nonlinearity of the form $g(t,\vec{x},\psi(\vec{x},t))\psi(\vec{x},t) = V(\vec{x},t)\psi(\vec{x},t)$. We suppose that $V(\vec{x},t)$ takes the form $V_0(x-(e/\omega^2)\cos(\omega t))$ for some smooth, rapidly decaying potential $V_0(x)$.

This system is equivalent, by a unitary gauge transformation, to the time dependent system with Hamiltonian $H(t) = -(1/2)\Delta + V_0(x) + e\cos(\omega t)\cdot x$ (c.f. [9], chapter 7).

Now, suppose further that the reference Hamiltonian $H_0 = -(1/2)\Delta + V_0(x)$ has a single bound state, having energy $-E_0$.

Consider an initial condition initially localized in this bound state.

In this case, Fermi's golden rule suggests that for e small and $\omega > |E_0|$, mass will be ejected from the bound state into the continuum[9], and will have energy $\omega - E_0$ after ejection. Thus, energy transitions from the bound state into frequencies localized near $\sqrt{\omega - E_0}$. By making ω sufficiently close to E_0, we can make this as small as possible.

Thus, in this scenario, $k_{\min} \ll \sqrt{\omega - E_0}$, i.e. $k_{\min}$ can be made as small as desired.

6 Lingering Waves (proof of theorem 5.12)

In this section, we construct a bound on the difference between the free propagator and the box propagator acting on waves which are not outgoing:

$$\|(\mathcal{U}(t) - \mathcal{U}_b(t)\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}\psi_0(x)\|_{H^s}$$

We do this by Duhamel's principle and Gronwall, and use the fact that the nonlinearity is locally Lipschitz (assumption 3). The bound on this term is summarized in theorem 5.12 in the next section.

We first define three functions, $E(t)$, $Q(t)$ and $Q_b(t)$ which we will use to construct error bounds.

Definition 6.1 *Let $\psi(\vec{x},t)$ be a solution to* (1.1) *on $\mathbb{R}^N$, and $\psi_b(\vec{x},t)$ be a solution to* (1.1) *on $[-L_{\mathrm{int}}, L_{\mathrm{int}}]^N$. Suppose that*

$$\psi(\vec{x},0) = \psi_b(\vec{x},0) = \mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}}\psi_0(x)$$

for some $\psi_0(x)$.

We define the free error function to be some function $E(t)$ for which:

$$\left\|(e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t})\psi(x,0)\right\|_{H^s_b} \leqslant E(t) \tag{6.1}$$

[9]This happens only generically. More precisely, it happens if $\langle u_0(x)|e\cdot xu(x,\omega - E_0)\rangle \neq 0$, where $u_0(x)$ is the bound state and $u(x,\omega - E_0)$ is the generalized eigenfunction at energy $\omega - E_0$.

We define the interaction error to be functions $Q(t)$ (or $Q_b(t)$) for which:

$$\left\| \int_0^t (e^{i(1/2)\Delta(t-t')} - e^{i(1/2)\Delta_b(t-t')}) g(t', \vec{x}, \psi(x,t'))\psi(x,t')dt' \right\|_{H_b^s} \leq Q(t) \quad (6.2a)$$

$$\left\| \int_0^t (e^{i(1/2)\Delta(t-t')} - e^{i(1/2)\Delta_b(t-t')}) g(t', \vec{x}, \psi_b(x,t'))\psi_b(x,t')dt' \right\|_{H_b^s} \leq Q_b(t) \quad (6.2b)$$

We will write our estimates in terms of these functions. We show that (5.37) is consistent with definition 6.1.

The rest of section 6 is devoted to proving various pieces of theorem 5.12. We prove (5.36) in section 6.1. The estimate (5.37a) is done in in section 6.2 (proposition 6.9) while (5.37b) is proved in section 6.3 (proposition 6.13).

6.1 Estimates in terms of $E(t)$, $Q(t)$

Here, we prove the estimates (5.36a) and (5.36b) assuming that $E(t)$ and $Q(t)$ are known.

We state the result in a more general manner, which we believe will also be useful for proving short time error bounds for other types of absorbing boundary conditions.

Theorem 6.2 *Let $\psi_0(x) \in H^s$. Let $g(t, \vec{x}, \cdot)$ satisfy assumption 3. Let $E(t)$ be defined by (6.1), and $Q(t), Q_b(t)$ by (6.2). Then the following holds:*

$$\|(\mathcal{U}(t) - \mathcal{U}_b(t))\psi_0(x)\|_{H_b^s} \leq (E(t)+Q(t)) + \mathbf{G}e^{\mathbf{G}t} \star (E(t)+Q(t)) \text{ (apriori)} \quad (6.3a)$$

$$\|(\mathcal{U}(t) - \mathcal{U}_b(t))\psi_0(x)\|_{H_b^s} \leq (E(t) + Q_b(t)) + \mathbf{G}e^{\mathbf{G}t} \star (E(t) + Q_b(t)) \text{ (aposteriori)} \quad (6.3b)$$

Lemma 6.3 (Gronwall) *Let $y(t)$ satisfy the inequality:*

$$y(t) \leq p(t) + C\int_0^t y(t)dt \quad (6.4)$$

$y(t)$ satisfies the bound:

$$y(t) \leq p(t) + Ce^{Ct}\int_0^t e^{-Cs}p(s)ds \quad (6.5)$$

Proof of Theorem 6.2. We use Duhamel. We observe the following equality:

$$\psi(t) - \psi_b(t) = e^{i(1/2)\Delta t}\varphi(x) - e^{i(1/2)\Delta_b t}\varphi(x) + i\int_0^t [e^{i(1/2)\Delta(t-s)}g(s,\vec{x},\psi(s))\psi(s) - e^{i(1/2)\Delta_b t-s}g(s,\vec{x},\psi_b(s))\psi_b(s)]ds$$

We then add and subtract $e^{i(1/2)\Delta(t-s)} g(s, \vec{x}, \psi_b(s))\psi_b(s)$ under the integral sign, and take norms in H^s to obtain:

$$\|\psi(t) - \psi_b(t)\|_{H^s_b} \leqslant E_s(t)$$
$$+ \left\| \int_0^t [e^{i(1/2)\Delta(t-s)} - e^{i(1/2)\Delta_b t - s}] g(s, \vec{x}, \psi_b(s))\psi_b(s) ds \right\|_{H^s_b} +$$
$$\left\| \int_0^t e^{i(1/2)\Delta(t-s)} [g(s, \vec{x}, \psi(s))\psi(s) - g(s, \vec{x}, \psi_b(s))\psi_b(s)] ds \right\|_{H^s_b}$$

We then observe that

$$\|g(s, \vec{x}, \psi(s))\psi(s) - g(s, \vec{x}, \psi_b(s))\psi_b(s)\|_{H^s} \leq \mathbf{G} \|\psi(s) - \psi_b(s)\|_{H^s}$$

and also that the first term is $Q_b(t)$. Gronwall's Lemma (6.3) gives us (6.3b). Estimate (6.3a) follows in much the same way, except that we add and subtract $e^{i(1/2)\Delta_b t - s} g(s, \vec{x}, \psi(s))\psi(s)$ instead. □

Proof of Lemma 6.3. In the case of equality, we have:

$$y(t) = p(t) + C \int_0^t y(t) dt$$

Laplace transformation yields:

$$Y(z) = P(z) - C \frac{Y(z)}{z}$$

Or equivalently:

$$Y(z) = \left(1 + \frac{C}{z + C}\right) P(z)$$

Inverting the Laplace transform and collecting residues yields the result we seek:

$$y(t) = e^{Ct} \int_0^t e^{-Cs} \frac{dp(s)}{ds} ds = p(t) + C e^{Ct} \int_0^t e^{-Cs} p(s) ds$$

□

In the event that $g(t, \vec{x}, \psi)\psi = V(x,t)\psi(x)$ a sharper estimate holds. This can not be shown to hold in the nonlinear case – indeed, counterexamples exist.

Theorem 6.4 *Let $\psi(x, t = 0) \in H^s$ be an initial condition of (1.1), where $g(t, \vec{x}, \psi)\psi = V(x,t)\psi(x)$ (that is, a "linear nonlinearity"). Suppose that the equation*

$$i\partial_t \psi_b(\vec{x}, t) = (-(1/2)\Delta_b + V(\vec{x}, t))\, \psi_b(\vec{x}, t)$$

satisfies the energy conservation law $\|\psi_b(x,t)\|_{H^s} \leqslant \alpha(t) \|\psi_b(x,0)\|_{H^s}$. Then we find:

$$\|\psi(\vec{x}, t) - \psi_b(\vec{x}, t)\|_{H^s_b}$$
$$\leq \alpha(t) \|\psi(x,0) - \psi_b(x,0)\|_{H^s_b} + \int_0^t \alpha(t - t') \|S(\vec{x}, t)\|_{H^s_b} dt' \quad (6.6)$$

where:

$$S(x,t) = \Big[(e^{i(1/2)\Delta_b t} - e^{i(1/2)\Delta t})\psi(x,0) \\ + i\int_0^t \left(e^{i(1/2)\Delta_b(t-t')} - e^{i(1/2)\Delta(t-t')}\right) V(x,t')\psi(x,t')dt\Big] \quad (6.7a)$$

$$s(x,t) = i\partial_t S(x,t) \quad (6.7b)$$

In particular, observe that $\|S(x,t)\|_{H^s} \leqslant E(t) + Q(t)$, so to bound the error, it is sufficient to construct $E(t)$ and $Q(t)$.

Proof. We write $\psi_b(x,t) = \psi(x,t) + e(x,t)$ where $e(x,t)$ is the error. We then subtract the Duhamel equation for $\psi_b(x,t)$ from the Duhamel equation for $\psi(x,t)$ to obtain:

$$e(x,t) = e^{i(1/2)\Delta_b(t-t')}e(x,0) + i\int_0^t e^{i(1/2)\Delta_b(t-t')}V(x,t')e(x,t')dt' \\ + (e^{i(1/2)\Delta_b t} - e^{i(1/2)\Delta t})\psi(x,0) \\ + i\int_0^t \left(e^{i(1/2)\Delta_b(t-t')} - e^{i(1/2)\Delta(t-t')}\right) V(x,t')\psi(x,t')dt'$$

If we apply $i\partial_t$ to this equation, we observe that:

$$i\partial_t e(x,t) = \left(-(1/2)\Delta_b + V(x,t)\right)e(x,t) + S(x,t)$$

Taking norms and bringing them under the integral sign gives us the result we seek. □

6.2 Bounds on $E(t)$

Here, the bound (5.37a) on $E(t)$ is constructed from the framelet decomposition and the fact that $\psi(x,0)$ is given by framelets which are in NECC $\cap$ BB. We further split this up into framelets which are in BAD$^C \cap$ NECC $\cap$ BB and BAD $\cap$ NECC $\cap$ BB. We then add the results together to obtain the estimate.

Lemma 6.5 *Let $\{\phi_j\}$ be a frame with frame bounds A_F, B_F and with per-framelet error bounds $\{\mathcal{E}_j^s(t)\}$. Suppose J is a finite set of framelet indices. Then:*

$$\left\|(e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t})\sum_{j\in J}\psi_j\phi_j(x)\right\|_{H^s} \leq \sum_{j\in J}|\psi_j|\,\mathcal{E}_j^s(t) \\ \leq A_F^{-1}\sqrt{\sum_{j\in J}\left|\mathcal{E}_j^s(t)\right|^2}\,\|\psi\|_{L^2} \leq A_F^{-1}\sqrt{|J|}\sup_{j\in J}\mathcal{E}_j^s(t)\,\|\psi\|_{L^2} \quad (6.8)$$

Here, $|J|$ represents the cardinality of J. The same result holds if we replace $(e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t})$ by $\chi_{[-L_{\text{int}},L_{\text{int}}]^N}e^{i(1/2)\Delta t}$ and $\mathcal{E}_j^s(t)$ by $\mathcal{R}_j^s(t)$.

Proof. The triangle inequality yields:

$$\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \sum_{j \in J} \psi_j \phi_j(x) \right\|_{H^s} \leqslant \sum_{j \in J} |\psi_j| \, \mathcal{E}_j^s(t)$$

We have a sharp bound:

$$\leqslant \sum_{j \in J} |\psi_j| \, \mathcal{E}_j^s(t) \leq \sqrt{\sum_{j \in J} |\psi_j|^2} \sqrt{\sum_{j \in J} \left| \mathcal{E}_j^s(t) \right|^2} \leq A_F^{-1} \left\| \psi \right\|_{L^2} \sqrt{\sum_{j \in J} \left| \mathcal{E}_j^s(t) \right|^2}$$

We obtain a suboptimal (although still reasonably useful) bound:

$$\sqrt{\sum_{j \in J} \left| \mathcal{E}_j^s(t) \right|^2} \leq \sqrt{|J|} \sup_{j \in J} \mathcal{E}_j^s(t)$$

This yields the result we seek. The proof with $\mathcal{R}_j^s(t)$ instead of $\mathcal{E}_j^s(t)$ is identical, but with $e^{i(1/2)\Delta t}$ replacing $(e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t})$. □

Remark 6.6 For practical purposes, the estimate $\sqrt{\sum_{j \in J} \left| \mathcal{E}_j^s(t) \right|^2}$ should be used rather than $A_F^{-1} \sqrt{|J|} \sup_{j \in J} \mathcal{E}_j^s(t) \left\| \psi \right\|_{L^2}$. For any given set of parameters it is simple to compute, and gives a precise estimate (which does not grow with L). The cruder estimate is included to demonstrate that the estimate is nontrivial.

We now apply lemma 6.5 to obtain the following result dealing with framelets in $\mathrm{NECC} \cap \mathrm{BB} \cap \mathrm{BAD}^C$.

Proposition 6.7 *Let $\psi_0(x)$ satisfy assumption 2. Then we find:*

$$\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \mathcal{P}_{\mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \psi_0(x) \right\|_{H_b^s} \leq \widehat{\mathcal{E}}(t) \left\| \psi \right\|_{L^2} \tag{6.9}$$

Proof. Compute:

$$\begin{aligned}
&\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \sum_{(\vec{a},\vec{b}) \in \mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \psi_{0(\vec{a},\vec{b})} \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H_b^s} \\
&\quad \leq \sum_{(\vec{a},\vec{b}) \in \mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \left| \psi_{0(\vec{a},\vec{b})} \right| \left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H_b^s} \\
&\quad \leq \sqrt{\sum_{(\vec{a},\vec{b}) \in \mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \mathcal{E}_{(\vec{a},\vec{b})}(t)^2} \\
&\quad \times \sqrt{\sum_{(\vec{a},\vec{b}) \in \mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \left| \psi_{0(\vec{a},\vec{b})} \right|^2} \leq \widehat{\mathcal{E}}(t) \left\| \psi_0 \right\|_{L^2}
\end{aligned}$$

Here we used the fact that

$$\sqrt{\sum_{(\vec{a},\vec{b})\in \mathrm{BAD}^C \cap \mathrm{NECC} \cap \mathrm{BB}} \left| \psi_{0\,(\vec{a},\vec{b})} \right|^2} \leq A_F^{-1} \left\| \psi_0 \right\|_{L^2}$$

and the definition of $\widehat{\mathcal{E}}(t)$ (definition 5.7 on page 63). □

Proposition 6.8 *Let the parameters* $k_{\min}$, w *and* T_{step} *satisfy* (5.35). *Let* $\psi_0(x)$ *satisfy assumption 6. Then the following estimate holds:*

$$\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \mathcal{P}_{\mathrm{BAD} \cap \mathrm{NECC} \cap \mathrm{BB}} \psi_0(x) \right\|_{H_b^s} \leq 2\delta_{\min} \tag{6.10}$$

This result is slightly trickier, and subsubsection 6.2.1 is devoted to the proof. We now arrive at the bound on $E(t)$:

Proposition 6.9 *Let* $\psi_0(x)$ *satisfy assumption 6, and let* L_{int}, T_{step} *and* w *satisfy* (5.35). *Then:*

$$\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \mathcal{P}_{\mathrm{BB} \cap \mathrm{NECC}} \psi_0(x) \right\|_{H_b^s} \leq \widehat{\mathcal{E}}(t) \left\| \psi_0(x) \right\|_{L^2} + 2\delta_{\min} = E(t) \tag{6.11}$$

Proof. Observe that

$$\mathcal{P}_{\mathrm{BB} \cap \mathrm{NECC}} \psi_0(x) = \mathcal{P}_{\mathrm{BAD} \cap \mathrm{BB} \cap \mathrm{NECC}} \psi_0(x) + \mathcal{P}_{\mathrm{BAD}^C \cap \mathrm{BB} \cap \mathrm{NECC}} \psi_0(x) \tag{6.12}$$

We therefore apply $(e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t})$ to (6.12), then take the norm in H_b^s and use the triangle inequality, to obtain:

$$\begin{aligned} &\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \mathcal{P}_{\mathrm{BB} \cap \mathrm{NECC}} \psi_0(x) \right\|_{H_b^s} \\ &\quad \leq \left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \mathcal{P}_{\mathrm{BAD} \cap \mathrm{BB} \cap \mathrm{NECC}} \psi_0(x) \right\|_{H_b^s} \\ &\quad\quad + \left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \mathcal{P}_{\mathrm{BAD}^C \cap \mathrm{BB} \cap \mathrm{NECC}} \psi_0(x) \right\|_{H_b^s} \end{aligned} \tag{6.13}$$

Then apply proposition 6.7 to the last term and proposition 6.8 to the first term on the right side of (6.13). □

6.2.1 Slowly Moving Waves

We now prove proposition 6.8.

The idea of the proof is to show that for any $(\vec{a},\vec{b}) \in \mathrm{BAD} \cap \mathrm{NECC} \cap \mathrm{BB}$, $(\vec{a},\vec{b})$ satisfies (5.7). This, combined with $\mathrm{BAD} \cap \mathrm{NECC} \cap \mathrm{BB}$ implies that:

$$\left\| \mathcal{P}_{\mathrm{BAD} \cap \mathrm{NECC} \cap \mathrm{BB}} \psi_0(x) \right\|_{H_b^s} \leq \delta_{\min}$$

Thus we need only prove that $(\vec{a}, \vec{b}) \in \mathrm{BAD} \cap \mathrm{NECC} \cap \mathrm{BB}$ satisfies (5.7).

We prove first a technical lemma, showing that a given framelet is either incoming or outgoing (not both) if it has velocity sufficiently fast.

Lemma 6.10 *Assume that w, T_{step} satisfy* (5.35b) *and* (5.35c). *Then for*

$$(\vec{a}x_0, \vec{b}k_0) \in [-(L_{\text{int}} + w/3), (L_{\text{int}} + w/3)]^N \times [-k_{\max}, k_{\max}]^N,$$

we find that $(\vec{a}, \vec{b}) \notin \mathrm{BAD}(\epsilon, s, T_{\text{step}})$.

Proof. By lemma 4.9, it suffices to show that $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon, t) \subset [-(L_{\text{int}} + w), (L_{\text{int}} + w)]^N$.

Note that:

$$\begin{aligned}\vec{a}x_0 + \vec{b}k_0 t &\in [-(L_{\text{int}} + w/3 + k_{\max}t), (L_{\text{int}} + w/3 + k_{\max}t)]^N \\ &\subseteq [-(L_{\text{int}} + w/3 + k_{\max}T_{\text{step}}), (L_{\text{int}} + w/3 + k_{\max}T_{\text{step}})]^N\end{aligned}$$

Consider $\vec{x} \in \mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon, t)$. By definition 4.7 (the definition of $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon, t)$), we find that:

$$|\vec{x} - \vec{a}x_0 + \vec{b}k_0 t|_2 \leq \mathbf{w}_i^s(\vec{b}, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)t$$

Thus, since $\vec{a}x_0 + \vec{b}k_0 t \in [-(L_{\text{int}} + w/3 + k_{\max}T_{\text{step}}), (L_{\text{int}} + w/3 + k_{\max}T_{\text{step}})]^N$, and $\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon, t)$ is contained in a ball of radius $\mathbf{w}_i^s(\vec{b}, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)T_{\text{step}}$ about $\vec{a}x_0 + \vec{b}k_0 t$, we find that:

$$\begin{aligned}\mathrm{BB}_{(\vec{a},\vec{b},\sigma)}(\varepsilon, t) \subseteq [&-(L_{\text{int}} + w/3 + k_{\max}T_{\text{step}} + \mathbf{w}_i^s(\vec{b}, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)T_{\text{step}}), \\ &(L_{\text{int}} + w/3 + k_{\max}T_{\text{step}} + \mathbf{w}_i^s(\vec{b}, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)T_{\text{step}})]^N\end{aligned}$$

Then applying (5.35b) and (5.35c), we find that:

$$\begin{aligned}&[-(L_{\text{int}} + w/3 + k_{\max}T_{\text{step}} + \mathbf{w}_i^s(\vec{b}, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)T_{\text{step}}), \\ &(L_{\text{int}} + w/3 + k_{\max}T_{\text{step}} + \mathbf{w}_i^s(\vec{b}, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)T_{\text{step}})]^N \subseteq [-(L_{\text{int}} + w), (L_{\text{int}} + w)]^N\end{aligned}$$

Lemma 4.9 implies the result we seek. □

Lemma 6.11 *Assume w and T_{step} satisfy* (5.35b) *and* (5.35c).

Fix $(\vec{a}, \vec{b}) \in \mathbb{Z}^N \times \mathbb{Z}^N$. Suppose that $(\vec{a}, \vec{b})$ satisfies:

$$\exists j \in 1 \ldots N, |\vec{a}_j x_0| \geq L_{\min} \text{ and } \vec{b}_j k_0(\vec{a}_j / |\vec{a}_j|) > k_{\min} \tag{6.14}$$

Suppose also that L_{int}, w and $L_{\min}$ satisfy (5.35h), *that is $L_{\min} \geq L_{\text{int}} + w/3$.*

Then $(\vec{a}, \vec{b}) \notin \mathrm{NECC}(\epsilon, s, \infty)$.

Proof. For the duration of this proof, let j denote the (possibly nonunique) index j for which (6.14) holds.

Note that by (5.35b) and (5.35h), we find that $|\vec{a}_j x_0| \geq L_{\text{int}} + w/3$. For simplicity, suppose that $\vec{a}_j > 0$, and therefore that $\vec{b}_j > 0$.

Then note that:

$$\vec{a}_j x_0 + \vec{b} k_0 t \geq (L_{\text{int}} + w/3) + \mathbf{w}_v^s(\vec{b}, \epsilon) t$$

The constant term was obtained by using (5.35h) while the t term was obtained using (5.35a).

Thus, we find that:

$$d(\vec{a}x_0 + \vec{b}k_0 t, [-L_{\text{int}}, L_{\text{int}}]^N) \geq w/3 + \mathbf{w}_v^s(\vec{b}, \epsilon)t \geq \mathbf{w}_i^s(vb, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)t$$

The last inequality follows by applying (5.35b). Applying lemma 4.10 implies that $(\vec{a}, \vec{b}) \notin$ NECC. □

Proof of proposition 6.8. We now wish to show that:

$$\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \mathcal{P}_{\text{BAD} \cap \text{NECC} \cap \text{BB}} \psi_0(x) \right\|_{H_b^s} \leq 2\delta_{\min} \tag{6.15}$$

We do this by showing that BAD ∩ NECC ∩ BB is a set which satisfies (5.7).

Fix $(\vec{a}, \vec{b}) \in$ BAD ∩ NECC ∩ BB. Note that since $(\vec{a}, \vec{b}) \in$ BB, we find that $|\vec{b}k_0|_\infty \leq k_{\max}$.

Applying the converse of lemma 6.10, we find that $|\vec{a}x_0|_\infty \geq L_{\text{int}} + w/3$.

Now suppose $(\vec{a}, \vec{b})$ satisfies (6.14). Then:

$$(\vec{a}, \vec{b}) \notin \text{NECC}(\epsilon, s, \infty) \supseteq \text{BAD} \cap \text{NECC} \cap \text{BB}$$

Thus, if $(\vec{a}, \vec{b}) \in$ BAD ∩ NECC ∩ BB, we find that:

$$!(\exists j \in 1 \ldots N, |\vec{a}_j x_0| \geq L_{\min} \text{ and } \vec{b}_j k_0 (\vec{a}_j / |\vec{a}_j|) > k_{\min})$$

This implies that BAD ∩ NECC ∩ BB is a set satisfying (5.7). Hence:

$$\left\| (e^{i(1/2)\Delta t} - e^{i(1/2)\Delta_b t}) \mathcal{P}_{\text{BAD} \cap \text{NECC} \cap \text{BB}} \psi_0(x) \right\|_{H_b^s} \leq 2 \left\| \mathcal{P}_{\text{BAD} \cap \text{NECC} \cap \text{BB}} \psi_0(x) \right\|_{H_b^s} \leq 2\delta_{\min}$$

Thus, we have proved proposition 6.8. □

6.3 Bounds on $Q(t)$

We now attempt to determine bounds on $Q(t)$ and $Q_b(t)$ based on apriori and aposteriori knowledge of $\psi(x,t)$ and $g(t, \vec{x}, \cdot)$. This is where we use assumption 4.

The main tool is phase space localization based on the WFT and assumption 4. In particular, we wish to treat $g(t, \vec{x}, \psi(t))\psi(t)$ as a source term and then figure out how much of it's mass can leave $[-L_{\text{int}}, L_{\text{int}}]^N$. We will decompose $\mathbb{Z}^N \times \mathbb{Z}^N = \text{NL} \cup \text{NL}^C$ (with the set NL defined as in assumption 4), and write:

$$g(t, \vec{x}, \psi)\psi = \sum_{(\vec{a}, \vec{b}) \in \text{NL}} g_{(\vec{a}, \vec{b})}(t)\phi_{(\vec{a}, \vec{b})}(\vec{x}) + \sum_{(\vec{a}, \vec{b}) \in \text{NL}^C} g_{(\vec{a}, \vec{b})}(t)\phi_{(\vec{a}, \vec{b})}(\vec{x})$$

The last term is small by assumption 4. We now come up with sufficient conditions on L_{int} and T_{step} (depending on $k_{\max,\text{NL}}$ and L_{NL}) so that framelets in NL are not bad.

Proposition 6.12 *Let T_{step}, L_{int} satisfy* (5.35e), (5.35f) *and* (5.35g). *Then* $\text{NL} \cap \text{BAD}(\epsilon, s, T_{\text{step}}) = \emptyset$.

Proof. Fix $(\vec{a}, \vec{b}) \in \text{NL}$.

Note that $\text{BB}_{(\vec{a}, \vec{b}, \sigma)}(\varepsilon, t)$ is a ball of radius $\mathbf{w}_i^s(\vec{b}, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)t$ around the point $\vec{a}x_0 + \vec{b}k_0 t$. Thus, if $\vec{x} \in \text{BB}_{(\vec{a}, \vec{b}, \sigma)}(\varepsilon, t)$, then:

$$\begin{aligned}
|\vec{x}|_\infty \leq |\vec{a}x_0|_\infty + |\vec{b}k_0|_\infty t + \mathbf{w}_i^s(\vec{b}, \epsilon) + \mathbf{w}_v^s(\vec{b}, \epsilon)t \\
\leq L_{\text{int}} + k_{\max,\text{NL}} T_{\text{step}} + w/2 + \mathbf{w}_v^s(\vec{b}, \epsilon) T_{\text{step}} \\
\leq L_{\text{int}} + w/2 + (L_{\text{int}} + w/2 - L_{\text{NL}})
\end{aligned}$$

This calculation follows by applying (5.35e) to $(k_{\max,\text{NL}} + \mathbf{w}_v^s(\vec{b}, \epsilon))T_{\text{step}}$ and (5.35g) to $\mathbf{w}_i^s(\vec{b}, \epsilon)$.

Note that (5.35f) is needed only to insure that (5.35e) is possible to satisfy, i.e. that $L_{\text{int}} - L_{\text{NL}} > 0$.

This implies that $\vec{x} \in [-(L_{\text{int}} + w), (L_{\text{int}} + w)]^N$, hence

$$\text{BB}_{(\vec{a}, \vec{b}, \sigma)}(\varepsilon, t) \subset [-(L_{\text{int}} + w), (L_{\text{int}} + w)]^N$$

Applying lemma 4.9 implies that $(\vec{a}, \vec{b}) \notin \text{BAD}(\epsilon, s, T_{\text{step}})$. The only assumption on $(\vec{a}, \vec{b})$ was $(\vec{a}, \vec{b}) \in \text{NL}$, hence $\text{NL} \cap \text{BAD}(\epsilon, s, T_{\text{step}}) = \emptyset$. □

We can now compute a bound on $Q(t)$ for $Q(t)$ satisfying assumption 4.

Proposition 6.13 *Let $g(t, \vec{x}, \psi)\psi$ satisfy assumption 4. Suppose that L_{int} and T_{step} satisfy* (5.35e), (5.35f) *and* (5.35g). *Then $Q(t)$ satisfies:*

$$Q(t) \leq (\widehat{\mathcal{Q}}(t)\mathbf{G} + t\delta_{\text{NL}}) \sup_{t' \in [0,t]} \|\psi(x, t')\|_{H^s} \tag{6.16}$$

Proof. We note that:

$$\left\| \int_0^t (e^{i(1/2)\Delta(t-t')} - e^{i(1/2)\Delta_b(t-t')}) g(t,\vec{x},\psi(\vec{x},t'))\psi(\vec{x},t')dt' \right\|_{H_b^s}$$
$$\leq \int_0^t \left\| (e^{i(1/2)\Delta(t-t')} - e^{i(1/2)\Delta_b(t-t')}) \sum_{(\vec{a},\vec{b})\in \mathrm{NL}} g_{(\vec{a},\vec{b})}(t)t')\phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H_b^s} dt'$$
$$+ \int_0^t \left\| (e^{i(1/2)\Delta(t-t')} - e^{i(1/2)\Delta_b(t-t')}) \sum_{(\vec{a},\vec{b})\in \mathrm{NL}^C} g_{(\vec{a},\vec{b})}(t)t')\phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H_b^s} dt'$$

By assumption 4, for any fixed t, the last term satisfies:

$$\left\| (e^{i(1/2)\Delta(t-t')} - e^{i(1/2)\Delta_b(t-t')}) \sum_{(\vec{a},\vec{b})\in \mathrm{NL}^C} g_{(\vec{a},\vec{b})}(t)t')\phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H_b^s}$$
$$\leq 2\delta_{\mathrm{NL}} t \sup_{t'\in[0,t]} \|\psi(x,t')\|_{H^s} \quad (6.17)$$

The first term satisfies (at each fixed $t \leq T_{\mathrm{step}}$):

$$\left\| (e^{i(1/2)\Delta(t-t')} - e^{i(1/2)\Delta_b(t-t')}) \sum_{(\vec{a},\vec{b})\in \mathrm{NL}} g_{(\vec{a},\vec{b})}(t)t')\phi_{(\vec{a},\vec{b})}(\vec{x}) \right\|_{H_b^s}$$
$$\leq \|g(t,\vec{x},\psi(\vec{x},t))\psi(\vec{x},t)\|_{L^2} A_F^{-1} \sqrt{\sum_{(\vec{a},\vec{b})\in \mathrm{NL}} \left|\mathcal{E}_{(\vec{a},\vec{b})}(t)\right|^2}$$
$$\leq \mathbf{G} \|\psi(\vec{x},t)\|_{H^s} A_F^{-1} \sqrt{\sum_{(\vec{a},\vec{b})\in \mathrm{NL}} \left|\mathcal{E}_{(\vec{a},\vec{b})}(t)\right|^2}$$

We then integrate this result over time:

$$\int_0^t \mathbf{G} \|\psi(\vec{x},t)\|_{H^s} A_F^{-1} \sqrt{\sum_{(\vec{a},\vec{b})\in \mathrm{NL}} \left|\mathcal{E}_{(\vec{a},\vec{b})}(t)\right|^2}$$
$$\leq \mathbf{G} t \sup_{t'\in[0,t]} \|\psi(\vec{x},t)\|_{H^s} A_F^{-1} \sqrt{\sum_{(\vec{a},\vec{b})\in \mathrm{NL}} \left|\mathcal{E}_{(\vec{a},\vec{b})}(t)\right|^2} = \mathbf{G} \|\psi(\vec{x},t)\|_{H^s} \widehat{\mathcal{Q}}(t) \quad (6.18)$$

Adding (6.17) and (6.18) yields the result we seek. $\square$

7 Exterior Waves

In this section, we prove theorems 5.10 and 5.11.

We first prove a technical result, that the waves outside $[-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N$ and also the waves of high frequency are small. We will use this result in the proof of both theorem 5.10 and 5.11.

Now we will show that $f(x)$ is localized. We assume throughout this section that $f(x)=\mathcal{U}(T_{\text{step}})\mathcal{P}_{\text{NECC}\cap\text{BB}}h(x)$ for some $h(x)\in H^s$.

Proposition 7.1 *The following inequality holds.*

$$\|f(x)\|_{H^s(\mathbb{R}^N\setminus[-L_{\text{comp}},L_{\text{comp}}]^N)} \leq \widehat{\mathcal{E}}(T_{\text{step}})\,\|h(x)\|_{L^2}+\widehat{\mathcal{Q}}(T_{\text{step}}) \tag{7.1}$$

where $E(t)$ and $Q(t)$ are given by (5.37a) *and* (5.37b) *with $h(x)$ replacing $\psi(x)$.*

Proof. Recall that the per-framelet error functions, used to construct $\widehat{\mathcal{E}}(t)\,\|h(x)\|_{L^2}$ and $\widehat{\mathcal{Q}}(t)$ are nothing more than the mass (in H^s) outside $[-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N$. Thus, the proofs of propositions 6.9 and 6.13 apply without change, and we can merely add $\widehat{\mathcal{E}}(T_{\text{step}})\,\|h(x)\|_{L^2}$ and $\widehat{\mathcal{Q}}(T_{\text{step}})$ to get our bound. □

Proposition 7.2 *The framelet coefficients of $f(x)$ satisfy:*

$$\|\mathcal{P}_{\text{BB}^C}f(x)\|_{H^s} \leq \mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2})[\widehat{\mathcal{E}}(T_{\text{step}})\,\|h(x)\|_{L^2}+\widehat{\mathcal{Q}}(T_{\text{step}})+\epsilon]+\delta_{\max} \tag{7.2}$$

Proof. Note that BB^C Cconsists of framelets moving faster than $k_{\max}$, or outside the region $[-L_{\text{comp}},L_{\text{comp}}]^N$. We apply corollary 3.21.

Assumption 2 can be invoked to bound $\left\|\mathcal{P}_{\text{HF}(k_{\max})}f(x)\right\|_{H^s}$ by $\delta_{\max}$. To bound the spatial component, we apply proposition 7.1.

$$\begin{aligned}\|\mathcal{P}_{\text{BB}}f(x)\|_{H^s} \leq \mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2})[E(T_{\text{step}})+Q(T_{\text{step}})+\epsilon]\\ +\left\|\mathcal{P}_{\text{HF}(k_{\max})}f(x)\right\|_{H^s}\end{aligned} \tag{7.3}$$

□

7.1 Outgoing Waves (Proof of theorem 5.10)

In this section we prove theorem 5.10, concerning the outgoing wave term:

$$\|\mathcal{U}(t|f)\mathcal{P}_{\text{NECC}^C}f(x)\|_{H_b^s}$$

Our goal is to show that because the waves are outgoing, this term remains small for a long time. The function $f(x)$ will be assumed to satisfy assumptions 2, and also satisfy the assumption that $f(x)=\mathcal{U}(t)\mathcal{P}_{\text{NECC}\cap\text{BB}}h(x)$.

This is where we use assumption 5. Assumption 5 states that:

$$\|\mathcal{U}(t|f)\mathcal{P}_{\text{NECC}^C}f(x)\|_{H_b^s} \leq \delta_{\text{F}}\,\|\mathcal{P}_{\text{NECC}^C}f(x)\|_{H_b^s}$$

We first add and subtract $e^{i(1/2)\Delta t}\mathcal{P}_{\mathrm{NECC}} f$ under the norm, and apply the triangle inequality:

$$\begin{aligned}
\|\mathcal{U}(t|f)\mathcal{P}_{\mathrm{NECC}^C} f(x)\|_{H^s_b} \\
&\leq \left\|\mathcal{U}(t)\mathcal{P}_{\mathrm{NECC}^C} f(x) - e^{i(1/2)\Delta t}\mathcal{P}_{\mathrm{NECC}^C} f(x)\right\|_{H^s_b} \\
&\quad + \left\|e^{i(1/2)\Delta t}\mathcal{P}_{\mathrm{NECC}^C} f(x)\right\|_{H^s_b} \qquad (7.4)
\end{aligned}$$

The first term is bounded by $\delta_{\mathrm{F}} \|\mathcal{P}_{\mathrm{NECC}^C} f(x)\|_{H^s}$, by assumption 5. This is true provided $L_{\mathrm{int}} \geq L_F$, since in this case

$$\left\|e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{H^s([-L_F,L_F]^N)} \leq \left\|e^{i(1/2)\Delta t}\phi_{(\vec{a},\vec{b})}(\vec{x})\right\|_{H^s([-L_{\mathrm{int}},L_{\mathrm{int}}]^N)} \leq \varepsilon$$

for any $(\vec{a},\vec{b}) \in \mathrm{NECC}^C$.

Thus we need only compute a bound on $\left\|e^{i(1/2)\Delta t}\mathcal{P}_{\mathrm{NECC}^C} f(x)\right\|_{H^s_b}$.We break up $\mathcal{P}_{\mathrm{NECC}^C} f(x)$ further:

$$\mathcal{P}_{\mathrm{NECC}^C} f(x) = \mathcal{P}_{\mathrm{NECC}^C \cap \mathrm{HF}(k_{\max}) \cup B} f(x) + \mathcal{P}_{\mathrm{NECC}^C \cap (\mathrm{HF}(k_{\max}) \cup B)^C} f(x)$$

Proposition 7.2 provides a bound on the first term. To bound the second, we need merely count the framelets in $(\mathrm{HF}(k_{\max}) \cup B)^C$ and apply lemma 6.5.

We observe that B^C consists only of framelets with $|\vec{a}|_\infty x_0 \leq L_{\mathrm{comp}} + \mathbf{X}^s(\epsilon, k_{\max})$, while $\mathrm{HF}(k_{\max})^C$ consists only of framelets with $\left|\vec{b}\right|_\infty x_0 \leq k_{\max}$. It is easy to see that there are only $(2k_{\max}/k_0)^N(2[L_{\mathrm{comp}} + \mathbf{X}^s(\epsilon, k_{\max})]/x_0)^N$ such framelets. Thus, we obtain the result of theorem 5.10:

$$\begin{aligned}
\|\mathcal{U}(t|f)\mathcal{P}_{\mathrm{NECC}^C} f(x)\|_{H^s_b} &\leq \delta_{\mathrm{F}} \|\mathcal{P}_{\mathrm{NECC}^C} f(x)\|_{H^s_b} \\
&\quad + \mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})[E(T_{\mathrm{step}}) + Q(T_{\mathrm{step}}) + \epsilon] + \delta_{\max} \\
&\quad + A_F^{-1}\left(\sum_{(\vec{a},\vec{b})\in \mathrm{NECC}^C \cap (\mathrm{HF}(k_{\max})\cup B)^C} \left|\mathcal{R}_{(\vec{a},\vec{b})}(s)t\right|^2\right)^{1/2} \|f(x)\|_{L^2} \\
&= \delta_{\mathrm{F}} \|\mathcal{P}_{\mathrm{NECC}^C} f(x)\|_{H^s_b} + \widehat{\mathcal{R}}(t) \|f(x)\|_{L^2} \\
&\quad + \mathbf{H}^s_+(\tilde{g}(\vec{x}))\mathbf{H}^{-s}_+(e^{-x^2/\sigma^2})[\widehat{\mathcal{E}}(T_{\mathrm{step}}) \|h(x)\|_{L^2} + \widehat{\mathcal{Q}}(T_{\mathrm{step}}) + \epsilon] + \delta_{\max} \qquad (7.5)
\end{aligned}$$

Here, we used definition of $\widehat{\mathcal{R}}(t)$ to simplify the inequality.

7.2 Residual Waves

In this section, we wish to show that

$$\|\mathcal{U}(t)\mathcal{P}_{\mathrm{NECC}} f(x) - \mathcal{U}(t)\mathcal{P}_{\mathrm{NECC}\cap \mathrm{BB}} f(x)\|_{H^s_b} = \left\|\mathcal{U}(t)\mathcal{P}_{\mathrm{NECC}\setminus \mathrm{BB}} f(x)\right\|_{H^s_b}$$

is small, provided $f(x) = \Psi(x, nT_{\text{step}})$ for some n.

The residual waves consist of waves which are located outside the box, but are moving in a direction that will take them into the box at some future point. They can be thought of as outgoing waves that have turned around outside the box, and are returning.

Remark 7.3 This proof does not use the fact that the waves are off the propagation set. It merely uses the fact that BB^C consists of framelets which are localized outside the box, and it takes a moderate amount of time to reach them.

Proof of theorem 5.11. By proposition 7.2, and the observation that

$$\mathrm{NECC} \setminus \mathrm{BB} \subset \mathrm{BB}^C$$

we observe that:

$$\begin{aligned}
&\left\|\mathcal{P}_{\mathrm{NECC}\setminus\mathrm{BB}} f(x)\right\|_{H^s} \\
&\qquad \leq \mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2})[E(T_{\text{step}}) + Q(T_{\text{step}}) + \epsilon] \\
&\qquad\qquad + \left\|\mathcal{P}_{\mathrm{HF}(k_{\max})} f(x)\right\|_{H^s}
\end{aligned}$$

We then observe that:

$$\begin{aligned}
&\|\mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}} f)\mathcal{P}_{\mathrm{NECC}} f(x) - \mathcal{U}(t|\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}})\mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}} f(x)\|_{H_b^s} \\
&\qquad \leq \mathbf{L}(t)\,\|\mathcal{P}_{\mathrm{NECC}} f(x) - \mathcal{P}_{\mathrm{NECC}\cap\mathrm{BB}} f(x)\|_{H_b^s} \\
&\qquad \leq \mathbf{L}(t)\Big(\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2})[E(T_{\text{step}}) + Q(T_{\text{step}}) + \epsilon] \\
&\qquad\qquad + \left\|\mathcal{P}_{\mathrm{HF}(k_{\max})} f(x)\right\|_{H^s}\Big)
\end{aligned}$$

This is the result we seek, after substituting the definitions of $E(T_{\text{step}})$ and $Q(T_{\text{step}})$ in. □

8 Validation of the Assumptions: Some Simple Examples

In this section we verify that the assumptions hold for certain common examples.

8.1 Time Independent Potentials

In this section, we consider the case where $g(t, \vec{x}, \psi(\vec{x}, t))\psi(\vec{x}, t)$ is merely a time independent linear potential. That is, $g(t, \vec{x}, \psi(\vec{x}, t))\psi(\vec{x}, t) = V(x)\psi(\vec{x}, t)$ for $V(x)$ an analytic, short range potential which is real-valued. More precisely, we demand the following:

$$\left|\partial_x^j V(x)\right| \leq C_V \langle x \rangle^{-(1+\beta)} \tag{8.1a}$$

$$\hat{V}(k) \leq C'_V e^{-\alpha|\vec{k}|} \tag{8.1b}$$

Assumption 1

This follows trivially from standard functional analysis. The operator $H = -(1/2)\Delta + V(x)$ is self adjoint and bounded below, so e^{iHt} is an isometric semigroup on L^2. Thus, the solution exists and is unique. This also implies that $\mathbf{L}(t) = 1$.

Assumption 2

This assumption holds due to conservation of energy, which allows us to prove that $\|\psi(\vec{x},t)\|_{H^1}$ is bounded.

Lemma 8.1 *We have the following bound on* $\|\psi(\vec{x},t)\|_{H^1}$*:*

$$\|\psi(\vec{x},t)\|_{H^1} \leq \sqrt{2}\sqrt{|E_0| + \|\psi(x,0)\|_{L^2}^2 \left(\|V(x)\|_{L^\infty} + 1/2\right)} \tag{8.2}$$

E_0 *is the energy of the system, i.e.* $E_0 = \langle \psi(x,0) | H_0 \psi(x,0)\rangle$.

Proof. Since $V(x)$ is real valued, (1.1) becomes a Hamiltonian system. Thus, $\langle \psi(\vec{x},t) | H\psi(\vec{x},t)\rangle$ is a conserved quantity. Therefore:

$$\langle \psi(\vec{x},t)| - (1/2)\Delta\psi(\vec{x},t)\rangle = \langle \psi(x,0)|H\psi(x,0)\rangle - \langle\psi(\vec{x},t)|V(x)\psi(\vec{x},t)\rangle$$

Multiplying by 2, adding $\|\psi(x,0)\|_{L^2}^2$ to both sides and then taking absolute values yields:

$$\|\psi(\vec{x},t)\|_{H^1}^2 \leq 2\langle\psi(x,0)|H\psi(x,0)\rangle + 2\|\psi(\vec{x},t)\|_{L^2}^2 \|V(x)\|_{L^\infty}^2 + \|\psi(\vec{x},t)\|_{L^2}$$

Applying conservation of mass to the $\psi(\vec{x},t)$ terms on the right, and then taking square roots yields the result we seek. □

We note that $\left\|[1 - P^0_{[-K,K]^N;0}(k)]f(x)\right\|_{L^2} \leq \langle K\rangle^{-1}\|f(x)\|_{H^1}$. Combining this with proposition 5.2 on page 59, we have verified assumption 2. Thus:

$$\left\|[1 - P^0_{[-K,K]^N;0}(k)]\psi(\vec{x},t)\right\|_{L^2} \leq K^{-1}\sqrt{2}\sqrt{|E_0| + \|\psi(x,0)\|_{L^2}^2\left(\|V(x)\|_{L^\infty} + 1/2\right)} \tag{8.3}$$

Now, given $\delta_{\max}$, we let

$$k_{\max} - \mathbf{k}^s(k_{\max}) = \delta_{\max}^{-1} 2^{3/2} \mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2})\sqrt{|E_0| + \|\psi(x,0)\|_{L^2}^2\left(\|V(x)\|_{L^\infty} + 1/2\right)}$$

Substituting this definition of $k_{\max}$ into (8.3), we find that proposition 5.2 is satisfied and therefore assumption 2 is also satisfied.

One can, of course, use energy estimates (based on the fact that $\langle\psi(\vec{x},t)|H^s\psi(\vec{x},t)\rangle$ is conserved) in higher order Sobolev spaces to bound $k_{\max}$ as well. In general, one can show that $k_{\max} \sim \delta_{\max}^{s-t}$ where s is the sobolev space in which we measure the error, and $t > s$ is some higher Sobolev space. However, the constants are difficult to control, due to the need to estimate many commutators, e.g. $[-(1/2)\Delta^a, V(x)^b]$ (and the like).

Assumption 3

Since $V(x)$ is a bounded linear operator, we find that $\mathbf{G} = \|V(x)\|_{\mathcal{L}(H^s,H^s)}$. But $\|V(x)\|_{\mathcal{L}(H^s,H^s)}$ is given merely by $\|V(x)\|_{\mathcal{L}(H^s,H^s)} = \|V(x)\|_{W^{s,\infty}}$. In the case when $s=0$, we find simply that $\|V(x)\|_{\mathcal{L}(L^2,L^2)} = \|V(x)\|_{L^\infty}$.

Assumption 4

This follows from assumption 2 combined with the fact that the potential is smooth and decays rapidly in space. We use the alternative assumption to assumption 4 found on page 59. We need to verify (5.9a) and (5.9b).

Bounds in Momentum

To verify (5.9a), we need to compute a bound on:

$$\left\|(1 - P^s_{[-M,M]^N;k_0}(\vec{x}))V(x)\psi(\vec{x},t)\right\|_{L^2}$$

We do this by using the fact that $\hat{V}(k)$ decays rapidly, combined with (8.3). We write:

$$\begin{aligned}
&\left\|(1 - P^0_{[-M,M]^N;k_0}(\vec{x}))V(x)\psi(\vec{x},t)\right\|_{L^2} \\
&\quad\leq \left\|(1 - P^0_{[-M,M]^N;k_0}(\vec{x}))[\hat{V}(k) \star P^0_{[-K,K]^N;k_0}(\vec{x})\hat{\psi}(k,t)]\right\|_{L^2} \\
&\quad + \left\|(1 - P^0_{[-M,M]^N;k_0}(\vec{x}))[\hat{V}(k) \star (1 - P^0_{[-K,K]^N;k_0}(\vec{x}))\hat{\psi}(k,t)]\right\|_{L^2} \\
&\quad\leq \left\|(1 - P^0_{[-M,M]^N;k_0}(\vec{x}))[\hat{V}(k) \star P^0_{[-K,K]^N;k_0}(\vec{x})\hat{\psi}(k,t)]\right\|_{L^2} \\
&\qquad + \|V(x)\|_{L^\infty} \left\|(1 - P^0_{[-K,K]^N;k_0}(\vec{x}))\hat{\psi}(k,t)\right\|_{L^2} \\
&\quad\leq \left\|(1 - P^0_{[-M,M]^N;k_0}(\vec{x}))[\hat{V}(k) \star P^0_{[-K,K]^N;k_0}(\vec{x})\hat{\psi}(k,t)]\right\|_{L^2} \\
&\qquad + \|V(x)\|_{L^\infty} K^{-1}\sqrt{2}\sqrt{|E_0| + \|\psi(x,0)\|^2_{L^2}(\|V(x)\|_{L^\infty} + 1/2)}
\end{aligned} \tag{8.4}$$

The last term can be made as small as necessary by making K large, which we will do shortly. We can calculate this by:

$$\begin{aligned}
&\left\|(1 - P^0_{[-M,M]^N;k_0}(\vec{x}))[\hat{V}(k) \star P^0_{[-K,K]^N;k_0}(\vec{x})\hat{\psi}(k,t)]\right\|^2_{L^2} \\
&\quad\leq \int_{([-(M+k_0),(M+k_0)]^N)^C} \left| \int_{[-(K+k_0),(K+k_0)]^N} C'_V e^{-\alpha|\vec{k}-\vec{k}'|}\hat{\psi}(\vec{k}',t)d\vec{k}' \right|^2 d\vec{k}
\end{aligned} \tag{8.5}$$

The inner integral is the convolution of a compactly supported function with an exponentially decaying one. The result is exponentially decaying. The outer integral is then integrated over the tail of this exponentially decaying function, and is therefore exponentially small.

Lemma 8.2 *Suppose $|\vec{k}|_\infty \geq (K+k_0)$, in particular suppose that $|\vec{k}_j| \geq K+k_0$ with $j \in 1 \ldots N$. We have the following bound on the inner integral:*

$$\left| \int_{[-(K+k_0),(K+k_0)]^N} C'_V e^{-\alpha|\vec{k}-\vec{k}'|} \hat{\psi}(\vec{k}', t) d\vec{k}' \right|^2$$
$$\leq (C'_V)^2 2(K+k_0) e^{-2\alpha(|\vec{k}|_\infty - K - k_0)} \|\psi(x,0)\|_{L^2}^2 \alpha^{-N+1}$$

Proof. Since $|\vec{k}|_\infty \geq (K+k_0)$, there exists j so that $\left|\vec{k}_j\right| \geq K+k_0$. Suppose, without loss of generality, that $\vec{k}_j \geq K+k_0$ (the case when $\vec{k}_j \leq -K-k_0$ is just a change of coordinates). We can then calculate:

$$\left| \int_{[-(K+k_0),(K+k_0)]^N} (C'_V)^2 e^{-\alpha|\vec{k}-\vec{k}'|} \hat{\psi}(\vec{k}', t) d\vec{k}' \right|^2 \leq$$
$$\int_{[-(K+k_0),(K+k_0)]^N} (C'_V)^2 e^{-2\alpha|\vec{k}-\vec{k}'|} \left\| \hat{\psi}(\vec{k}, t) \right\|_{L^2}^2$$
$$\leq 2(K+k_0) e^{-2\alpha(\vec{k}_j - K - k_0)} \left\| \hat{\psi}(\vec{k}, t) \right\|_{L^2}^2 \int_{[-(K+k_0),(K+k_0)]^{N-1}} e^{-2\alpha|\vec{k}-\vec{k}'|_1} d\vec{k}'$$
$$\leq 2(K+k_0) e^{-2\alpha(\vec{k}_j - K - k_0)} \left\| \hat{\psi}(\vec{k}, t) \right\|_{L^2}^2 \int_{\mathbb{R}^{N-1}} e^{-2\alpha|\vec{k}-\vec{k}'|_1} d\vec{k}'$$
$$\leq 2(K+k_0) e^{-2\alpha(\vec{k}_j - K - k_0)} \left\| \hat{\psi}(\vec{k}, t) \right\|_{L^2}^2 \alpha^{-N+1}$$

Finally, note that $\left\| \hat{\psi}(\vec{k}, t) \right\|_{L^2} = \|\psi(x,0)\|_{L^2}$ and we are done. □

Lemma 8.3 *The following equation holds.*

$$\int_{([-(M+k_0),(M+k_0)]^N)^C} e^{-2\alpha(|\vec{k}|_\infty - K - k_0)} d\vec{k}$$
$$= 2N(2\alpha)^{-N} e^{2\alpha(K-k_0)} \Gamma(N, 2\alpha(M+k_0))$$
$$\sim M^N e^{-2\alpha(M-K)} 2N(2\alpha)^{-N} \quad (8.6)$$

In particular, (8.6) *vanishes faster than $e^{-(2\alpha-\delta)M}$ for any $\delta > 0$.*

Proof. The set $\{\vec{k} : |\vec{k}|_\infty = u\}$ has surface area $2Nu^{N-1}$. Thus, we find that:

$$\begin{aligned}
&\int_{([-(M+k_0),(M+k_0)]^N)^C} e^{-2\alpha(|\vec{k}|_\infty - K - k_0)} d\vec{k} \\
&= \int_{M+k_0}^{\infty} 2Nu^{N-1} e^{-2\alpha(u-K-k_0)} du = 2Ne^{2\alpha(K-k_0)} \int_{M+k_0}^{\infty} u^{N-1} e^{-2\alpha u} du \\
&\qquad = 2Ne^{2\alpha(K-k_0)} \int_{2\alpha(M+k_0)}^{\infty} (v/2\alpha)^{N-1} e^{-v} \frac{dv}{2\alpha} \\
&\qquad = 2N(2\alpha)^{-N} e^{2\alpha(K-k_0)} \int_{2\alpha(M+k_0)}^{\infty} v^{N-1} e^{-v} dv \\
&\qquad\qquad = 2N(2\alpha)^{-N} e^{2\alpha(K-k_0)} \Gamma(N, 2\alpha(M+k_0))
\end{aligned}$$

The asymptotics follow by applying (4.15) to $\Gamma(N, 2\alpha M)$. $\square$

We now apply lemma 8.2 to the inner integral of (8.5), and lemma 8.3 to the outer integral. We thus find that:

$$\begin{aligned}
(8.5) \leq &(C_V')^2 2\alpha^{-N+1} 2N(2\alpha)^{-N} \\
&\times \left\| \hat{\psi}(\vec{k}, t) \right\|_{L^2}^2 (K+k_0) e^{2\alpha(K-k_0)} \Gamma(N, 2\alpha(M+k_0))
\end{aligned} \tag{8.7}$$

Thus:

$$\begin{aligned}
(8.4) \leq &C_V' 2\alpha^{-(N+1)/2} N^{1/2} (2\alpha)^{-N/2} \\
&\times \|\psi(x,0)\|_{L^2} \sqrt{K+k_0} e^{\alpha(K-k_0)} \sqrt{\Gamma(N, 2\alpha(M+k_0))} \\
&+ \|V(x)\|_{L^\infty} K^{-1} \sqrt{2} \sqrt{|E_0| + \|\psi(x,0)\|_{L^2}^2 (\|V(x)\|_{L^\infty} + 1/2)}
\end{aligned} \tag{8.8}$$

We will now make K and M sufficiently large.

We choose K in order to obtain:

$$\begin{aligned}
&\|V(x)\|_{L^\infty} K^{-1} \sqrt{2} \sqrt{|E_0| + \|\psi(x,0)\|_{L^2}^2 (\|V(x)\|_{L^\infty} + 1/2)} \\
&\qquad \leq \frac{1}{2} \frac{\delta_{\mathrm{NL}} \|\psi(\vec{x}, t)\|_{L^2}}{(4\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}))}
\end{aligned}$$

This yields:

$$\begin{aligned}
K = &2^{3/2} (4\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2})) \\
&\times \frac{\|V(x)\|_{L^\infty} \sqrt{|E_0| + \|\psi(x,0)\|_{L^2}^2 (\|V(x)\|_{L^\infty} + 1/2)}}{\delta_{\mathrm{NL}} \|\psi(x,0)\|_{L^2}}
\end{aligned}$$

We now select M so that:

$$C_V' 2\alpha^{-(N+1)/2} N^{1/2} (2\alpha)^{-N/2} \times \|\psi(x,0)\|_{L^2} \sqrt{K+k_0} e^{\alpha(K-k_0)} \sqrt{\Gamma(N, 2\alpha(M+k_0))} \leq \frac{1}{2} \frac{\delta_{\mathrm{NL}} \|\psi(\vec{x},t)\|_{L^2}}{(4\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}))}$$

This yields:

$$M = k'_{\max,\mathrm{NL}} = -k_0 + (2\alpha)^{-1}\Gamma^{-1}\left(N, \frac{\delta_{\mathrm{NL}} 2^{N-7} \alpha^{2N-1} e^{-2\alpha(K-k_0)}}{(C_V')^2 N (K+k_0) (\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}))^2}\right) \quad (8.9)$$

In terms of asymptotics, we find that $K = O(\delta_{\mathrm{NL}}^{-1})$ and $M = \Gamma^{-1}(N, e^{-2\alpha K}/K) = \Gamma^{-1}(N, e^{-2\alpha\delta_{\mathrm{NL}}^{-1}}\delta_{\mathrm{NL}})$, thus $M = k'_{\max,\mathrm{NL}}$ grows at most $\delta_{\mathrm{NL}}^{-1-\delta}$ for any $\delta > 0$. Thus we have satisfied (5.9a).

Bounds in Space

To verify (5.9b), we need to compute a bound on

$$\left\| P^s_{[-L_{\mathrm{NL}},L_{\mathrm{NL}}]^N;x_0}(\vec{x})\psi(\vec{x},t) \right\|_{L^2},$$

where we are free to choose L'_{NL}.

We can bound this by $\left\|(1 - P^s_{[-L_{\mathrm{NL}},L_{\mathrm{NL}}]^N;x_0}(\vec{x}))V(x)\right\|_{L^\infty} \|\psi(\vec{x},t)\|_{L^2}$. Observe that:

$$\left\|(1 - P^s_{[-L_{\mathrm{NL}},L_{\mathrm{NL}}]^N;x_0}(\vec{x}))V(x)\right\|_{L^\infty} \leq \left\|1 - P^s_{[-L_{\mathrm{NL}},L_{\mathrm{NL}}]^N;x_0}(\vec{x})\right\|_{L^\infty} C_V \langle L'_{\mathrm{NL}}\rangle^{-1-\beta} \leq C_V \langle L'_{\mathrm{NL}}\rangle^{-1-\beta}$$

Therefore, we find that in order to make

$$\left\| P^s_{[-L_{\mathrm{NL}},L_{\mathrm{NL}}]^N;x_0}(\vec{x})\psi(\vec{x},t) \right\|_{L^2} \leq \frac{\delta_{\mathrm{NL}} \|\psi(\vec{x},t)\|_{L^2}}{(4\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}))},$$

we need only let

$$L_{\mathrm{NL}} = \left[\delta_{\mathrm{NL}}^{-1} C_V (4\mathbf{H}_+^s(\tilde{g}(\vec{x}))\mathbf{H}_+^{-s}(e^{-x^2/\sigma^2}))\right]^{\frac{1}{1+\beta}}$$

Asymptotically, $L_{\mathrm{NL}} = O((1/\delta_{\mathrm{NL}})^{\frac{1}{1+\beta}})$.

If $V(x)$ decays exponentially, one can prove a similar estimate in which L_{NL} will behave like $O(\ln(1/\delta_{\mathrm{NL}}))$.

Assumption 5

Various propagation estimates can be used to verify assumption 5 (using proposition 5.4) using propagation estimates, e.g. [27].

We would break the non-necessary waves involved in assumption 5 into waves which are pointing away from $\vec{x} = 0$, waves which are pointing towards $\vec{x}$ but do not have enough velocity to reach $[-L_{\text{int}}, L_{\text{int}}]^N$ before $t = T_{\max}$, and those waves for which $\vec{x} \cdot \vec{k} = 0$ (waves moving in the angular direction).

The outgoing waves can be treated by using minimal velocity bounds on the positive spectral subspace of the dilation generator $(-i/2[\vec{x} \cdot \nabla + \nabla \cdot \vec{x}])$.

The waves which are moving inward, but too slowly too reach the computational region, are controlled by maximal velocity bounds.

The treatment of the third type of waves is more intricate, which requires the use of velocity bounds with modified dilation operators and covering arguments in phase space. The idea is that they are contained in regions of phase space for which $[-L_{\text{comp}}, L_{\text{comp}}]^N$ is outside the propagation set.

It is our intent to calculate this all explicitly at some later point.

Assumption 6

This is, we believe, the most difficult assumption to verify.

Assumption 6 has two components which need to be verified. We only know of a general argument which is capable of dealing with one of them.

The basic tool for verifying assumption 6 is proposition 5.5. Proposition 5.5 says that all we need to do is verify that framelets which are outside the box have $|\vec{b}k_0|_2 \geq 2\sqrt{N}k_{\min}$, and for which $\vec{a}x_0$ is located cone around $\vec{b}k_0$.

This means that we need to show that framelets which are far from this cone have small mass, and framelets below $2\sqrt{N}k_{\min}$ have small mass.

We believe the first can be verified by using pseudoconformal-type estimates, which we will sketch out below. We are uncertain at this time how to show that the amount of mass below $2\sqrt{N}k_{\min}$ is small. For this reason, we are developing a multiscale algorithm capable of handling low frequency waves [37].

We now sketch an argument suggesting that waves cluster on waves where $\vec{x} \parallel \vec{k}$. Recall that in remark 5.6, we provided an argument suggesting that if $\|(\vec{x} - it\nabla)f(\vec{x})\|_{L^2}$ was bounded, then the mass of $f(\vec{x})$ sitting on framelets with $|\vec{a}x_0 - \vec{b}k_0 t|_2 \gg 0$ is small.

We now suppose that $\psi(x,t)$ is located strictly on positive energies, i.e. $\chi_{[k_{\min},\infty)}(H)\psi(x,t) = \psi(x,t)$. Let us also suppose that $\langle\vec{x}\rangle^2 V(\vec{x})$ decays rapidly. This suggests to us that $\left\| |\vec{x}|_2^2 V(\vec{x})\psi(x,t) \right\|_{L^2} \leq \text{const}\, t^{-3/2}$.

We can then decompose $\psi(x,t)$ by Duhamel in the following way:

$$\psi(x,t) = e^{i(1/2)\Delta t}\psi(x,0) + \int_{jt/n}^{(j+1)t/n} e^{i(1/2)\Delta(t-t')} V(x)\psi(x,t')dt'$$

We then observe that:

$$\left\| (x - it\nabla)e^{i(1/2)\Delta t}\psi(x,0) \right\|_{L^2} = \left\| |\vec{x}|_2^2 \psi(x,0) \right\|_{L^2}$$

In addition, we find that:

$$\left\| (x - i(t-t')\nabla)e^{i(1/2)\Delta(t-t')}V(x)\psi(x,t') \right\|_{L^2} = \left\| e^{i(1/2)\Delta(t-t')} |\vec{x}|_2^2 V(x)\psi(x,t') \right\|_{L^2}$$
$$= \left\| |\vec{x}|_2^2 V(x)\psi(x,t') \right\|_{L^2} \leq \text{const}(t')^{-3/2}$$

We then observe that this suggests that the framelet coefficients of $e^{i(1/2)\Delta(t-t')}V(x)\psi(x,t')$ are also small when $\vec{a}x_0 \perp \vec{b}k_0$.

This indicates that:

$$\left\|\mathcal{P}_{\vec{a}\perp\vec{b}}\psi(x,t)\right\|_{L^2} \leq \text{small}\left\||\vec{x}|_2^2\psi(x,0)\right\|_{L^2} + \text{small}\int_0^t \text{const}(t')^{-3/2}dt' \quad (8.10)$$

This argument, which we believe can be made rigorous, suggests why we believe that all of our assumptions can be verified for the case of linear, time independent potentials.

9 Numerical Tests

In this section we discuss the results of our numerical tests.

We built and implemented the algorithm in the program Kitty . Kitty is implemented in the Python programming language, with external libraries (written in C) handling the expensive numerical computations. The external libraries used are FFTW (Fastest Fourier Transform in the West), and Numarray (support for large arrays in Python, at C-like speeds). Kitty also calls the external programs Gnuplot to generate graphs and ImageMagick/gifsicle in order to produce movies for 2-dimensional simulations.

Kitty is licensed under the GPL. It is very much a work in progress. Kitty comes with little documentation and no warranty. Use it at your own risk.

Various test cases, spanning many types of parameters, are also available for download from the author's webpage, http://math.rutgers.edu/˜stucchio.

9.1 $T + R = E$: Simple Tests

The standard method for testing absorbing boundaries is simply to throw coherent states (which are well localized in frequency) at the boundary. After the collision, the amount transmitted (if absorbing potentials are used – for Dirichlet-to-Neumann and other boundaries nothing is transmitted) and the amount reflected are measured.

This is a useful test, although it is by no means completely characterizes the errors. We explain why, and provide an example where this method fails in section 9.2.

9.2 $T + R \neq E$: A trickier test

We describe in this section a scenario in which computing a bound on $T + R$ provides no useful estimate.

Consider the following linear Schrödinger equation (with $(\vec{x},t) \in \mathbb{R}^{2+1}$):

$$\begin{aligned} i\partial_t\psi(x,t) &= \left[-(1/2)\Delta - \frac{15}{0.05|\vec{x}|_2^2+1}\right]\psi(x,t) \quad (9.1) \\ \psi(x,0) &= e^{i7\vec{x}_2}e^{-|\vec{x}|_2^2/20} + e^{i4\vec{x}_1}e^{-|\vec{x}|_2^2/20} \end{aligned}$$

Observe that the initial condition consists of two coherent states of equal mass, one with velocity 4 and one with velocity 7. The notable fact about this particular potential is that the fast gaussian has enough kinetic energy to (mostly) escape from the binding potential. The slow gaussian does not. The slow gaussian moves toward the boundary, turns around and returns.

The problem with the absorbing potential approach is that the absorbing potential does not distinguish between incoming and outgoing waves. It dissipates everything on the boundary including the waves that should have returned. This will occur even if one can construct a complex potential for which $T + R = 0$!

We ran three simulations of (9.1). The first was performed using the TDPSF with $\sigma = 2.0$. The region of computation was $[-25.6, 25.6]^2$ The second was performed (on the same region) with an absorbing potential

$$V_1(\vec{x}) = -20ie^{-(\vec{x}_1 \pm 25.6)^2/36} - 20ie^{-(\vec{x}_2 \pm 25.6)^2/36}.$$

The third was solved with periodic boundary conditions on the region $[-102.4, 102.4]^2$. This boundary is sufficiently distant so that the outgoing waves cannot return to the origin for a time $204.8/7.0 \approx 29$. Thus, we will take the distant boundaries simulation as our benchmark, at least for $t \leq 29$.

After $t = 29$, we have some qualitative knowledge of the behavior. We expect that the solution consists of continuum and bound states. Over a short time, the continuum will disperse, leaving only the bound states. The bound states will remain forever.

In all three cases, the quantity $M(t) = \|\psi(x,t)\|_{L^2([-10,10]^2)}$ was computed. The simulation using the TDPSF agreed with the simulation on the larger region to within 1.25% for $t < 29$[10].The simulation using complex potentials had an error of 4% for $t < 29$, and the error appears to increase after that.

In fact, examining the graphs of $M(t)$ (see figure 1) part of the bound states appear to be dissipating. In fact, we believe that this dissipation will continue and the error will only get worse with time.

The reason the TDPSF performs so much better than the complex potential is that it distinguishes outgoing waves from incoming waves on the boundary. The TDPSF only removes waves which sit on the boundary and are also outgoing with sufficiently high velocity. The trapped waves, although they sit on the boundary, do not have high outgoing velocity, and thus are not removed.

9.3 Violations of Assumption 4: Soliton Filtering

Numerical experiments suggest that in some cases, assumption 4 can be relaxed. Consider $g(t, \vec{x}, \psi(\vec{x},t))\psi(\vec{x},t)$ of the form $f(|\psi(\vec{x},t)|^2)\psi(\vec{x},t)$, where $f(|\psi(\vec{x},t)|^2)\psi(\vec{x},t)$ is some nonlinearity that supports solitons.

[10] In fact, the 1.25% is much better than one might otherwise expect. A simple calculation shows that the potential is equal to -0.44 on the boundary. Therefore, assumption 4 is not satisfied, since the "nonlinearity" is not contained inside the box. Additional simulations using the domain $[-51.2, 51.2]^2$ yielded almost complete agreement with the simulation using distant boundaries, and had the correct qualitative behavior after that.

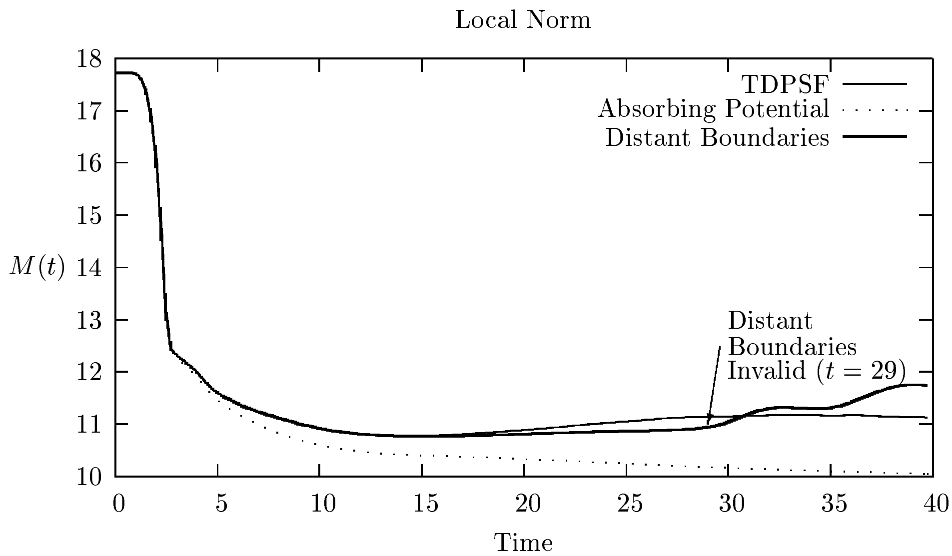

Figure 1: A graph of $M(t) = \|\psi(x,t)\|_{L^2([-10,10]^2)}$ vs t. The distant boundary simulation is invalid at time $t = 29$, due to the fact that the outgoing pulse returns at this time.

It turns out that solitons moving with sufficiently high velocity are filtered by our boundary conditions as well. The reason is simply the fact that an outgoing soliton is localized in phase space on outgoing waves. Consider a soliton, taking the form $e^{i(vx-\omega t)}\phi(x-vt)$, for some smooth, well localized $\phi(x)$ (e.g. $\phi(x) = \cosh(x)^{-1}$).

The Fourier transform of the soliton is also well localized around frequency v. If v is sufficiently large, then the framelet coefficients of $e^{i(vx-\omega t)}\phi(x-vt)$ will cluster around (x,v). When x is near the boundary, these framelets will all be outgoing under the free flow $e^{i(1/2)\Delta t}$.

The soliton is also leaving the box under the full flow $\mathcal{U}(t)$. Although $e^{i(1/2)\Delta t}$ and $\mathcal{U}(t)$ move the soliton very differently (one dispersively, one coherently), they both move it out of the box and in nearly the same direction.

We ran numerical tests to demonstrate this as follows. We solved the Schrödinger equation

$$i\partial_t \psi(x,t) = -(1/2)\Delta - |\psi(x,t)|^2 \psi(x,t)$$

on the region $[-51.2, 51.2]$. The TDPSF was placed on the boundary. The initial condition was taken to be $\psi(x,0) = 2^{-1/2}e^{ivx}/\cosh(x-15)$ for $v = 1..15$. We then computed:

$$E(v) = \sup_{t<200/v} \frac{\|\psi(x,t) - \psi_{ex}(x,t)\|_{L^2([-10,10])}}{\|\psi_{ex}(x,0)\|_{L^2(\mathbb{R})}} \tag{9.2}$$

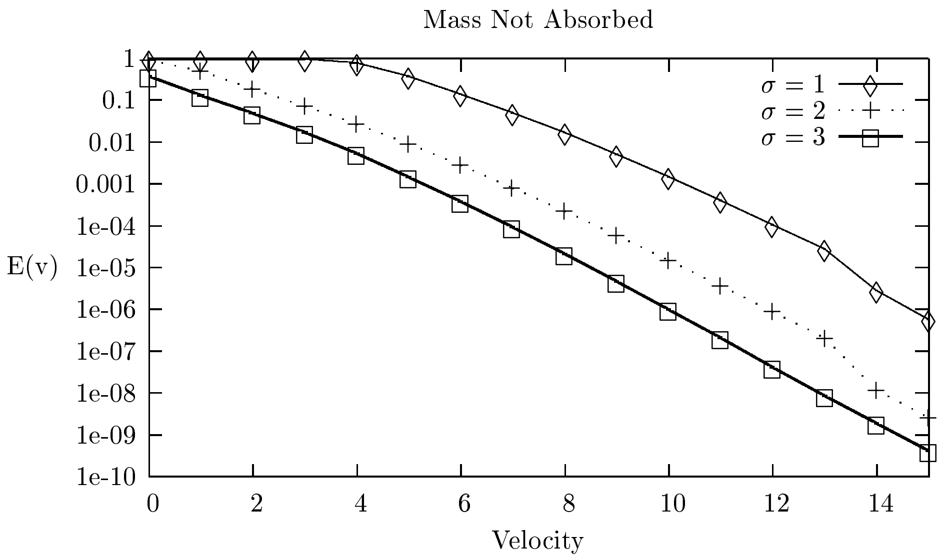

Figure 2: A plot of the error (defined as in (9.2)) as a function of velocity. Note the exponential improvement in accuracy with velocity.

The function $\psi_{ex}(x,t)$ is the exact solution. The result of this experiment is plotted in figure 9.3. The time $200/v$ was chosen since it is more than enough time for errors to return to the region $[-10, 10]$.

Remark 9.1 The paper [40] proposes an alternative method of absorbing boundaries (namely the paradifferential strategy), based on a novel method of approximating the Dirichlet-to-Neumann operator. A similar numerical test was performed for those boundary conditions. For a soliton at velocity 15, Szeftel obtained $E(15) = 0.08$ at best. For comparison, we obtain $E(v) = 2.86 \times 10^{-6}$ for $\sigma = 1$ and $E(v) = 1.88 \times 10^{-09}$ for $\sigma = 3$. It is worth noting that the methodology we use differs somewhat from that of [40] (amoung other things, we used spectral methods to solve the interior problem rather than FTDT).

It is somewhat surprising that this occurs, since the method described in [40] actually takes the nonlinearity into account. In contrast, our method actually assumes the nonlinearity is nearly zero on the boundary. In spite of that, we have an error which is of order $10^{-6} - 10^{-7}$ as opposed to 0.08.

9.3.1 A Coincidence, not a Conjecture

This is not a general phenomenon, however, as illustrated by the following example. Consider the KdV equation, and suppose a scheme similar to ours were implemented. That is, we decompose the solution into gaussian framelets, and filter them if they are leaving under the free flow. If a soliton exists, and is sitting near the right boundary, it too will be filtered, since it is leaving under the free flow. But under the full flow, the soliton will not leave the box, since solitons propagate leftward while free waves propagate rightward.

The fact that our method succesfully filters outwardly moving solitons is a consequence of the fact that fast-moving solitons have very little incoming waves. For some nonlinearities, a soliton or soliton-like object at position $(\vec{a}x_0, \vec{b}k_0)$ in phase space actually propagates along the trajectory $\vec{a}x_0 + t\vec{b}k_0$. However, not all solitons have this feature, and when they lack it, there is no reason to believe our method will be effective.

9.3.2 Soliton Filters

Our motivation in constructing the TDPSF was the following. Nonreflecting boundary conditions are possible because we understand the motion of waves away from the support of the nonlinearity. So we used that knowledge to determine what to filter, and what not to filter.

We propose that a practical way to filter outgoing solitons is simply to identify them and remove them. That is, at a time T_{step}, we determine whether $\psi(x, T_{\text{step}})$ might have a soliton located near the boundary. If so, use the decomposition $\psi(x, T_{\text{step}}) = S(x) + R(x)$, where $S(x)$ is the soliton and $R(x)$ is the remainder. We then determine whether $S(x)$ is outgoing. If it is, we then set $\psi(x, T_{\text{step}_+}) = R(x)$. Thus, the soliton has been filtered.

This does, of course, depend on an explicit knowledge of what solitons look like. But that information is available in many cases, so assuming it to be available is not unreasonable.

10 Comparison to Other Methods

A variety of other approaches have been proposed for open boundaries. They fall into two main categories, and we discuss them both briefly.

10.1 Engquist-Majda type Boundaries, and Dirichlet-to-Neumann Operators

The closest approach to ours is the original Engquist-Majda boundary conditions, found in [18, 16]. The principle that was guiding them was that near the boundary, the geometric optics approximation to wave flow is sufficiently accurate to filter off the outgoing waves.

Our result is a direct analogue of this - the gaussian framelet elements behave (under the free flow) like classically free particles. We use a different method to filter, but the guiding principle is the same.

In comparison, the approach that is farthest from ours are the various modern extensions to [18]. Modern approaches attempt to construct the exact solution on the boundary, and then impose it as a boundary condition. In principle, this is the best possible approach. However, in practice, this will be very difficult, because if the exact solution were known, we would not need a simulation!

In fact, this approach is sufficiently difficult that we know of few aproaches for the Schrödinger equation. We describe the two main approaches we are aware of, and remark that only the paradifferential strategy of J. Szeftel even attempts to deal with nonlinear equations.

10.1.1 Exact Dirichlet-Neumann maps for the Schrödinger Equation

To deal with the free Schrödinger equation (no nonlinearity or potential),Lubich and Schädle [28, 34, 33] constructed a novel method for using the exact boundary conditions rather than an approximate one. Their method consists of approximating the integral kernel by using a piecewise exponential approximation (in time) and the fact that convolution with an exponential can be done in linear rather than polynomial time. This approach appears to work nicely for the free Schrödinger equation, although it is uncertain that it could be applied to the full Dirichlet-to-Neumann operator of a nonlinear equation.

10.1.2 Paradifferential Strategy

The only fully nonlinear Dirichlet-to-Neumann operator that we are aware of was constructed by J. Szeftel in [41]. Szeftel constructs the Dirichlet-to-Neumann operator by a modified version of the paradifferential calculus (introduced in [4]). His methodology is demonstrated in 1 space dimension, with a nonlinearity that is C^∞ in x, $\psi(\vec{x},t)$ and $\partial_x \psi(\vec{x},t)$. He proves local well posedness of the boundary operator.

However, extensions to $\mathbb{R}^N$ appear highly nontrivial. The assumptions are significantly stronger than ours, and there are no error bounds. However, the numerical experiments look promising and the results appear accurate for radiative problems (see also remark 9.1).

10.2 Absorbing Potentials/ PML

10.2.1 Absorbing Potentials

Absorbing (complex) potentials, described in [29], are the current "industry standard". The approach consists of the following. Instead of solving (1.1) on the box $[-L_{\text{int}}, L_{\text{int}}]^N$, we solve

$$i\partial_t \Psi(\vec{x},t) = -(1/2)\Delta\Psi(\vec{x},t) + g(t,\vec{x},\Psi(\vec{x},t))\Psi(\vec{x},t) + -ia(x)\Psi(\vec{x},t)$$

on the region $[-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N$. The function $a(x)$ is a positive function supported in $[-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N \setminus [-L_{\text{int}}, L_{\text{int}}]^N$. The term $-ia(x)$ is a dissipative term which is localized on waves which have left the region $[-L_{\text{int}}, L_{\text{int}}]^N$. Thus, it (partially) absorbs waves which have left the domain of interest.

This approach is the mainstay of absorbing boundaries, due to it's generality and simplicity. One important reason for the attractiveness is that they are compatible with the FFT/Split Step algorithm (algorithm 2.2), with minimal difficulty of programming.

Of course, the potential $a(x)$ must be tuned to the given problem. Given $k_{\min}$, $k_{\max}$, one must select the height and width of the absorber so that it kills most of the wave between $k_{\min}$ and $k_{\max}$, resulting in an error τ.

Waves with momentum lower than $k_{\min}$ are mostly reflected, and waves with momentum higher than $k_{\max}$ are mostly transmitted (and therefore wrap around the computational domain).

Heuristic calculations and numerical experiments suggest that the absorber must have width proportional to $Ck_{\max}\ln(\epsilon)/k_{\min}$, with C depending on the precise shape of the potential. In contrast, our method works on a boundary layer of width $C\ln(\epsilon)/k_{\min}$, which is smaller by a factor of $k_{\max}$.

An additional problem with absorbing potentials is that they kill everything on the boundary. They make no distinction between incoming and outgoing waves, and thus they absorb some waves which should return to the region of interest. This poses a fundamental limitation on their use, especially in problems where the nonlinearity creates long range effects, which was illustrated in section 9.2.

10.2.2 Perfectly Matched Layers

Perfectly Matched Layers (PML) are a variation on this approach, proposed in [24] for the Schrödinger equation (see also [3], where they are first proposed for Maxwell's equations). In [24], they are tested for the 1 dimensional free Schrödinger equation, and the result appears reasonably accurate.

To use a PML, instead of solving (10.2.1), we solve:

$$i\partial_t\Psi(\vec{x},t) = -(1+ia(x))(1/2)\Delta\Psi(\vec{x},t) + g(t,\vec{x},\Psi(\vec{x},t))\Psi(\vec{x},t)$$

where $a(x)$ is now a function chosen rather carefully (see below).

The PML has two main advantages over complex absorbing potentials. First, the fact that $ia(x)$ is now in the coefficient of Δ now means that high momentum waves are dissipated more strongly than low momentum ones. Thus, fast waves do not pass through the absorbing potential without being dissipated.

Second, the function $a(x)$ can be chosen precisely so that there is no reflection at the interface (the boundary of $[-L_{\text{int}}, L_{\text{int}}]^N$). However, this does not eliminate all reflections, as some reflections will be created in the region $[-(L_{\text{int}}+w),(L_{\text{int}}+w)]^N \setminus [-L_{\text{int}}, L_{\text{int}}]^N$.

The PML has the same problem as complex absorbing potentials with regards to dissipating incoming waves on the boundary.

Lastly, some PML methods are unstable. Numerical experiments in [32] suggest that the PML for 2 dimensional Maxwell's Equations exhibit a long time instability. It is possible that this effect occurs for the Schrödinger equation as well.

The PML method for the Schrödinger equation is still very much undeveloped. This makes a more detailed comparison difficult to make.

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