Original Research Article

# A Wavelets based scheme for solving Schrödinger's equation.

**Abstract**

We present numerical approaches to Schrödinger's equation based on standard Galerkin techniques and wavelet functions. The orthonormal wavelet basis is found to stably represent the solution for small viscosity. The oscillations at a shock are, in comparison with finite difference and spectral approximations, reduced and confined to the vicinity of the shock. Numerical results and comparison with classical algorithms are provided.

## 1 Introduction

The general one dimensional Schrödinger equation is given as follows:

$$\hat{H}\psi(x,t) = E\psi(x,t)$$

Where $\hat{H}$ is the Hamiltonian operator, $\psi$ is the wave function, and $E$ is the energy. In atomic units, the Hamiltonian operator for a particle in a potential is:

$$\hat{H} = - \bigtriangledown^2 + V(x)$$

The time-independent Schrödinger equation (TISE) bounded inside a potential becomes:

$$\psi_x x(x,0) + V(x)\psi(x,0) = E\psi_t(x,0)$$

($\psi$ is the time-independent wave function) For a particle in a time-dependent potential, the one-dimensional Schrödinger equation is

$$\frac{-h^2}{2m}\psi_x x(x,t) + V(x)\psi(x,t) = E\psi_t(x,t)$$

where $m$ is the mass of the particle, $V(x)$ is the potential that the particle moves in, and $\psi(x,t)$ is the particle's wave function. The physical interpretation of the wave function is that $\psi^*(x,t)\psi(x,t)dx$ is the probability of finding the particle between $x$ and $x + \Delta x$. The notation $\psi^*$ denotes taking the complex conjugate. In general the wave function $\psi(x,t)$ will be complex, not real.

For bound state problems we generally require that the wave function be normalized, which is to say that $\int \psi^*(x,t)\psi(x,t)dx = 1$ where the integral runs over all possible values of $x$. This condition simply means that if we look everywhere, we find the particle once and only once.

In quantum mechanics a particle does not have a definite position (at least not until we measure the particles position) but only has a probability of being found at a position. If we have a million hydrogen atoms all in the ground state and we measure the position of the electron in all million atoms, we will get a different answer for each atom. It does not make sense to talk about a definite position in a quantum system but only an average position. Since $\psi^*(x,t)\psi(x,t)$ is the probability distribution, the average position of a particle is $< x >= \int \psi^*(x,t)\psi(x,t)dx$ . In quantum mechanics angular brackets are used to denote an average. In general, the average or expectation value of an observable $O$ is $< O >= \int \psi^* O \psi dx$ and order matters! You cannot interchange the $O$ and $\psi^*$ or $\psi$ except in special cases.

## 2 Algorithm of Standard Galerkin

The formulation of the algorithm of Galerkin from just the following series of spaces $V_j$ of a multi-resolution analysis is presented as follows:

To find $u_p(x,t) = \sum_{k=0}^{2^p-1} C_{pk}(t)\phi_{pk}(x)$ where

$$\forall k, \qquad \frac{\partial}{\partial t}C_{pk}(t) + \sum_l C_{pk} < u^* \frac{\partial \phi_{pl}}{\partial x}, \phi_{pk} >= -\nu \sum_l C_{pl} < \frac{\partial \phi_{pl}}{\partial x}, \frac{\partial \phi_{pk}}{\partial x} > \tag{2.1}$$

where $< ., . >$ stands for the $L^2(\mathbb{R})$ inner product.

If $C_p = (C_{pk})_{k=0,2^p-1}$ then

$$\frac{\partial}{\partial t}C_p(t) + AC_p(t) = 0 \tag{2.2}$$

where $A$ is a matrix with the general term

$$A_{kl} =< u^* \frac{\partial \phi_{pl}}{\partial x}, \phi_{pk} > -\nu \sum_l C_{pl} < \frac{\partial \phi_{pl}}{\partial x}, \frac{\partial \phi_{pk}}{\partial x} >$$

Many solutions are enabled to integrate those differential equation (system):

1. Direct integration while using $e^{-tA}$.
2. Numerical integration after discretization by finite difference.

In this second case we use often some implicit schemes for the term of diffusion (elliptical) and we will be therefore leaded to inverse an ill conditioned matrix. It is useful to use in the place of the basis of $(\phi_{pk})_{0\leq k\leq 2^p-1}$ those of $(\psi_{jk})_{0\leq j\leq p-1}^{0\leq k\leq 2^j-1}$, to reformulate and preconditioning the problem with the diagonal matrix of the operator $\Gamma^2$: $\psi_{jk} \mapsto 2^j\psi_{jk}$.

The formulation of Galerkin use a particular approximation of the operator of evolution $u^*\frac{\partial}{\partial x} - \nu\frac{\partial^2}{\partial x^2}$. It is not very well adapted in case that the space of the approximation space is adapted to the solution because in this case it's necessary to recalculate all the matrix (or at least a part).

# 3 Wavelet approaches

## 3.1 first approach

We write a weak formulation while using one family of functions $(\theta_\lambda(x))$:

$$\frac{\partial}{\partial t} < u, \theta_\lambda > + \frac{1}{2} < \frac{\partial u}{\partial x} u^*, \theta_\lambda > - \nu < \frac{\partial^2 u}{\partial x^2}, \theta_\lambda >= 0 \tag{3.3}$$

and we discretize directly in time for example by an implicit Euler's scheme for the term of diffusion and explicit for the term $u^* \frac{\partial u}{\partial x}$.
If $(< u^n, \theta_\lambda >)$ are the news unknowns we have:

$$\frac{< u^{n+1}, \theta_\lambda > - < u^n, \theta_\lambda >}{\Delta t} + < \frac{1}{2} \frac{\partial u}{\partial x} u^*, \theta_\lambda > - \nu < \frac{\partial^2 u}{\partial x^2}, \theta_\lambda >= 0 \tag{3.4}$$

that we write

$$< (I - \Delta t \nu \frac{\partial^2}{\partial x^2}) u^{n+1}, \theta_\lambda >= -\Delta t < (\frac{1}{2} \frac{\partial u}{\partial x} u^*)^n, \theta_\lambda > + < u^n, \theta_\lambda >= 0. \tag{3.5}$$

We will choose now $\theta_\lambda$ such that $< (I - \Delta t \nu \frac{\partial^2}{\partial x^2}), \theta_\lambda >= \psi_\lambda$ where $\psi_\lambda$ is a family of $r$-regular wavelets $(r \geq 2)$), then

$$< u^{n+1}, \psi_\lambda >= -\Delta t < (\frac{1}{2} \frac{\partial u}{\partial x} u^*), \theta_\lambda > + < u^n, \theta_\lambda >, \tag{3.6}$$

and

$$u^{n+1} = \sum_\lambda (-\Delta t < (\frac{1}{2} \frac{\partial u}{\partial x} u^*), \theta_\lambda > + < u^n, \theta_\lambda >) \psi_\lambda. \tag{3.7}$$

$u^{n+1}$ is the exact solution of the discretized problem in time and $\lambda$ describe a family of indices $\Lambda_V$ then $u^{n+1} = \sum_\lambda (u^n - \Delta t < (\frac{1}{2} \frac{\partial u}{\partial x} u^*), \theta_\lambda > + < u^n, \theta_\lambda >) \psi_\lambda$ is the orthogonal propagation of $u^{n+1}$ in $V$.

We know that some rapid algorithms of reconstruction allow to get $u_V^{n+1}$ from its wavelets coefficients $(u^n - \Delta t < (\frac{1}{2} \frac{\partial u}{\partial x} u^*), \theta_\lambda >)$.
The computation of these scalar products can be speedily done, indeed $\theta_\lambda$ follows $\psi_\lambda$. Then, For all $\epsilon$, there exist one constant $n_\epsilon$ such that, for all function $f$,

$$| < f - \pi_{V_{j+n_\epsilon}} f, \theta_{jk} > | \leq C(f) \epsilon. \tag{3.8}$$

$n_\epsilon$ is independent of $j$ which for a given $\epsilon$, some rapid algorithms (in tree) can be used to compute the scalar product $< f, \theta_{jk} >$.

This approach leads to some rapid and adaptative algorithms. The obtained numerical results compare favorably to those obtained by classical approaches in term of precision and cost (see Table 1).

The computation of some nonlinear terms in the initial equation $(u^2)$ is a real difficulty in the case of adaptative spaces. Indeed, in this case, the collocation approaches are difficult even though there are the most efficient in the case of regular spaces $(V_j)$ holding interpolative functions.

| Algorithm | $2\pi\ T_{max}$ | $S_{max}/2$ | | dimension |
|---|---|---|---|---|
| $V^{(n)} = V_8$ | 1.64 | 150.3 | no oscillations | 256 |
| $V^{(n)} = V_7$ | 1.63 | 135.0 | localized oscillations | 128 |
| $V^{(n)}$ adapted | 1.64 | 150.3 | no oscillations | $\leq 104$ |
| Fourier pseudospectral $n = 128$ | 1.62 | 134.8 | spread oscillations | 128 |

Table 1: Comparison of some different methods

### 3.2 Second approach

Starting from the discretized equation in time and for $\theta_\lambda = \psi_\lambda$ we write

$$< (I - \Delta t\nu \frac{\partial^2}{\partial x^2})u^{n+1}, \psi_\lambda >= -\Delta t < \frac{1}{2}\frac{\partial (u^* u)^n}{\partial x}, \psi_\lambda > + < u^n, \psi_\lambda >= 0, \tag{3.9}$$

and if we define $(I - \Delta t\nu \frac{\partial^2}{\partial x^2})\psi_\lambda = \theta'_\lambda$, we have:

$$< u^{n+1}, \theta'_\lambda >= -\Delta t < (\frac{1}{2}\frac{\partial uu^*}{\partial x}), \psi_\lambda > + < u^n, \psi_\lambda > \tag{3.10}$$

$\theta'_\lambda$ and $\theta_\lambda$ are two bi-orthogonal families and $\Pi_\Lambda u^{n+1} = \sum_{\lambda\in\Lambda} < u^{n+1}, \theta'_\lambda > \theta_\lambda$.

As compared to the first approach, the difficulty is not to compute the scalar product $< u^{n+1}, \theta_\lambda >$ since it is the wavelets coefficients of $u^n - \frac{\Delta t}{2}\frac{\partial}{\partial x}(uu^*)$ but to "rebuild" $\Pi_\Lambda u^{n+1}$ from the sum $\sum < u^{n+1}, \theta'_\lambda > \theta_\lambda$.
Rapid algorithms are still available and inspired from those defined for homogeneous operators and the associated bi-orthogonal multi-resolutions analysis .

## 4 Algorithm for variable coefficient problem

For a bounded Lipschitzienne real function $a(x)$, consider the problem:

$$\begin{cases} (I - \frac{\partial}{\partial x}(a(x)\frac{\partial}{\partial x}))u = f \\ u(0) = u(1). \end{cases} \tag{4.11}$$

The localization of the wavelets $\psi_{jk}$ for big $j$, allows us to think that in order to such values of $j$, the operator $(-a(k2^{-j}\frac{\partial^2}{\partial x^2})$ is close to the operator $L^{-1}$ when we apply it to the wavelets $\psi_{jk}$. This is not realistic only for big $j$ and, for the smooth part of the problem it's necessary to use a more classical approach.
In fact, we build an approximation of $L^{-1}$ from the following theorem:

**Theorem 1** *: Consider $A_q$ the approximation of Galerkin of $L^{-1}$ in $V_q$ by:*

$$A_q = \Pi_q^*(\Pi_q L \Pi_q^*)\Pi_q$$

*where $\Pi_q$ termed the projection in $V_q$ and $\Pi_q^*$ the extension of $V_q$ in $L^2$.*
*Define $P_q$ the operator as:*

$$\psi_{jk} \mapsto P_q(\psi_{jk}) = \theta_{jk}, \qquad where\ -a(k2^{-j})\frac{\partial^2}{\partial x^2}\theta_{jk} = \psi_{jk},\ \forall j \geq q$$

$$P_q = 0 \text{ on } V_q$$

*so if* $L(A_q + P_q) = I - u$, *there exists a constant* $C$ *dependent of* $a(x)$ *and of the multi-resolutions analysis such that* $\|u^2\|_{L^2,L^2} \leq C2^{-q}$. *We get then* $P(u) \leq C2^{-q/2}$ *and the Neumann's serie* $\sum_{k=0}^{\infty} u^k$ *converge, it means that* $L^{-1} = (A_q + P_q)\sum_{k=1}^{\infty} u^k$.

A numerical algorithm is then possible and provides an approximation of $L$ in $V_p$ from the approximation of Galerkin of $f$ in $V_q$ $(q < p)$ and the diagonal operator of constant coefficients in the basis some $(\psi_{jk})_{j\geq q, j\leq p-1}$.

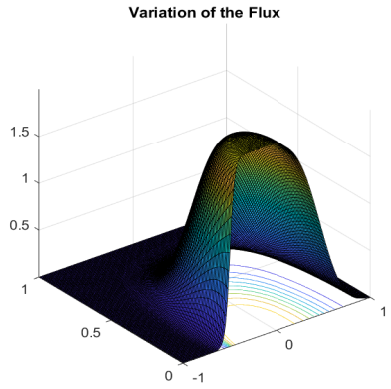


Figure 1: Time evolution of the numerical solution

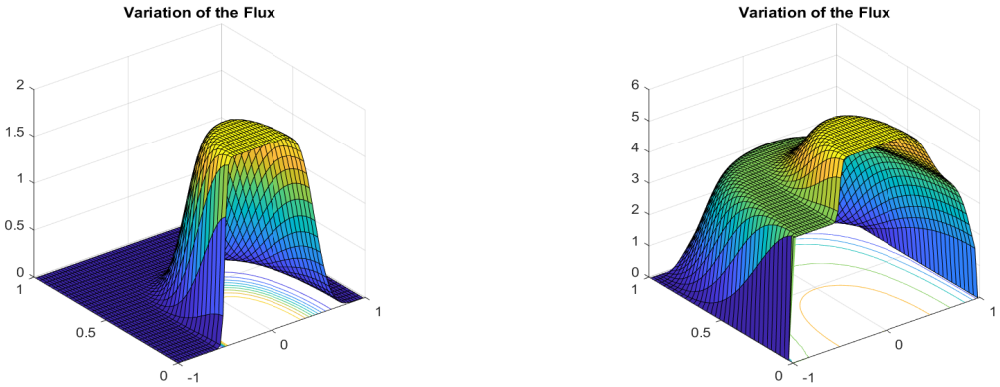


Figure 2: Schrödinger's equation solution at various times.

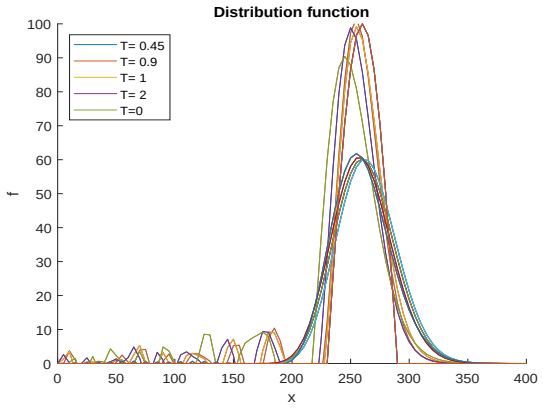


Figure 3: distribution function.

## 5 Conclusion

The numerical resolution of Schrödinger's equation has been performed using different approaches. These approaches are based on the wavelet representation of the space of the approximation. Comparison with other classical algorithms is given and an approach for the variable coefficient problem is proposed. Extensions to realistic problems with different boundary conditions and multidimension are our future research.

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