Numerical studies for Nonlinear Schrödinger equations: the Schrödinger-Poisson-Xα model and Davey-Stewartson systems

C. Besse [*], *N.J. Mauser*, [†] *H. P. Stimming* [‡]

Abstract. We study the numerical approximation and analysis of two different time dependent Nonlinear Schrödinger equations (NLS) : the "Schrödinger-Poisson-Xα" equation, which plays a role in the modeling of quantum particle dynamics, and the Davey-Stewartson system, which is a 2-d equation modeling unidirectional water surface waves. For both equations we use a Time Splitting Spectral scheme, which had previously shown to be a good tool for numerical simulation of cubic NLS. This scheme is particularly useful for calculations in the "semi-classical regime", where the scaled Planck constant is taken to be small. Extensive numerical results of position density and Wigner measures in 1d, 2d and 3d for the S-P-Xα model with/without an external potential are presented. These results give an insight to understand the interplay between the nonlocal ("weak") and the local ("strong") nonlinearity.

For the Davey-Stewartson system, we give a convergence analysis for the semi-discrete version of the scheme. Numerical results are presented for various blow-up phenomena of the equation, including blow-up of defocusing, elliptic-elliptic Davey-Stewartson systems and simultaneous blow-up at multiple locations in the focusing elliptic-elliptic system. Also the modeling of exact soliton type solutions for the hyperbolic-elliptic (DS2) system is studied.

1. Introduction

In the recent mathematics literature the name "Nonlinear Schrödinger equation" (NLS) mostly refers to the following class of Schrödinger equations with a particular "local nonlinearity" :

$$i\varepsilon\partial_t u + \frac{\varepsilon^2}{2}\Delta u = \pm\,\varepsilon^\alpha |u|^p u, \quad \mathbf{x}\in I\!R^d,\ t\in I\!R. \tag{1.1}$$

Here u is the (complex valued) "wave function" and ε is the scaled Planck constant. The equation is called "focusing NLS" for the minus sign in front of the nonlinear term and "defocusing NLS" for the plus sign. Existence and uniqueness results on

the initial value problem (IVP) have first been obtained by Ginibre and Vélo [19]. Much work has been done on this equation since, for an extensive coverage of the subject we refer to [14] and [37]. For short times, existence and uniqueness of a solution in the energy space H^1 holds if $p < 4/(d-2)$ if $d \geq 3$, and for all $p < \infty$ for $d = 1,\ 2$. The long term behaviour depends on whether the nonlinearity has focusing or defocusing sign. For defocusing NLS, the short time solution extends to all times. For the focusing NLS, this is true only if the power p is below the critical value $4/d$; for p at or above this value, finite time blowup can occur.

A quite difficult and mostly open question is the "(semi-)classical" limit of nonlinear Schrödinger equations, i.e. the passage to the limit when the "scaled Planck constant" tends to zero ($\varepsilon \to 0$). For the NLS (1.1), some results on particular cases are known. For for one dimensional defocusing cubic NLS ($p = 2$), Levermore, D. McLaughlin and Jin obtained that limit by using inverse scattering theory [22], which works for integrable systems only. Kamvissis, K. McLaughlin and Miller obtained the limit for the focusing cubic NLS by the same method [23]. Carles used a geometric argument to obtain the limit in cases where the scale exponent α is large enough and a particular geometry is given e.g. by a harmonic potential [15]. For other cases, the semiclassical limit is an open problem.

The first model we investigate is the "Schrödinger-Poisson-Xα" (S-P-Xα) equation, which is proposed as a "local one particle approximation" of the time dependent Hartree-Fock equations. It describes the time evolution of electrons in a quantum model respecting the Pauli principle in an approximate fashion [28]. It reads

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi \ + \ CV_{\text{Hartree}}\psi \ - \ \alpha|\psi|^{2/d}\psi, \quad \mathbf{x} \in I\!R^d,\ t \in I\!R\,, \tag{1.2}$$

$$\Delta V_{\text{Hartree}} = -|\psi|^2 \tag{1.3}$$

It is an NLS with two nonlinear terms of different nature: the nonlocal Hartree potential and a local power term, with focusing sign and an exponent that is subcritical for finite time blowup. Such "time dependent density functional theory" models yield approximations of the time-dependent Hartree-Fock (TDHF) equations that are much easier to solve numerically: firstly, for large number of particles N the system of coupled NLS of the TDHF system becomes too large, and secondly, the exchange terms are very costly to calculate. We will discuss the derivation of this equation in section 1.1.

The "semiclassical limit" for equation (1.2) is mostly an open problem, rigorous results have recently been given by Carles, Mauser, Stimming for a model with quadratic confinement potential only in the case of a scaling where α is $o(\epsilon)$ [16].

Our numerical approximations yield interesting insight in the behaviour of the solution in the limit, in particular they indicate the critical relative scaling of the 2 nonlinearities.

In the regime of "small" ε, it would be desirable that a numerical scheme permits a choice of discretization steps that is independent of the scale ε. Studies on finite difference discretizations of linear Schrödinger equations [29], [30] show that in

this case this is not possible, on the contrary the scale ε has to be over-resolved, which means discretization steps have to be of order $o(\varepsilon)$ to guarantee a correct approximation. On the other hand, for a scheme like ours, the work of Bao et al. [13] shows that it is possible to choose the time-step independent of ε while the space discretization step can be $O(\varepsilon)$. This scheme has proven to be a quite efficient method and hence is the method of choice for the problem. We have developed a parallel version of the scheme that also allows for 3-d semiclassical simulations of time dependent NLS.

The second model equation treated here is the Davey-Stewartson (DS) system, which is a 2-dimensional Nonlinear Schrödinger equation coupled to a potential equation. It reads, in dimensionless form,

$$\begin{aligned} i\partial_t u + \lambda\partial_x^2 u + \partial_y^2 u = \nu|u|^2 u + u\,\partial_x\phi\,, \\ \alpha\partial_x^2\phi + \partial_y^2\phi = \chi\partial_x(|u|^2)\,, \qquad (x,y) \in I\!R^2\,; t \in I\!R. \end{aligned} \tag{1.4}$$

Here u is the (complex) amplitude of the wave and ϕ the (real) potential which is generated by the mean velocity. The parameters α and λ can have both signs, according to which the system can be classified as elliptic-elliptic (E-E), elliptic-hyperbolic (E-H), hyperbolic-elliptic (H-E) and hyperbolic-hyperbolic (H-H). This system is a model for a surface wave of a fluid over a flat ground which is propagating mostly in one direction. It is valid in a situation where both gravity and the surface tension of the fluid influence the motion.

The equations can be viewed as a generalization of the cubic NLS (1.1) ($p = 2$ in (1.1)). Like the 1-d cubic NLS, the 2-d Davey-Stewartson system is (for specific values of the parameters) integrable by inverse scattering methods ([1], [2]). With respect to finite time blowup, the focusing cubic NLS is the critical case in 2 space dimensions, and hence an interesting question is given by the blowup behaviour of (focusing) DS equations and its relations to the NLS case.

We use the same time-splitting spectral scheme as before. In the present work we show numerical results for the blowup of focusing E-E equations and for exact soliton type solutions of the H-E system. We add a study of multi-focusing of the E-E system and an investigation of blowup in the H-E system, which are treated for the first time in this work (to our knowledge).

1.1. The Schrödinger-Poisson-Xα equation : a NLS for one-particle quantum dynamics of electrons

The (nonrelativistic) quantum dynamics of a system of N electrons is given by the linear N particle Schrödinger equation with Coulomb interaction. However, even for moderate N a numerical solution of this equation is out of question. A successful method to rigorously derive "mean field approximations" and other non-local "one particle" Schrödinger equations from a (linear) many-particle equation is "weak interaction limits" (see e.g. [4], [6]), i.e. a limit where the number of

particles N tends to infinity and the interaction potential among the particles is rescaled with $1/N$. Depending on the "ansatz" for the (initial) N particle wave function, different asymptotic limits of the linear N particle Schrödinger equation are obtained. For the Hartree ansatz, the case of a bounded interaction potentials has been solved as well as the Coulomb interaction case which leads to the Schrödinger-Poisson equation [4], [6].

By the Hartree-Fock ansatz, in which the antisymmetrized wave function of N fermions is taken as a "Slater determinant", a minimization of total energy yields the Hartree-Fock (HF) equations for the time-independent case. For a rigorous analysis of this stationary Hartree-Fock system and references see e.g. [27].

For the time-dependent case, the rigorous derivation of the HF equations, by means of "mean field limits", is given in [5] for the bounded potential case.

The HF exchange potential, which is the key part of this equation (system) presents a problem in numerical simulations since it is very costly to calculate, especially if the number of particles in the model becomes large. An approximation of the exchange potential is due to Slater [36] who replaces it by the local density taken to the power 1/3. This expression was first given implicitly by Dirac in the context of the exchange energy as a correction in the Thomas-Fermi model. It is also named after Gaspar and Kohn-Sham [25] where it appears with a difference of 2/3 in the factor in front. By the name "$X\alpha$ method" [17, 35], these expressions are summarized in the sense that the value of the factor is named α and taken as parameter tunable in a certain range.

Despite the successful use of this kind of local approximations of the HF exchange potential, rigorous derivations are still missing. In a particular setting of a high density limit on the torus a rigorous version of Slater's heuristic arguments to derive the $X\alpha$ exchange potential was given in [10],[11].

In order to take into account exchange effects in a time-dependent one-particle approximation, we can most simply take the more or less rigorously derived expression of the stationary case and hence add the "$X\alpha$" term, with t as additional variable, to the effective potential in the Schrödinger-Poisson model. This corresponds to "time dependent density functional theory", where the energy is expressed in terms of the local density $n(x,t)$. This yields a NLS with a "weak" nonlocal nonlinearity, and a "strong" local nonlinearity with a potential that is a power of the local density.

In a model with d space dimensions, the approximated exchange term is proportional to $n^{1/d}$, according to the derivation in [10]. In 1d, i.e. $d = 1$ in (1.5), the $X\alpha$ term is exactly what is called the "focusing cubic NLS", i.e. $-\alpha\,|\psi|^2\psi$.

We call the equations (1.5), (1.6) the "Schrödinger-Poisson-$X\alpha$" (S-P-Xα) model :

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi + C\,V_{\rm Hartree}\psi - \alpha|\psi|^{2/d}\psi + V_{\rm ext}\psi,\ \mathbf{x}\in I\!R^d,\ t\in I\!R, \quad (1.5)$$

$$\Delta V_{\rm Hartree} = -|\psi|^2, \quad (1.6)$$

$$\psi(\mathbf{x}, t=0) = \psi_I(\mathbf{x}), \quad \mathbf{x}\in I\!R^d\,; \quad (1.7)$$

where $C > 0$ is a fixed constant, $\alpha > 0$ a parameter and V_{ext} is a given external potential, for example a confining potential.

Since $C > 0$ and $\alpha > 0$, we have a repulsive Hartree interaction and a focusing local nonlinearity. The wave function ψ is used to compute the physical observables, e.g. the position density

$$n(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2, \qquad \mathbf{x} \in I\!R^d, \quad t \geq 0. \tag{1.8}$$

At ε fixed, the analysis of equation (1.5)-(1.7) in 3-d can be done by a straightforward application of standard results on NLS [14], [19], [24].

For the 1-d case, the existence and uniqueness analysis of the S-P-Xα equation is given in [39]. For the case of 2 space dimensions, the analysis of the S-P-Xα equation is open.

1.2. Davey-Stewartson systems : NLS for surface waves

Davey-Stewartson equations model free surface waves subject to the effects of both gravity and capillarity ("Gravity-Capillary waves"). In dimensionless form, they read

$$\begin{aligned} i\partial_t u + \lambda \partial_x^2 u + \partial_y^2 u &= \nu |u|^2 u + u\, \partial_x \phi \,, \\ \alpha \partial_x^2 \phi + \partial_y^2 \phi &= \chi \partial_x (|u|^2) \,, \qquad (x, y) \in I\!R^2 \,; t \in I\!R. \end{aligned} \tag{1.9}$$

u is the (complex) amplitude of the wave and ϕ the (real) potential which is generated by the mean velocity. The parameters α and λ can have both signs, according to which the system can be classified as elliptic-elliptic (E-E), elliptic-hyperbolic (E-H), hyperbolic-elliptic (H-E) and hyperbolic-hyperbolic (H-H).

The equations can be viewed as a generalization of the cubic Nonlinear Schrödinger equation (NLS)

$$i\partial_t u + \Delta u = \nu |u|^2 u. \tag{1.10}$$

The 2-d Davey-Stewartson (DS) system is (for specific values of the parameters) integrable by inverse scattering methods ([2]), as is the cubic NLS in 1-d. Therefore it generalizes the inverse Scattering theory in 2 dimensions [1]. With respect to finite time blowup, the focusing cubic NLS is the critical case in 2 space dimensions, and an interesting question is the blowup behaviour of (focusing) DS equations and its relations to the NLS case.

For the following invariance properties to hold we need to assume that the solution (u, ϕ) of (1.9) is sufficiently smooth and decaying at infinity. This restricts the result to the case $\alpha > 0$ where the equation for ϕ is of elliptic type. If this

assumption is satisfied, then the following functionals are independent of time:

$$N(u) = \int_{\mathbb{R}^2} |u|^2 dxdy \tag{1.11}$$

$$J_x(u) = \int_{\mathbb{R}^2} (u\overline{\partial_x u} - \overline{u}\partial_x u)dxdy \tag{1.12}$$

$$J_y(u) = \int_{\mathbb{R}^2} (u\overline{\partial_y u} - \overline{u}\partial_y u)dxdy \tag{1.13}$$

$$H(u) = \int_{\mathbb{R}^2} \mu|\partial_x u|^2 + \lambda|\partial_y u|^2 + \frac{1}{2}(\nu|u|^4 - \nu_1\beta(\partial_x\phi^2 + \alpha\partial_y\phi^2))dxdy \tag{1.14}$$

The (straightforward) proof is omitted here and can be found for example in [37].

For the derivation from a physical model and an overview of existence results by Ghidaglia *et al.* and Hayashi *et al.* we refer to [9], [18], [20].

The paper is organized as follows: in section 2, we will discuss the time splitting scheme and give a convergence proof for the DS equations for the Strang splitting method. In section 1.1, we consider the S-P-Xα model and present numerical results of position density and Wigner measures with/without an external potential. Section 1.2 deals with the DS system, where we present numerical results on H-E DS and focusing and defocusing E-E DS.

2. Time splitting spectral methods for Nonlinear Schrödinger equations

In order to approximate (1.2) and (1.4) numerically, we adapt the time-splitting spectral code of [13] ("Fourier split-step method" [40]). The method goes back to the '70 s ([21]) and was recently used and studied for NLS in the semi-classical regime. It showed much better spatial and temporal resolution than finite difference methods [29], [30]. It is hence also the method of choice for the equations treated here. White and Weideman [41] applied it for the first time to DS systems in the E-H and H-E cases.

The semi-discrete version of the splitting method was recently proved convergent for Nonlinear Schrödinger equations with local Lipschitz nonlinearities [7]. In [34], Papanicolaou *et al.* studied the self-focusing of E-E DS equations by a numeric resolution of the blowup. Besse and Bruneau [8] have successfully applied a finite difference method with time relaxation to the general DS equations.

The idea behind the time-splitting method is to decouple the nonlinear system into a linear PDE with constant coefficients, which can be discretized in space by a spectral method or by a classical finite difference method, and a nonlinear equation which can be solved exactly.

Let us consider a very general form of the NLS, which allows to summarize both models we consider, i.e. (1.5) and (1.9):

$$\begin{cases} i\varepsilon\partial_t u + \varepsilon^2 L_\lambda u = F(u), & \mathbf{x} \in I\!R^d,\ t > 0, \\ u(\mathbf{x}, 0) = u_0(\mathbf{x}), & \mathbf{x} \in I\!R^d, \end{cases} \tag{2.1}$$

Here, $L_\lambda = \Delta$ in case of (1.2) or $L_\lambda = \lambda\partial_x^2 + \partial_y^2$, with $\lambda = \pm 1$, for (1.4). ε is set to one in (1.4), and $F(u)$ denotes the nonlinear terns in the respective equations. The split-step method is based on a decomposition of the flow of (2.1).

Indeed, let us define the flow X^t of the linear Schrödinger equation

$$\begin{cases} i\varepsilon\partial_t v + \varepsilon^2 L_\lambda v = 0, & \mathbf{x} \in I\!R^2,\ t > 0, \\ v(\mathbf{x}, 0) = v_0(\mathbf{x}), & \mathbf{x} \in I\!R^2, \end{cases} \tag{2.2}$$

and Y^t as the flow of the nonlinear differential equation

$$\begin{cases} i\varepsilon\partial_t w = F(w) & \mathbf{x} \in I\!R^2,\ t > 0, \\ w(\mathbf{x}, 0) = w_0(\mathbf{x}), & \mathbf{x} \in I\!R^2. \end{cases} \tag{2.3}$$

Then, the splitting method consists of combining the two flows X^t and Y^t. The best known methods are the following: the most simple "Lie formula" given by $Z^t_{L_1} = X^t Y^t$ (or $Z^t_{L_2} = Y^t X^t$) and the "Strang splitting" $Z^t_S = Y^{t/2} X^t Y^{t/2}$ (or $X^{t/2} Y^t X^{t/2}$), which usually yields a higher order of convergence.

2.1. Convergence of the split-step method for DS systems

In this section, we are concerned with equation (1.9) (so ε is set to 1) in the case of a subsonic wave packet, that is the E-E or H-E versions of the DS system. This system can then be written as a single equation for u (see [18]). We set $\phi_x = E(|u|^2)$, where the singular integral operator E is defined in Fourier variables by

$$\widehat{E(f)}(\xi_1, \xi_2) = \frac{\xi_1^2}{\xi_1^2 + \xi_2^2} \hat{f}(\xi_1, \xi_2). \tag{2.4}$$

Therefore, the E-E or H-E DS system reduces to a nonlinear, non-local Schrödinger equation

$$i\partial_t u + L_\lambda u = \nu|u|^2 u + \nu_1 E(|u|^2) u = F(u) \tag{2.5}$$

where $L_\lambda = \lambda\partial_x^2 + \partial_y^2$ with $\lambda = \pm 1$.

We use the first Strang formulation $Z^t_S = Y^{t/2} X^t Y^{t/2}$. For a general nonlinear Schrödinger equation, the convergence proof for this method has been done in [7]. Note that there Besse *et al.* actually prove the convergence result only for initial data belonging to H^4, which does not work for E-E or H-E versions of DS. Hence the proof must be adapted for initial data belonging to H^2.

To state the convergence result, we define a new flow S^t which gives the solution of (2.5) as

$$u(\mathbf{x},t) = S^t u_0(\mathbf{x}) = X^t u_0(\mathbf{x}) - i\int_0^t X^{t-s} F(u(\mathbf{x},s))ds. \tag{2.6}$$

The result, proven in [9], is:

Theorem 2.1. *For all u_0 in H^2 and for all $0 < T < T^*$, there exists C and h_0 such that for all $h \in (0, h_0]$, for all n such that $nh \leq T$*

$$\left\| \left(Z_S^h\right)^n u_0 - S^{nh} u_0 \right\| \leq C(\|u_0\|_{H^2})h\|u_0\|_{H^2}. \tag{2.7}$$

Here $\|\cdot\|$ denotes the L^2 norm. We will give a sketch of the proof which is done in [9].

The key of the proof is to prove that the nonlinearity $F(u)$ is Lipschitz, and an applicatoin of the following estimates of the separated flows:

2.1.1. Estimates on the flows X^t and Y^t From the definition of the Schrödinger flow, we first have

$$\dot{X}^t = iL_\lambda X^t = iX^t L_\lambda. \tag{2.8}$$

As the flow X^t is a unitary group on H^2, we have

$$\|X^t u_0\|_{H^2} = \|u_0\|_{H^2} \tag{2.9}$$

For the nonlinear flow Y^t, by a simple calculation ([13]), it follows from (2.3) and the explicit form of F that

$$|Y^t w| = |w|,$$

and with this result, an alternative way to define it is

$$Y^t w = e^{-i(\nu|w|^2 + \nu_1 E(|w|^2))t} w. \tag{2.10}$$

We immediately get for all $t \in [0, T]$

$$\|Y^t w\|_{H^2} \leq \|w\|_{H^2}. \tag{2.11}$$

By a Gronwall argument and the above results, the error for a single step of length t of the Lie method L_ν can be bounded by a $O(t^2)$ term. From this the same can be deduced for the Strang splitting.

Next it is shown that the Strang method Z_S^t is Lipschitz, with a Lipschitz constant $1 + C_0 t$. By an expansion via the triangle inequality, the error term in (2.7) is expressed by the single step error which gives the result.

2.2. The time splitting spectral scheme for DS Systems

The crucial advantages of the time-splitting spectral method are that it is fully explicit, unconditionally stable, time reversible, and time-transverse invariant [13].

We use the Strang splitting method, $Z_S^t = Y^{t/2} X^t Y^{t/2}$. The linear flow X^t is solved by a spectral Fourier method and the nonlinear flow Y^t by exact integration via formula (2.4).

We choose a square domain $[a,b]^2$ and the same grid size in x- and y-direction, $\Delta x = \Delta y = (b-a)/M$ for an even, positive integer M. The time step is Δt and the grid points are $(x_j, y_k) = (a + j\Delta x, a + k\Delta x)$, $t_n = n\Delta t$. The approximation of $u(x_j, y_k, t_n)$ is denoted u_{jk}^n, and u^n is the solution matrix at time t_n with components u_{jk}^n. We impose periodic boundary conditions for a sufficiently fast decaying u in order to apply the spectral method.

In detail, the method is:

$$
\begin{aligned}
\mathtt{u}_{jk}^* &= \frac{1}{M^2} \sum_{l=-M/2}^{M/2-1} \sum_{m=-M/2}^{M/2-1} e^{-i(\alpha\mu_l^2+\mu_m^2)\,\Delta t/2}\ \widehat{(u^n)}_{lm}\ e^{i(\mu_l(x_j-a)+\mu_m(x_k-a))}, \\
& j,k = 0,1,2,\cdots,M-1, \\
E_{jk}^* &= \frac{1}{M^2} \sum_{-M/2\le l,m\le M/2-1,(l,m)\neq(0,0)} \frac{\beta\nu_1\mu_l^2}{\mu_l^2+\mu_m^2} \widehat{(|u^*|^2)}_{lm}\ \ e^{i(\mu_l(x_j-a)+\mu_m(x_k-a))}, \\
& j,k = 0,1,2,\cdots,M-1, \\
u_{jk}^{**} &= e^{-i(E_{jk}^*+\nu|u_{jk}^*|^2)\ \Delta t}\ u_{jk}^*, \qquad j,k = 0,1,2,\cdots,M-1, \\
\mathtt{u}_{jk}^{n+1} &= \frac{1}{M^2} \sum_{l=-M/2}^{M/2-1} \sum_{m=-M/2}^{M/2-1} e^{-i(\alpha\mu_l^2+\mu_m^2)\,\Delta t/2}\ \widehat{(u^{**})}_{lm}\ e^{i(\mu_l(x_j-a)+\mu_m(x_k-a))}, \\
& j,k = 0,1,2,\cdots,M-1.
\end{aligned}
$$

Here $\widehat{U}_{l,m}$ $(l,m = -M/2,\cdots,M/2-1)$ is the 2-D discrete Fourier transform of a (periodic) matrix U:

$$
\widehat{U}_{l,m} = \sum_{j=0}^{M-1} \sum_{k=0}^{M-1} U_{jk}\ e^{-i(\mu_l(x_j-a)+\mu_m(x_k-a))}, \quad \mu_l = \frac{2\pi}{b-a} l, \quad l,m = -\frac{M}{2},\cdots,\frac{M}{2}-1.
$$

2.3. Time-splitting spectral scheme for the Schrödinger-Poisson-Xα equation

As for the previous equation, we impose periodic boundary conditions for convenience to use the spectral method. By choosing a sufficiently large domain of computation we can avoid spurious effects for the time regime we regard.

For simplicity of notation we introduce the method in one space dimension $(d = 1)$. Generalizations to $d > 1$ are immediate for tensor product grids.

We choose the spatial mesh size $h = \Delta x = (b-a)/M > 0$ with M an even positive integer, the time step $k = \Delta t > 0$, and denote $x_j = a + jh$ $(j = 0,\ldots,M)$,

$t_n = nk$ $(n = 0, 1, \ldots)$ the grid points. Let u_j^n be the approximation of $u(x_j, t_n)$ and u^n be the solution vector with components u_j^n.

The linear flow X^t will be discretized in space by the Fourier spectral method due to the periodic boundary conditions and integrated in time exactly. For $t \in [t_n, t_{n+1}]$, the nonlinear flow Y^t leaves $|u|$ invariant in t [13] and therefore becomes

$$\partial_{xx} V_{\text{Hartree}} = -|u(x,t_n)|^2, \tag{2.12}$$

$$i\varepsilon \partial_t u(x,t) = C V_{\text{Hartree}}\ u(x,t) - \alpha |u(x,t_n)|^{2/d} u(x,t) + V_{\text{ext}} u(x,t). \tag{2.13}$$

Equation (2.12) will be discretized by the Fourier spectral method when $|u|$ is given and (2.13) can be integrated exactly. From time $t = t_n$ to $t = t_{n+1}$, we use the Strang splitting formula:

$$u_j^* = \frac{1}{M} \sum_{l=-M/2}^{M/2-1} e^{-i\varepsilon \mu_l^2\, k/4}\ \widehat{(u^n)}_l\ e^{i\mu_l (x_j - a)}, \quad j = 0, 1, 2, \cdots, M-1,$$

$$(V_{\text{Hartree}})_j^* = \frac{1}{M} \sum_{-M/2 \le l \le M/2-1,\ l \neq 0} \widehat{(|u^*|^2)}_l / \mu_l^2\ \ e^{i\mu_l (x_j - a)},$$

$$j = 0, 1, 2, \cdots, M-1,$$

$$u_j^{**} = e^{-i[C\ (V_{\text{Hartree}})_j^* + V_{\text{ext}}(x_j) - \alpha |u_j^*|^{2/d}] k/\varepsilon}\ u_j^*, \qquad j = 0, 1, 2, \cdots, M-1,$$

$$u_j^{n+1} = \frac{1}{M} \sum_{l=-M/2}^{M/2-1} e^{-i\varepsilon \mu_l^2\, k/4}\ \widehat{(u^{**})}_l\ e^{i\mu_l (x_j - a)}, \quad j = 0, 1, 2, \cdots, M-1;$$

where $\widehat{U}_l$ $(l = -M/2, \cdots, M/2-1)$, the Fourier coefficients of a vector $U = (U_0, U_1, \cdots, U_M)^T$ with $U_0 = U_M$, are defined as

$$\mu_l = \frac{2\pi l}{b-a}, \qquad \widehat{U}_l = \sum_{j=0}^{M-1} U_j\ e^{-i\mu_l (x_j - a)}, \quad l = -\frac{M}{2}, \cdots, \frac{M}{2} - 1. \tag{2.14}$$

2.4. Realization on a parallel machine

For simulations in 3 space dimensions with a satisfactory space resolution a large amount of memory is needed, exceeding the limitations of standard single processor computers. For such simulations parallel computers are very appropriate. This requires of course an adaptation of the code which can not be done automatically.

We are using the cluster "Schrödinger 2" of the University of Vienna, which currently features 192 Pentium IV processors, with about 1 GB memory each, linked by a switched gigabit network. The machine's LINPACK performance ranges among the fastest available.

As the above table shows, 64 nodes of this parallel machine are sufficient for 3-d simulations with a resolution with about 1000 points in each space dimension.

Table 1: Memory requirement for 3-d calculation

Resolution	Memory requirement
256 points per dimension	$8 \cdot 10^8$ byte = 768 MB
512 points per dimension	$6.4 \cdot 10^9$ byte = 6.4 GB
1024 points per dimension	$5.1 \cdot 10^{10}$ byte = 48 GB
16 byte numbers (type 'double complex'), 3 instances needed	

We use the MPI parallelization interface to adapt the code for distributed memory parallelization and compile it with "ifc", a Fortran compiler made by Intel. Hence both the compiler and the processor hardware come from the same manufacturer, which made it relatively easy to generate code optimized specifically for the used processor type and to obtain a quite good performance.

The main workload of the scheme, and the only part of the actual algorithm which needs to be adapted for parallelization, consists of Fast Fourier transforms. We implemented a parallel version FFT code on the cluster "Schrödinger 2" and test the performance of the parallelization which is listed in Table 2.

We see from table 2 that the code has a good degree of parallelization in the sense that most of the work seems to be evenly distributed among the nodes and calculation time decreases linearly with the number of nodes used. (The final version of the machine is actually faster than in table 2, reducing the required CPU time once more.)

Table 2: Performance

	256^3 grid points, walltime	
Number of nodes	50 time steps	500 time steps
2	1527 s	14760 s
4	812 s	7860 s
8	432 s	4020 s

In all our 3d simulations, we use the parallel code of the time-splitting spectral method (TSSP) to compute our numerical results. We also used the parallel version of the scheme for the study of blow-up in E-E DS systems.

3. Numerical results

3.1. Numerical results for S-P-Xα

In this section, we will present 1-d and 3-d numerical results of the S-P-Xα model (1.2) by using the time-splitting spectral discretization.

In our computations, the initial condition (1.7) for (1.5) is always chosen in WKB form:

$$\psi(\mathbf{x}, t=0) = \psi_I(\mathbf{x}) = A_I(\mathbf{x}) e^{i\, S_I(\mathbf{x})/\varepsilon}, \qquad \mathbf{x} \in I\!R^d, \tag{3.1}$$

with A_I and S_I real valued, regular and with A_I decaying to zero sufficiently fast as $|\mathbf{x}| \to \infty$. We always compute on a domain which is large enough (as controlled by the initial data and how long in time to compute) such that the periodic boundary conditions do not introduce a significant aliasing error relative to the whole space problem. To visualize our numerical results, we consistently present the position density $n(\mathbf{x}, t)$ which is defined as

$$n(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2, \qquad \mathbf{x} \in I\!R^d.$$

Example 1. 1-d S-P-Xα model, i.e. we choose $d = 1$, $V_{\text{ext}} \equiv 0$, $C = 1$ in (1.5). Note that the local interaction term in (1.5) is the "focusing cubic NLS interaction" in the case $d = 1$. The initial condition (3.1) is hence taken the same as in the simulations of [32]:

$$A_I = e^{-x^2}, \qquad \frac{d}{dx} S_I(x) = -\tanh(x), \qquad -\infty < x < \infty. \tag{3.2}$$

Note that S_I is such that the initial phase is "compressive". This means that even the linear evolution develops caustics in finite time. We solve this problem either on the interval $x \in [-4, 4]$ or on $x \in [-8, 8]$ depending on the time for which the solution is calculated.

We present numerical results for four different regimes of α:

Case I. $\alpha = 0$, i.e Schrödinger-Poisson regime;
Case II. $\alpha = \varepsilon$, i.e. Schrödinger-Poisson equation with $O(\varepsilon)$ cubic nonlinearity;
Case III. $\alpha = \sqrt{\varepsilon}$, i.e. Schrödinger-Poisson equation with $O(\sqrt{\varepsilon})$ cubic nonlinearity;
Case IV. $\alpha = 1$, i.e. Schrödinger-Poisson equation with $O(1)$ cubic nonlinearity.

Figure 1 displays comparisons of the position density $n(x, t)$ at fixed time for the above four different parameter regimes with different ε. Figure 2 plots the evolution of the position density and the Wigner transforms of the wave function for $\alpha = 1$ and $\varepsilon = 0.025$. Figure 3 shows the analogous results for attractive Hartree interaction, i.e. $C = -1$, $\alpha = 0.5$ and $\varepsilon = 0.025$.

From Figure 1, we can see that before the break (part a) and b)), the result is essentially independent of ε. After the break the behavior of the position density changes substantially with respect to the different regimes of α. For $\alpha = 0$ the solution stays smooth. For $\alpha = \varepsilon$ it stays also smooth, but it concentrates at the origin. For $\alpha = \sqrt{\varepsilon}$ a pronounced structure of peaks develop, that look like the

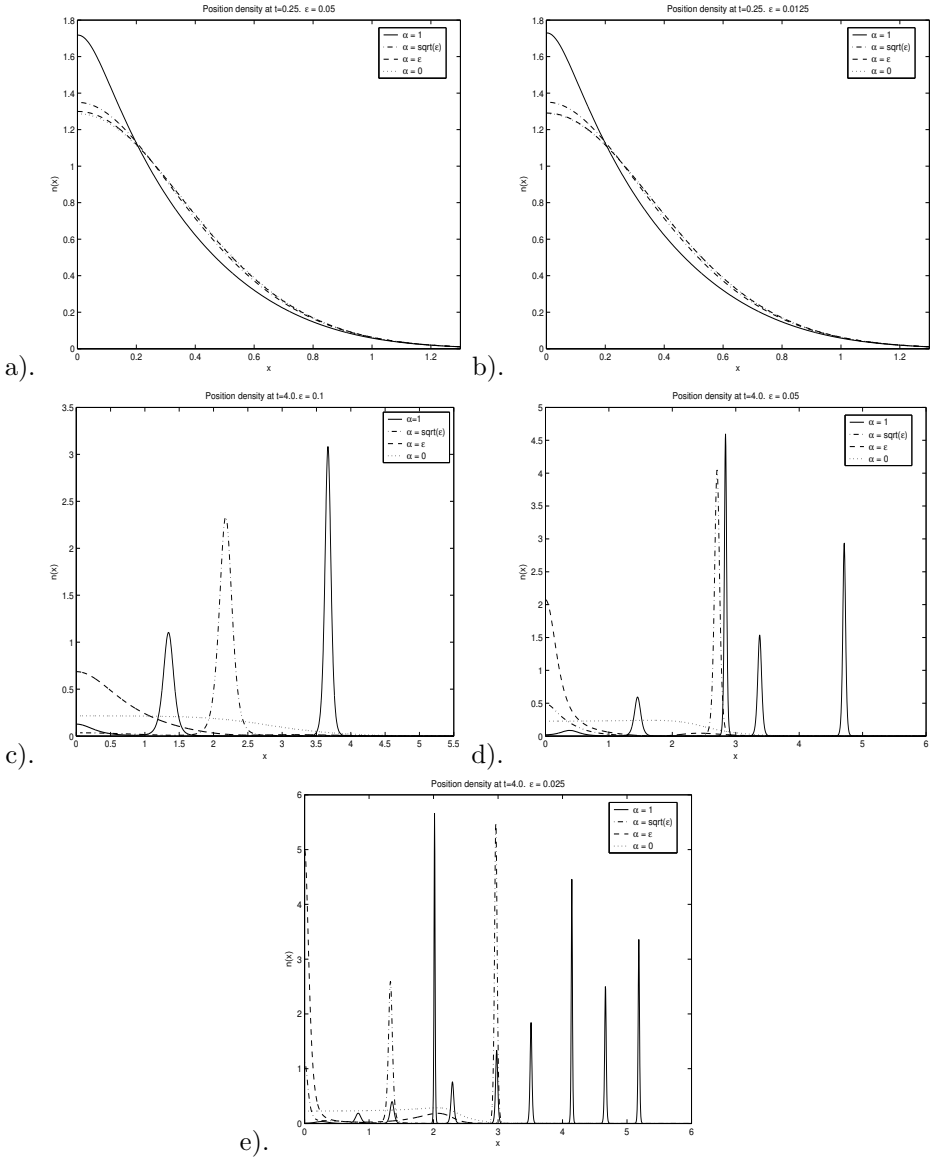


Figure 1: Numerical results for different scales of the Xα term, i.e. $\alpha = 1,\ \sqrt{\varepsilon},\ \varepsilon,\ 0.$ a) and b): small time $t = 0.25$, pre-break, a) for $\varepsilon = 0.05$, b) for $\varepsilon = 0.0125$. c) - e): large time, $t = 4.0$, post-break. c) for $\varepsilon = 0.1$, d) for $\varepsilon = 0.05$, e) for $\varepsilon = 0.025$.

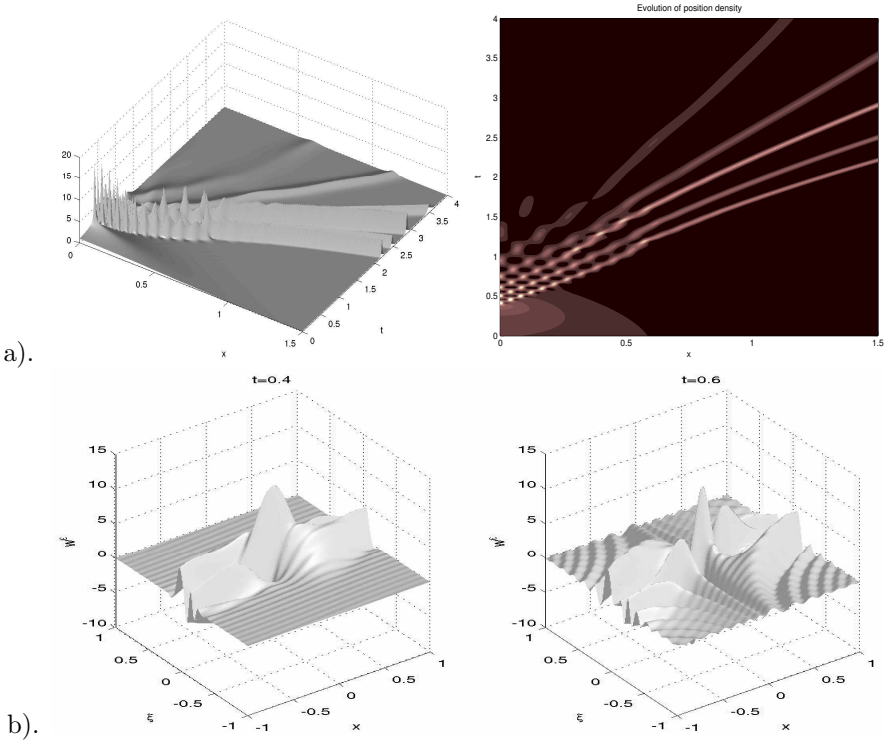


Figure 2: Numerical results for Xα term at $O(1)$, i.e. $\alpha = 0.5$, with $\varepsilon = 0.025$, $h = 1/512$ and $k = 0.0005$. a). Time evolution of the position density $n(x,t) = |\psi(x,t)|^2$: Left: surface plot; Right: pseudocolor plot. b). Wigner function $W[\psi(x,t)]$ at different times.

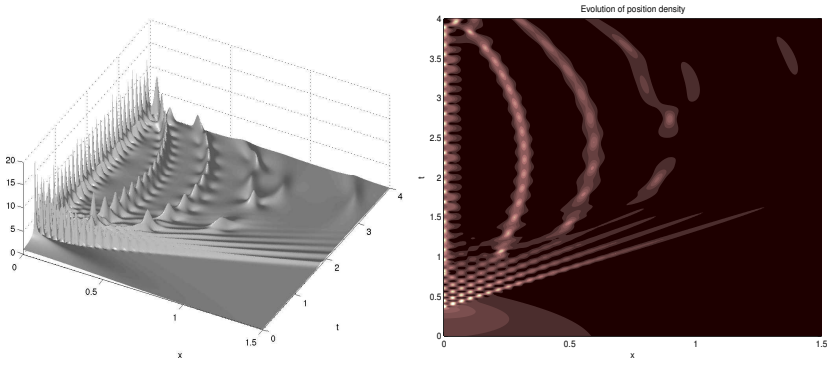


Figure 3: Time evolution of the position density for attractive Hartree interaction, i.e. $C = -1$, $\alpha = 0.5$, $\varepsilon = 0.025$, $\Delta t = 0.00015$. Left: surface plot; right: pseudocolor plot.

soliton structure typical for the NLS [23]. The number of peaks is doubled when ε is halved. For $\alpha = 1$, the number of peaks increases again and they occur at different locations than for $\alpha = \sqrt{\varepsilon}$.
We can see that the scaling $\alpha = \mathrm{O}(\sqrt{\varepsilon})$ is critical in the sense that the solution has a substantially different behavior than for the smaller scales of α. Beyond this scaling, the semiclassical limit cannot be obtained by naive numerics.

Figure 2 b) shows how the Wigner function completely changes its qualitative behaviour after the "break time" ("caustic") and develops a rich structure of oscillations.

Figure 3 is a test to see what happens if the Hartree potential is attractive instead of repulsive, with all other parameters kept the same, i.e. Figure 2 a) and Figure 3 differ only by the sign of C. The resulting effect corresponds to the physical intuition that the pattern of caustics that is typical for the focusing NLS would be enhanced and focused in physical space by an additional attractive force.

Example 2. 3-d S-P-Xα model, i.e. we choose $d = 3$, $V_{\text{ext}} \equiv 0$, $C = 1$ in (1.5). We consider the following initial data with nonzero phase:

$$A_I(x, y, z) = e^{-(x^2+y^2+z^2)}, \quad S_I(x, y, z) = -\ln\cosh\left(\sqrt{x^2 + y^2 + z^2}\right). \tag{3.3}$$

We solve this problem on the box $[-8, 8]^3$. We present numerical results for four different regimes of α:

Case I. $\alpha = 0$, i.e Schrödinger-Poisson regime;
Case II. $\alpha = \varepsilon$, i.e. Schrödinger-Poisson equation with Xα nonlinearity at $O(\varepsilon)$;
Case III. $\alpha = \sqrt{\varepsilon}$, i.e. Schrödinger-Poisson equation with Xα nonlinearity at $O\left(\sqrt{\varepsilon}\right)$;
Case IV. $\alpha = 1$, i.e. Schrödinger-Poisson equation with Xα nonlinearity at $O(1)$.

Figure 4 displays comparisons of the position density $n(x, y, z = 0, t = 4)$ and evolution of the position density $n(x, 0, 0, t)$ for the 4 different parameter regimes case I to IV, with $\varepsilon = 0.1$.

The simulations of figure 4 show again that the critical scaling is at $\alpha = O(\sqrt{\varepsilon})$ - a careful examination of figure b) shows also a less regular behaviour than for c) and d). For $\alpha = O(\varepsilon^2)$ the figure is virtually the same as for $\alpha = 0$, so we skipped that plot. Hence in some physical situations, we can conclude that in case that the "local exchange term" occurs only at $O(\varepsilon^2)$ the effect of the Pauli principle can be neglected and the Schrödinger-Poisson model is sufficiently precise.

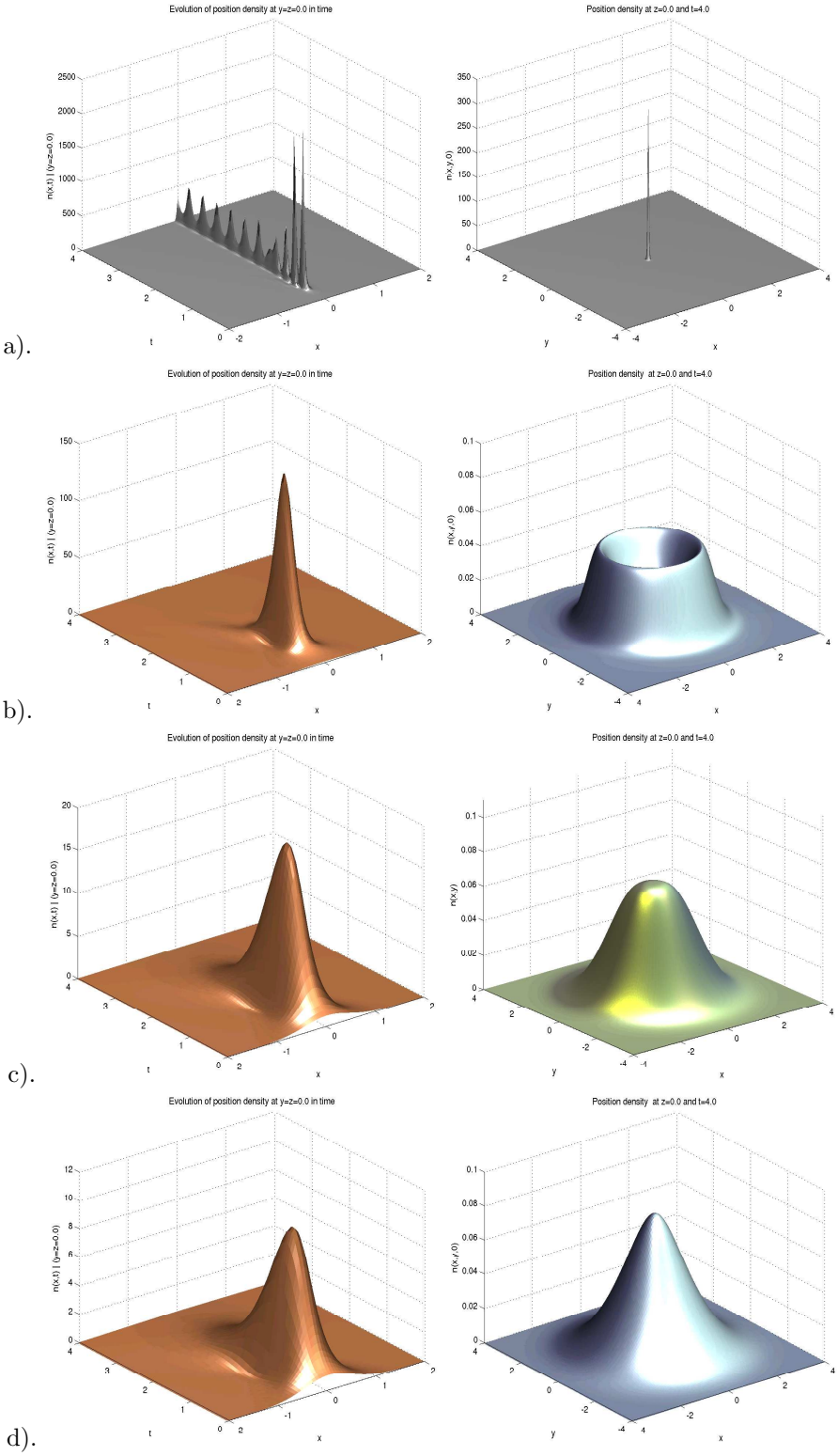


Figure 4: Numerical results for 3d S-P-Xα model in example 3 with $C = 1$, $\varepsilon = 0.1$, $V_{\text{ext}} \equiv 0$ for different regime of the parameter α. Left: Evolution of position density on $y = z = 0$, i.e. $n(x, 0, 0, t)$; Right: Position density at time $t = 4$ on $z = 0$, i.e. $n(x, y, 0, t = 4)$. a). $\alpha = 1$; b). $\alpha = \sqrt{\varepsilon}$; c). $\alpha = \varepsilon$; d). $\alpha = 0$.

3.2. Numerical Results for Davey-Stewartson systems

3.2.1. Hyperbolic-Elliptic DS System

Exact solutions In the long wavelength limit, the system (1.9) becomes

$$i\partial_t\psi - \sigma_1\partial_\xi^2\psi + \partial_\eta^2\psi = \sigma_1|\psi|^2\psi + \psi\partial_\xi\phi\,, \tag{3.1}$$

$$\sigma_1\partial_\xi^2\phi + \partial_\eta^2\phi = \partial_\xi(|\psi|^2)\,, \qquad \mathbf{x}\in I\!R^d\,; t\in I\!R. \tag{3.2}$$

where $\sigma_1 = \pm 1$. This system has the remarkable property of being integrable by inverse scattering and is called "DS1" or "DS2" system according to the value of σ_1.

The Hyperbolic-Elliptic system (3.1)-(3.2) with $\sigma_1 = 1$, is called "DS2". Arkadiev et al. [2] proved, by inverse scattering methods, the existence of a class of exact solutions. These show localized structures getting displaced without dispersion and for this reason are said to be of "Soliton type". To formulate these solutions we first rewrite the equation as

$$iu_t + \partial_x^2 u - \partial_y^2 u = -2\chi|u|^2u - u\phi_x$$
$$\Delta\phi = -4\chi(|u|^2)_x.$$

Then the exact solution is

$$u(x,y,t) = \frac{2\bar\nu\exp(x(\lambda-\bar\lambda) + iy(\lambda+\bar\lambda) + 2it(\lambda^2+\bar\lambda^2))}{|x+iy+\mu-2i\lambda t|^2 - \chi|\nu|^2}.$$

where $\nu, \mu, \lambda \in \mathcal{C}$ are parameters. We choose $\chi = -1$ and $\nu = \mu = \lambda = 1$. With this choice the expression of the solution is

$$u(x,y,t) = \frac{4\exp(iy+2it)}{(x+1)^2 + (y-2t)^2 + 1}.$$

Figure 5 shows the initial data at $t_0 = -3.5$, it is a hump centered at $x = -1$, $y = -7 = 2\cdot t_0$. This solution has only geometric decay towards infinity, which poses a problem for our scheme which needs to rely on a rapid decay of solutions to prevent errors from the artificial periodic boundary conditions. To prevent such errors we need to take a rather large domain, we choose $\Omega = [-16, 16]^2$. Figure 6 shows contour plots of $|u|$ at different times during the evolution. We can see that the "soliton structure" is traveling in y-direction at speed 2 as required. Also the shape of the solution is preserved accurately.

Blowup of H-E System The next test case for the DS2 equation is the case of a finite time blowup studied by Ozawa [33], where an exact solution is constructed which blows up at a given time. The initial data are $u_0(x,y) = \frac{\exp(i(x^2-y^2))}{1+x^2+y^2}$, which is a localized lump with algebraic decay (as in the previous case). By the construction we know that the blowup time is $t_* = 0.25$ and $\|u(t)\|_{L_\infty} = 1/(1-4t)$ holds for he exact solution.

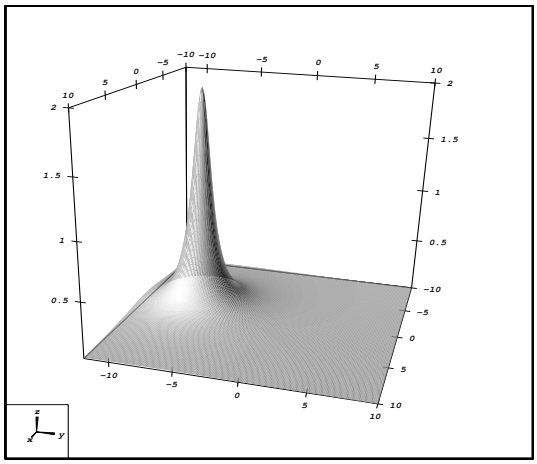


Figure 5: Exact solution at time $t_0 = -3.5$.

In this test we found the code to be very sensitive to cutoff errors from the artificial boundary conditions. We need to calculate on the domain $[-40, 40]^2$ to get reasonable results. Figure 7 shows the blowup for three different choices of the resolutions (upper line $\Delta x = 0.01953$, $\Delta t = 10^{-4}$, middle line $\Delta x = 0.039$, $\Delta t = 2.5 \cdot 10^{-4}$, lower line $\Delta x = 0.0781$, $\Delta t = 5 \cdot 10^{-4}$), and the exact rate stated above as a dashed line. We can see that, if the discretization is chosen fine enough, we can recover the correct blowup rate. Figure 8 shows the position density close to the blowup time.

3.2.2. Elliptic-Elliptic DS System

Finite time blowup In this section we treat the elliptic - elliptic DS system

$$\begin{aligned} iu_t + \Delta u &= \chi |u|^2 u + u\phi_x \\ \Delta \phi &= -\gamma (|u|^2)_x. \end{aligned} \tag{3.3}$$

Finite time blowup of this system was studied by Ghidaglia and Saut [18]. As mentioned in section 1, (3.3) always leads to blow-up either if $\chi = -1$, for any γ, or if $\chi = 1$ and $\gamma > \chi$. We choose the initial data profile

$$u_I(x, y) = 4 \exp\left(\frac{-x^2 - y^2}{4}\right).$$

First we investigate the case $\chi = -1$ (focusing nonlinearity) and set $\chi = -1$, $\gamma = 1$. This case is analogous to the focusing NLS, since for $\gamma = 0$, (3.3) reduces to the focusing cubic NLS, which in two space dimensions is the critical case for finite-time blowup. We expect the blowup mechanism to be similar to the one of that equation. We find that the solution blows up at time $t = 0.1311$. Figure 9 shows the L^∞-norm of u. Papanicolaou *et al.* ([34]) analytically found that the

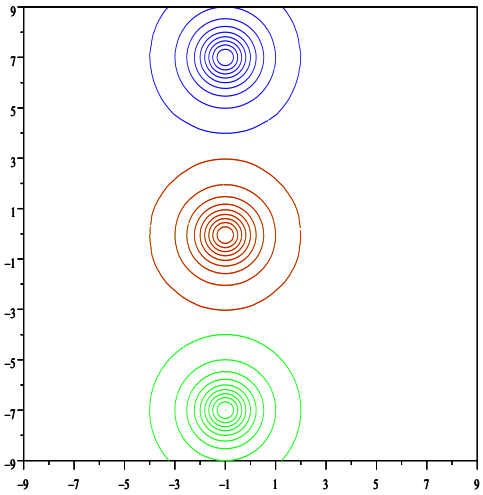


Figure 6: Traveling "soliton" at times $t = -3.5,\ 0,\ 3.5$.

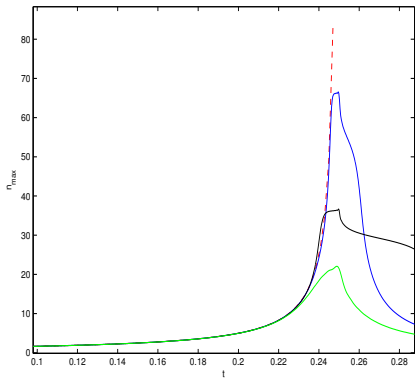


Figure 7: L^∞-norm of blowup solution for increasingly refined discretizations. Dashed line is analytic blowup rate.

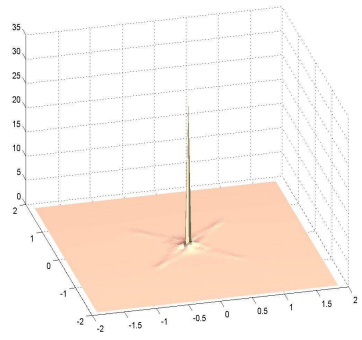


Figure 8: Position density close to blowup.

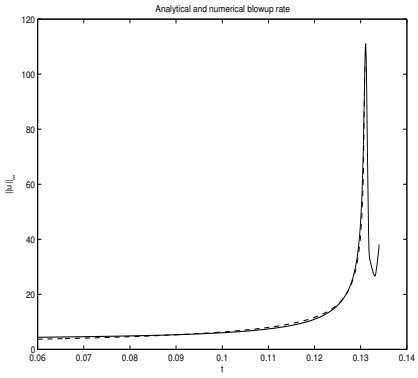


Figure 9: L^∞ norm of $|\Psi|$ and analytical blowup rate.

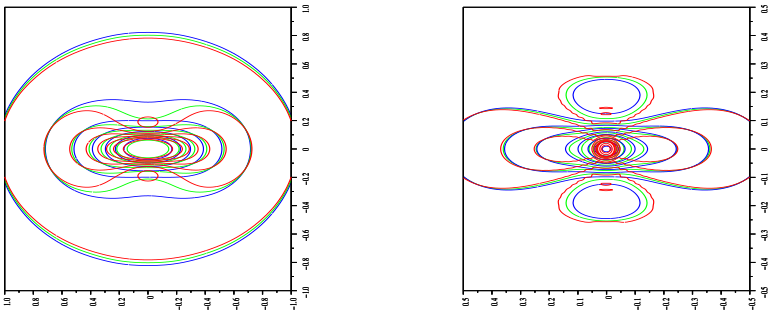
solution blows up at the rate

$$L(t) \approx (t_* - t)^{\frac{1}{2}} \left(\ln \ln \frac{1}{t_* - t} \right)^{-\frac{1}{2}} .$$

This rate is the same as the one for the critical NLS (Landman *et al.* [26], see also [37]). In figure 9, we added as a dashed line the analytic blowup by the above formula, with t_* at the value we found for our computation. It can be observed that the rate of blowup is recovered quite accurately.

Figure 10 shows contours of $|u|^2$ near the focus. A distinct anisotropy can be observed.

Next we investigate the case $\chi = 1$ (defocusing nonlinearity) and choose $\chi = 1$, $\gamma = 5$. In this case the second nonlinear term is causing the blowup. The corresponding L^∞-norm of u is shown in figure 11. In this case the blowup is more complicated, there is a first concentration at $t = 0.1$ before the blowup at



a) b)

Figure 10: Contour plot of position densities: a) before blowup, at $t = 0.12$, $t = 0.124$, $t = 0.128$, b) close to blowup, at $t = 0.1298$, $t = 0.1304$, $t = 0.1308$.

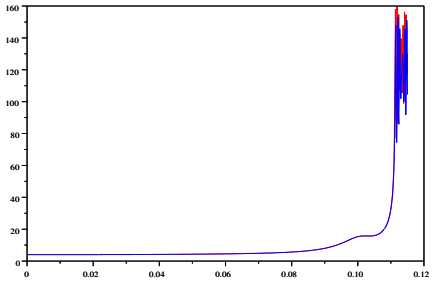


Figure 11: Blowup of defocusing ell.-ell. system ($\nu = 1$, $\beta = 5$). L^∞ norm of $|\Psi|$ for different time discretization steps. blue: $\Delta t = 5 \cdot 10^{-5}$; red: $\Delta t = 2.5 \cdot 10^{-5}$,

$t = 0.1115$. A much finer time and space resolution is needed to capture this blowup correctly. Figure 12 shows the maximum values of $|u|^2$ around the blowup time for several resolutions.

Figure 13 shows contours of $|u|^2$ close to the blowup, figure 14 shows surface plots. We can see that there is more anisotropy in the results for this case than in the previous, NLS-dominated case.

Multi-Focusing For the focusing critical NLS, according to a result of Merle [31] it is possible to construct a solution which blows up exactly at a prescribed set of points. We will state his result. Let, in $\mathbb{R}^d$ with a general dimension d, $R_0, R_1, \ldots$ be the infinite sequence of radial solutions to the equation

$$\Delta R - R + R^{\frac{4}{d}+1} = 0$$

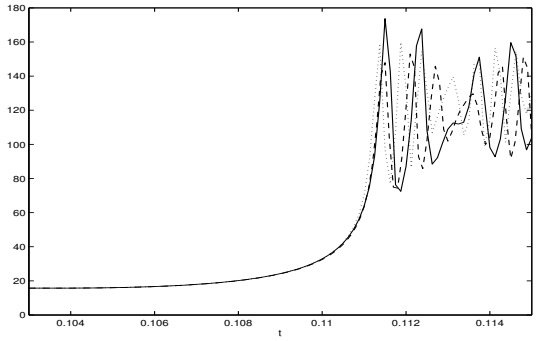
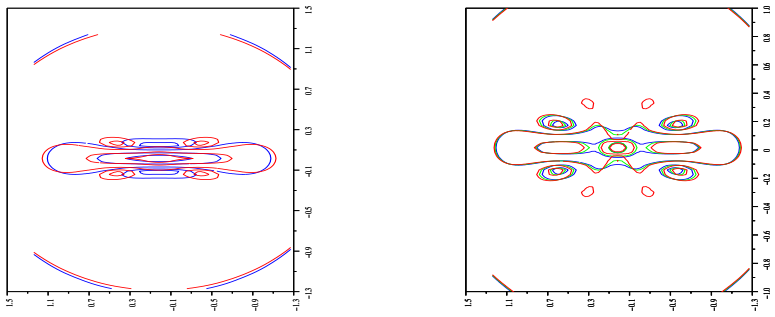
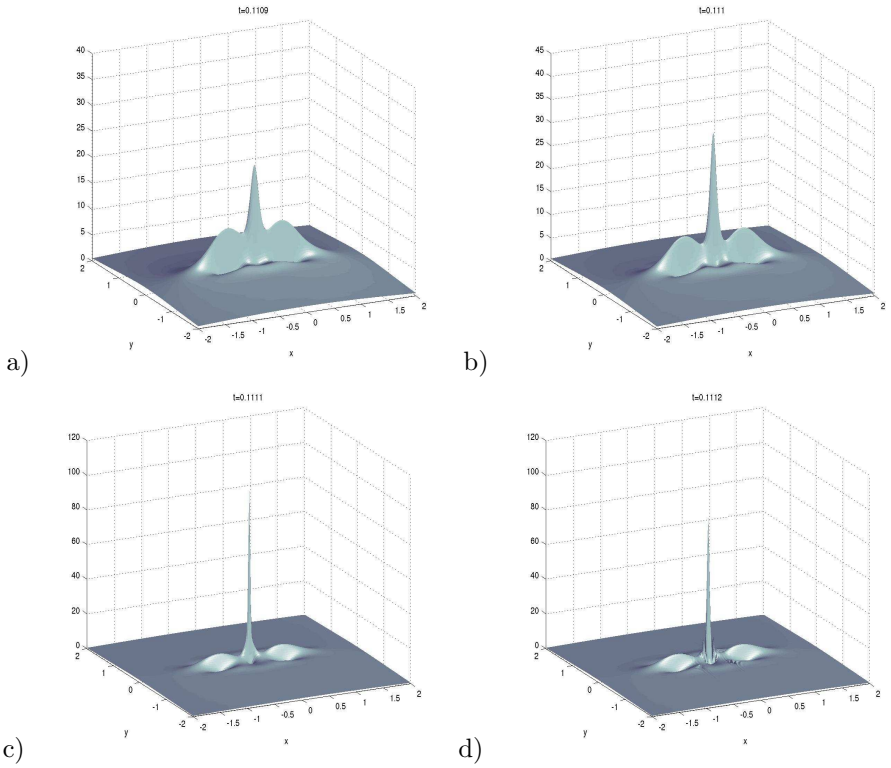


Figure 12: Blowup of defocusing ell.-ell. system. L^∞ norm of $|\Psi|$ for various space and time discretization steps, zoom. dashed line: $\Delta x = 0.0156, \Delta t = 5 \cdot 10^{-5}$; dotted line: $\Delta x = 0.0156, \Delta t = 2.5 \cdot 10^{-5}$, solid: $\Delta x = 0.00781, \Delta t = 2.5 \cdot 10^{-5}$



a) b)

Figure 13: a) Contour plot of position densities before blowup. $t = 0.099$, $t = 0.1045$. b) Contour plot of position densities close to blowup. $t = 0.1091$, $t = 0.1101$, $t = 0.111$.



a) b) c) d)

Figure 14: Position density at several times close to blowup. a) $t = 0.1109$, b) $t = 0.111$, c) $t = 0.1111$, d) $t = 0.1112$

such that R_k has exactly k nodes as a function of r and decreases exponentially at infinity.

Theorem 3.1 ([31]). *Let $\mathbf{x}_1, \ldots, \mathbf{x}_k$ be given in $\mathbb{R}^d$. There is a constant ω_0 such that for any constants $\omega_1, \ldots, \omega_k$ all strictly larger than ω_0, there exists a solution ψ of the critical (focusing) NLS that blows up in a finite time t_* such that:*

1. *The set of blowup points in $L^{2+4/d}$ and H^1 is $\{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$*
2. *For $i = 1, \ldots, k$ and all A such that the balls $B_i = B(\mathbf{x}_i, A)$ are disjoint, $\lim_{t \to t_*} \|\psi(t)\|_{L^2(B_i)} = \|R_i\|_{L^2}$*
3. *$\lim_{t \to t_*} \|\psi(t)\|_{L^2(\overline{B})} = 0$, where $\overline{B} = \mathbb{R}^d \setminus \cup_{i=1,\ldots,k} B_i$.*

In addition, there is a constant $\gamma > 0$ such that on $[0, t_*)$,

$$\left\| \psi(t) - \sum_{i=1}^{k} \frac{1}{|(t_* - t)\omega_i|^{d/2}} e^{\frac{-i}{(t_*-t)\omega_i^2} + \frac{i|\mathbf{x}|^2}{4(t_*-t)}} R_i\left(\frac{\mathbf{x} - \mathbf{x}_i}{\omega_i(t_* - t)}\right) \right\|_{L^{2+4/d}} \leq e^{-\frac{\gamma}{t_*-t}}.$$

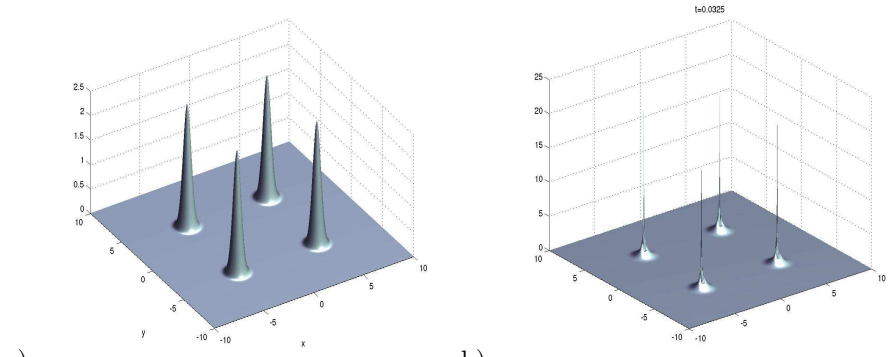
Papanicolaou *et al.* [34] proved that there is a ground state solution to the focusing E-E DS system (3.3). Since there is only one ground state, we decide instead of calculating with the exact ground-state profile to choose a test profile $Q(\mathbf{x}) = \exp(-|\mathbf{x}|^2)$, which is radial and decaying sufficiently fast. In order to realize the asymptotics described by the above result, we take the initial data as

$$u_I = \sum_{j=1}^{k} \frac{1}{\tilde{t}\omega} e^{-\frac{i}{\tilde{t}\omega^2} + i\frac{|\mathbf{x}|^2}{4\tilde{t}}} Q\left(\frac{\mathbf{x} - \mathbf{x}_j}{\tilde{t}\omega}\right)$$

where $\tilde{t}$ is an estimate of the blowup time and ω a constant (and $\mathbf{x} = (x, y) \in \mathbb{R}^2$). We solve the equation on the domain $[-10, 10]^2$, and choose the focus points $\mathbf{x}_1 = (4, 4)$, $\mathbf{x}_2 = (-4, 4)$, $\mathbf{x}_3 = (-4, -4)$, $\mathbf{x}_4 = (4, -4)$ and the constants $\tilde{t} = 0.03$, $\omega = 13.3$. We find that blowup occurs at $t_* = 0.032$. Figure 15 shows the position densities at initial time and at the blowup. We can see that the solution blows up exactly at the four chosen points.

3.3. Conclusion

We show that the "time splitting spectral method" is a very appropriate numerical method for a large class of time dependent nonlinear Schrödinger equations and that precise numerical simulations, even in 3 space dimensions and in the semi-classical regime are possible using modern parallel machines. The range of models we consider goes from the standard "cubic" NLS with its strong local nonlinearity to weakly nonlinear NLS of the Schrödinger-Poisson type and mixed versions of these two types, as well as generalizations like the different types of the Davey Stewartson system were the NLS structure as such is modified.



a) b)

Figure 15: Multi-focusing solution. a) Initial data, b) result shortly after blowup time.

Key properties of this numerical method are that it is explicit, unconditionally stable, time reversible and time transverse invariant. We use the code written by Bao et al that we have adapted for parallel computation. The adaption of this numerical code to the different types of NLS is relatively straightforward.

We present a first numerical study of the Schrödinger-Poisson-Xα (S-P-Xα) equation as a "local effective one particle approximation" of the time dependent Hartree-Fock equations. This particular NLS is the simplest model for quantum dynamics of electrons that respects the Pauli principle.

Thanks to 'good' ε-resolution of the numerical scheme we can study the S-P-Xα model in the semi-classical regime in 3 - d.
Extensive numerical results of position density and Wigner measures in and 3 space dimensions with/without an external potential are presented.

The interplay of the smoothing nonlocal nonlinearity - i.e. the repulsive "direct Coulomb interaction" ("Hartree potential") - with the strong local nonlinearity - i.e. the local approximation of the exchange interaction ("Xα potential")- is systematically studied by varying the scaling of the 2 nonlinearities between the Schrödinger-Poisson equation and an "exchange only" model. A critical scaling occurs when the Hartree term is $O(1)$ and the $X\alpha$ term is $O(\varepsilon)$.

In all simulations a critical time, the "break time", can be clearly distinguished and its "semiclassical limit" can be numerically estimated by comparing simulations with decreasing ε. Such simulations require a fine discretization which could be achieved also in 3-d by implementing the numerical code on a parallel machine.

The results in 1-d show a similarity to simulations of the "focusing cubic" NLS, with the smoothing effect of the additional Poisson equation nonlinearity. The well known "soliton" structure of the NLS (see e.g. [32]) is preserved in the S-P-Xα model when the cubic nonlinearity is dominant.

In 3-d, our simulations show a similarity with simulations of Bose-Einstein-Condensates modeled by the time dependent Gross-Pitaevski equation, where the third root of the density of the S-P-Xα model is replaced by the density itself

[12], i.e. a cubic NLS. In both cases, the local nonlinearity has the "focusing sign". However, the additional smoothing effect of the Hartree potential and the lower exponent of the local nonlinearity show a somewhat "smoother" structure of the solution unless the $X\alpha$ term and the Hartree term are of the same order of magnitude.

We have shown that the $S - P - X\alpha$ model allows for simulations of quantum dynamics in 3 dimensions, also in the semiclassical regime. The inclusion of the exchange interaction to the widely used Schrödinger-Poisson model leads to qualitative changes in the transient behaviour of the solution that become very pronounced beyond a relative scaling of $O(\varepsilon)$ and change the behaviour completely towards the typical "soliton-like structures" of the focusing cubic NLS beyond a relative scaling of $O(\sqrt{\varepsilon})$.

The second model we study numerically by the "time splitting spectral method" is the Davey-Stewartson (DS) system. The method was first used for the hyperbolic-elliptic (H-E) DS equations by White, Weideman [41] ten years ago. The new code we use has been developed independently of this previous work.

We not only study H-E DS systems, like White/Weideman, but also E-E DS systems. Exact soliton type solutions of H-E DS can be recovered accurately, eliminating numerical dispersion effects which appear in earlier results of [41] and [8]. For the finite time blowup solution of H-E DS, the blowup rate can be recovered.

For the E-E DS systems, we study finite time blowup of the focusing and defocusing equations. In the focusing case the analytic blowup rate is recovered accurately and blowup profiles are presented, in full agreement to the results in [8]. The blowup mechanism in this case is very similar to the one of critical focusing NLS. In the defocusing case, however, a resolution fine enough to approximate the blowup is new. High numerical resolution in the results admits a detailed representation of blowup profiles in both cases.

For the first time, we investigate the phenomenon of simultaneous blowup at a predefined, exact number of points. This is known for focusing NLS; we find that focusing E-E DS can show the same behaviour.

Continuation of the solution after the blowup time is a very demanding challenge for numerical simulations. Further work in this direction based on our code will be performed.

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