

1 Introduction

Let $\Omega \subseteq \mathbb{R}^n$, $V : \Omega \rightarrow \mathbb{R}$, $\kappa \in \mathbb{R}$, and $\psi : (0, T) \times \Omega \rightarrow \mathbb{C}$. The Nonlinear Schroedinger Equation (NSE) is given by:

$$-i\frac{\partial\psi}{\partial t} - \frac{1}{2}\Delta\psi + V\psi + \kappa|\psi|^2\psi = 0$$

With initial conditions:

$$\psi(0, \mathbf{x}) = \psi_0(\mathbf{x})$$

For all $\mathbf{x} \in \Omega$ and with boundary conditions:

$$\psi(t, \mathbf{x}) = 0$$

For all $(t, \mathbf{x}) \in (0, T) \times \partial\Omega$.

Because ψ is complex-valued, it is convenient to separate the equation into real and imaginary parts. If we take $\psi(t, \mathbf{x}) = u(t, \mathbf{x}) + iv(t, \mathbf{x})$ for $u, v : (0, T) \times \Omega \rightarrow \mathbb{R}$, we also have that $|\psi|^2 = u^2 + v^2$:

$$-i\frac{\partial}{\partial t}(u + iv) - \frac{1}{2}\Delta(u + iv) + V(u + iv) + \kappa(u^2 + v^2)(u + iv) = 0$$

So:

$$\begin{aligned}\frac{\partial v}{\partial t} - \frac{1}{2}\Delta u + Vu + \kappa(u^2 + v^2)u &= 0 \\ -\frac{\partial u}{\partial t} - \frac{1}{2}\Delta v + Vv + \kappa(u^2 + v^2)v &= 0\end{aligned}$$

2 Toy Problem

Let $\Omega = [-1, 1]^n$, and consider, for an example:

$$u(t, \mathbf{x}) = \cos(\pi t) \prod_{i=1}^n \cos(\pi x_i)$$

$$v(t, \mathbf{x}) = \sin(\pi t) \prod_{i=1}^n \cos(\pi x_i)$$

Then:

$$u(0, \mathbf{x}) = \prod_{i=1}^n \cos(\pi x_i)$$

$$v(0, \mathbf{x}) = 0$$

We have that:

$$u^2 + v^2 = \cos^2(\pi t) \prod_{i=1}^n \cos^2(\pi x_i) + \sin^2(\pi t) \prod_{i=1}^n \cos^2(\pi x_i)$$

$$= (\cos^2(\pi t) + \sin^2(\pi t)) \prod_{i=1}^n \cos^2(\pi x_i)$$

$$= \prod_{i=1}^n \cos^2(\pi x_i)$$

Note that $u^2 + v^2$ is independent of t . So:

Meanwhile:

$$\frac{\partial u}{\partial x_k} = -\pi \cos(\pi t) \sin(\pi x_k) \prod_{i \neq k} \cos(\pi x_i)$$

$$\frac{\partial^2 u}{\partial x_k^2} = -\pi^2 \cos(\pi t) \prod_{i=1}^n \cos(\pi x_i)$$

$$= -\pi^2 u$$

$$\Delta u = \sum_{k=1}^n \frac{\partial^2 u}{\partial x_k^2}$$

$$= -n\pi^2 u$$

Similarly:

$$\Delta v = -n\pi^2 v$$

And:

$$\begin{aligned}
\frac{\partial u}{\partial t} &= -\pi \sin(\pi t) \prod_{i=1}^n \cos(\pi x_i) \\
&= -\pi v \\
\frac{\partial v}{\partial t} &= \pi \cos(\pi t) \prod_{i=1}^n \cos(\pi x_i) \\
&= \pi u
\end{aligned}$$

Then, rewriting the first equation:

$$\begin{aligned}
Vu &= -\frac{\partial v}{\partial t} + \frac{1}{2}\Delta u - \kappa(u^2 + v^2)u \\
&= -\pi u - \frac{n}{2}\pi^2 u - \kappa(u^2 + v^2)u \\
V(\mathbf{x}) &= -\pi - \frac{n}{2}\pi^2 - \kappa(u^2 + v^2)
\end{aligned}$$

And the second equation:

$$\begin{aligned}
Vv &= \frac{\partial u}{\partial t} + \frac{1}{2}\Delta v - \kappa(u^2 + v^2)v \\
&= -\pi v - \frac{n}{2}\pi^2 v - \kappa(u^2 + v^2)v \\
V(\mathbf{x}) &= -\pi - \frac{n}{2}\pi^2 - \kappa(u^2 + v^2)
\end{aligned}$$

We see that the equations agree.

3 Spatial Discretization

Consider a set of basis function $\Phi_i : \Omega \rightarrow \mathbb{R}^2$, where each $\Phi_i(\mathbf{x}) = \varphi_{b_i} \hat{\mathbf{e}}_{c_i}$, where $\varphi_j : \Omega \rightarrow \mathbb{R}$ is a set of basis functions (b_i is the base index of the index i and c_i is the component index of i). We write $\mathbf{w} = \begin{bmatrix} u \\ v \end{bmatrix}$ and make the approximation $\mathbf{w} = W_j \Phi_j$ (Einstein summation); furthermore, we approximate $\frac{\partial \mathbf{w}}{\partial t} = \dot{W}_j \Phi_j$. Then, we have that:

$$\begin{aligned} u &= W_j \varphi_{b_j} \delta_{1,c_j} \\ v &= W_j \varphi_{b_j} \delta_{2,c_j} \\ \frac{\partial u}{\partial t} &= \dot{W}_j \varphi_{b_j} \delta_{1,c_j} \\ \frac{\partial v}{\partial t} &= \dot{W}_j \varphi_{b_j} \delta_{2,c_j} \end{aligned}$$

Then, we multiply and integrate the system with a basis function Φ_i :

$$\begin{aligned} \left\langle \Phi_i \mid \begin{array}{l} \partial_t v - \frac{1}{2} \Delta u + Vu + \kappa(u^2 + v^2)u \\ -\partial_t u - \frac{1}{2} \Delta v + Vv + \kappa(u^2 + v^2)v \end{array} \right\rangle &= 0 \\ i \left\langle \Phi_i \mid \begin{array}{l} \partial_t v \\ -\partial_t u \end{array} \right\rangle - \frac{1}{2} \left\langle \Phi_i \mid \begin{array}{l} \Delta u \\ \Delta v \end{array} \right\rangle + \left\langle \Phi_i \mid \begin{array}{l} Vu \\ Vv \end{array} \right\rangle + \kappa \left\langle \Phi_i \mid \begin{array}{l} u^3 \\ v^3 \end{array} \right\rangle + \kappa \left\langle \Phi_i \mid \begin{array}{l} uv^2 \\ u^2v \end{array} \right\rangle &= 0 \end{aligned}$$

We consider each form separately:

$$\begin{aligned} \left\langle \Phi_i \mid \begin{array}{l} \partial_t v \\ -\partial_t u \end{array} \right\rangle &= \delta_{1,c_i} \langle \varphi_{b_i} \mid \partial_t v \rangle - \delta_{2,c_i} \langle \varphi_{b_i} \mid \partial_t u \rangle \\ &= \delta_{1,c_i} \left\langle \varphi_{b_i} \mid \dot{W}_j \varphi_{b_j} \delta_{2,c_j} \right\rangle - \delta_{2,c_i} \left\langle \varphi_{b_i} \mid \dot{W}_j \varphi_{b_j} \delta_{1,c_j} \right\rangle \\ &= (\delta_{1,c_i} \delta_{2,c_j} - \delta_{2,c_i} \delta_{1,c_j}) \langle \varphi_{b_i} \mid \varphi_{b_j} \rangle \dot{W}_j \\ \left\langle \Phi_i \mid \begin{array}{l} \Delta u \\ \Delta v \end{array} \right\rangle &= \delta_{1,c_i} \langle \varphi_{b_i} \mid \Delta u \rangle + \delta_{2,c_i} \langle \varphi_{b_i} \mid \Delta v \rangle \end{aligned}$$

We note that:

$$\begin{aligned} \langle \varphi_{b_i} \mid \Delta f \rangle &= \int_{\Omega} \varphi_{b_i} \Delta f \, d\mathbf{x} \\ &= \oint_{\partial\Omega} \varphi_{b_i} \nabla f \cdot \hat{\mathbf{n}} \, d\mathbf{s} - \int_{\Omega} \nabla \varphi_{b_i} \cdot \nabla f \, d\mathbf{x} \\ &= \langle \varphi_{b_i} \hat{\mathbf{n}} \mid \nabla f \rangle_{\partial\Omega} - \langle \nabla \varphi_{b_i} \mid \nabla f \rangle \end{aligned}$$

And, because we have Dirichlet boundary conditions, we must have that $\varphi_{b_i}(t, \mathbf{x}) = 0$ for all $(t, \mathbf{x}) \in (0, T) \times \partial\Omega$. So:

$$\begin{aligned} \left\langle \Phi_i \mid \begin{array}{l} \Delta u \\ \Delta v \end{array} \right\rangle &= -\delta_{1,c_i} \langle \nabla \varphi_{b_i} \mid \nabla u \rangle - \delta_{2,c_i} \langle \nabla \varphi_{b_i} \mid \nabla v \rangle \\ &= -\delta_{1,c_i} \langle \nabla \varphi_{b_i} \mid W_j \nabla \varphi_{b_j} \delta_{1,c_j} \rangle - \delta_{2,c_i} \langle \nabla \varphi_{b_i} \mid W_j \nabla \varphi_{b_j} \delta_{2,c_j} \rangle \\ &= -(\delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \langle \nabla \varphi_{b_i} \mid \nabla \varphi_{b_j} \rangle W_j \end{aligned}$$

$$\begin{aligned}
\left\langle \Phi_i \mid \frac{Vu}{Vv} \right\rangle &= \delta_{1,c_i} \langle \varphi_{b_i} \mid Vu \rangle + \delta_{2,c_i} \langle \varphi_{b_i} \mid Vv \rangle \\
&= \delta_{1,c_i} \langle \varphi_{b_i} \mid W_j V \varphi_{b_j} \delta_{1,c_j} \rangle + \delta_{2,c_i} \langle \varphi_{b_i} \mid W_j V \varphi_{b_j} \delta_{2,c_j} \rangle \\
&= (\delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \langle \varphi_{b_i} \mid V \varphi_{b_j} \rangle W_j
\end{aligned}$$

We will not use the fact that $\mathbf{w} = W_j \Phi_j$ in considering the nonlinear forms at this time.

So:

$$\begin{aligned}
0 &= (\delta_{1,c_i} \delta_{2,c_j} - \delta_{2,c_i} \delta_{1,c_j}) \langle \varphi_{b_i} \mid \varphi_{b_j} \rangle \dot{W}_j \\
&\quad + \frac{1}{2} (\delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \langle \nabla \varphi_{b_i} \mid \nabla \varphi_{b_j} \rangle W_j \\
&\quad + (\delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \langle \varphi_{b_i} \mid V \varphi_{b_j} \rangle W_j \\
&\quad + \kappa \delta_{1,c_i} \langle \varphi_{b_i} \mid u^3 + uv^2 \rangle \\
&\quad + \kappa \delta_{2,c_i} \langle \varphi_{b_i} \mid v^3 + u^2 v \rangle
\end{aligned}$$

If we define:

$$\begin{aligned}
M_{ij} &= (\delta_{1,c_i} \delta_{2,c_j} - \delta_{2,c_i} \delta_{1,c_j}) \langle \varphi_{b_i} \mid \varphi_{b_j} \rangle \\
A_{ij} &= \frac{1}{2} (\delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \langle \nabla \varphi_{b_i} \mid \nabla \varphi_{b_j} \rangle \\
B_{ij} &= (\delta_{1,c_i} \delta_{1,c_j} + \delta_{2,c_i} \delta_{2,c_j}) \langle \varphi_{b_i} \mid V \varphi_{b_j} \rangle \\
C_i &= \kappa \delta_{1,c_i} \langle \varphi_{b_i} \mid u^3 + uv^2 \rangle + \kappa \delta_{2,c_i} \langle \varphi_{b_i} \mid v^3 + u^2 v \rangle
\end{aligned}$$

We rewrite the above equation as:

$$\mathbf{0} = M\dot{\mathbf{W}} + (\mathbf{A} + \mathbf{B})\mathbf{W} + \mathbf{C}$$

4 Time Stepping

In order to solve the monolithic system using an implicit Runge-Kutta method, we rewrite the equation from previous section:

$$\begin{aligned} M\dot{\mathbf{W}} &= -(\mathbf{A} + \mathbf{B})\mathbf{W} - \mathbf{C} \\ \dot{\mathbf{W}} &= -M^{-1}(\mathbf{A} + \mathbf{B})\mathbf{W} - M^{-1}\mathbf{C} \\ &= \mathbf{F}(\mathbf{W}) \end{aligned}$$

We must compute the action of $(\mathbf{I} - \tau\mathbf{J}[\mathbf{F}])^{-1}$ on a vector. We have that:

$$\begin{aligned} \mathbf{J}[\mathbf{F}] &= \frac{\partial \mathbf{F}}{\partial \mathbf{W}} \\ &= -\frac{\partial}{\partial \mathbf{W}}(M^{-1}(\mathbf{A} + \mathbf{B})\mathbf{W}) - \frac{\partial}{\partial \mathbf{W}}(M^{-1}\mathbf{C}) \\ &= -M^{-1}(\mathbf{A} + \mathbf{B}) - M^{-1}\mathbf{J}[\mathbf{C}] \end{aligned}$$

So, we must determine $\frac{\partial C_i}{\partial W_j}$:

$$\frac{\partial C_i}{\partial W_j} = \frac{\partial}{\partial W_j}(\kappa\delta_{1,c_i} \langle \varphi_{b_i} | u^3 + uv^2 \rangle + \kappa\delta_{2,c_i} \langle \varphi_{b_i} | v^3 + u^2v \rangle)$$

So, consider:

$$\begin{aligned} \frac{\partial}{\partial W_k} \langle \varphi_{b_i} | u^3 \rangle &= \frac{\partial}{\partial W_k} \langle \varphi_{b_i} | (W_j \varphi_{b_j} \delta_{1,c_j})^3 \rangle \\ &= \left\langle \varphi_{b_i} | \frac{\partial}{\partial W_k} (W_j \varphi_{b_j} \delta_{1,c_j})^3 \right\rangle \end{aligned}$$

What is the coefficient of W_k in $(W_j \varphi_{b_j} \delta_{1,c_j})^3$? First, note that:

$$\begin{aligned} (W_j \varphi_{b_j} \delta_{1,c_j})^3 &= (W_{j_1} \varphi_{b_{j_1}} \delta_{1,c_{j_1}})(W_{j_2} \varphi_{b_{j_2}} \delta_{1,c_{j_2}})(W_{j_3} \varphi_{b_{j_3}} \delta_{1,c_{j_3}}) \\ &= W_{j_1} W_{j_2} W_{j_3} \varphi_{b_{j_1}} \varphi_{b_{j_2}} \varphi_{b_{j_3}} \delta_{1,c_{j_1}} \delta_{1,c_{j_2}} \delta_{1,c_{j_3}} \end{aligned}$$