1 Constructing the Weak Formulation

Since FEniCS will be doign the heavy lifting for the matrix construction and equation solving, the weak formulation will be optimized to fit this framework. FEniCS is designed around elliptic-like problems, so the problem will be discretized in time first, then each update will be computed by solving an elliptic problem.

The time discretization applied to the Schrödinger equation gives

$$i\frac{\Psi^{n+1}(\mathbf{x})-\Psi^{n}(\mathbf{x})}{\Delta t}=\frac{1}{2}\left[-\nabla^2\Psi^{n+1}-\nabla^2\Psi^{n}+\nu V\Psi^{n+1}+\nu V\Psi^{n}\right].$$

Where $t^n = n\Delta t$ and $\Psi^n(\mathbf{x}) = \Psi(\mathbf{x}, t^n)$. Crank-Nicolson can be shown to be second order in time.

Rearranging this above expression gives

$$i\Psi^{n+1}+\frac{\Delta t}{2}\nabla^2\Psi^{n+1}-\frac{\nu\Delta t}{2}V\Psi^{n+1}=i\Psi^{n}-\frac{\Delta t}{2}\nabla^2\Psi^{n}+\frac{\nu\Delta t}{2}V\Psi^{n}.$$

At each time step, we can assume Ψ^n is known, with $\Psi^0 \equiv 0$ by the initial condition. Therefore this is now an elliptic problem for the $n+1$'st time step.

Next, for a quantum mechanical problem: the wavefunction must be continuously differentiable, which ensures that position and momentum are well defined everywhere. To guarentee this in $\mathbb{R}^2$ we require $\Psi \in H^4(\Omega)$.

To build the weak form, let

$$\mathcal{V}=\{u\in H^4(\Omega) : u|_{\Gamma_D\cup\Gamma_{\text{in}}}=0\}.$$

This will be our test function space. Let $\Phi \in \mathcal{V}$. Then the weak formulation comes from 3 terms:

$$\int_\Omega \Phi\Psi\,dx,\quad \int_\Omega \Phi\nabla^2\Psi\,dx,\quad \int_\Omega \Phi V\Psi\,dx.$$

Here we are considering the real and imaginary components of Ψ separately. In sticking with the quantum mechanical theme, I will be using bra-ket notation. That is Ψ will be known as $|\Psi\rangle$. The bar and angle denote that Ψ is an element of the Hilbert space $\mathcal{V}$. Next I will denote the linear functional:

$$\langle\Phi|\cdot=\int_\Omega \Phi\,\cdot\,dx.$$

That is $\langle\Phi|$ is the linear functional built by the L^2 inner product with $|\Phi\rangle$. Finally an inner product with an operator $\mathcal{O}$ will be denoted:

$$\langle\Phi|\,\mathcal{O}\,|\Psi\rangle=\int_\Omega \Phi\mathcal{O}(\Psi)\,dx.$$

The first and second components of the variational form are not interesting. Instead what is interesting is the middle term.

$$\begin{aligned}\int_\Omega \Phi\nabla^2\Psi\,dx &= \langle\Phi|\,\nabla^2\,|\Psi\rangle\\ &= \int_{\partial\Omega}\Phi\frac{\partial\Psi}{\partial n}\,d\sigma-\int_\Omega \nabla\Phi\cdot\nabla\Psi\,dx.\\ &= \int_{\Gamma_{\text{out}}}\Phi\frac{\partial\Psi}{\partial n}\,d\sigma-\langle\nabla\Phi|\nabla\Phi\rangle\end{aligned}$$

Due to the boundary condition on Γ_{out}, we know

$$\frac{\partial\Psi}{\partial t}=i\frac{\partial\Psi}{\partial n}.$$

Using the Crank-Nicolson time discretization on the boundary changes this to

$$\frac{\Psi^{n+1}-\Psi^{n}}{\Delta t}=\frac{i}{2}\left(\frac{\partial\Psi^{n+1}}{\partial n}+\frac{\partial\Psi^{n}}{\partial n}\right).$$

Therefore

$$\int_{\Gamma_{\text{out}}} \Phi\Psi^{n+1}\,d\sigma - \frac{i\Delta t}{2}\int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi^{n+1}}{\partial n}\,d\sigma = \int_{\Gamma_{\text{out}}} \Phi\Psi^{n}\,d\sigma + \frac{i\Delta t}{2}\int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi^{n}}{\partial n}\,d\sigma.$$

Giving

$$\int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi^{n+1}}{\partial n}\,d\sigma = \frac{2i}{\Delta t}\left(-\int_{\Gamma_{\text{out}}} \Phi\Psi^{n+1}\,d\sigma + \int_{\Gamma_{\text{out}}} \Phi\Psi^{n}\,d\sigma + \frac{i\Delta t}{2}\int_{\Gamma_{\text{out}}} \Phi\frac{\partial\Psi^{n}}{\partial n}\,d\sigma\right).$$

Therefore the weak form of the PDE reads

$$\begin{gathered} i\left\langle\Phi\middle|\Psi^{n+1}\right\rangle - \frac{\Delta t}{2}\left\langle\nabla\Phi\middle|\nabla\Psi^{n+1}\right\rangle - \frac{\nu\Delta t}{2}\left\langle\Phi\right|V\left|\Psi^{n+1}\right\rangle - i\int_{\Gamma_{\text{out}}}\Phi\Psi^{n+1}\,d\sigma = \\ i\left\langle\Phi|\Psi^{n}\right\rangle + \frac{\Delta t}{2}\left\langle\nabla\Phi|\nabla\Psi^{n}\right\rangle + \frac{\nu\Delta t}{2}\left\langle\Phi\right|V\left|\Psi^{n}\right\rangle - i\int_{\Gamma_{\text{out}}}\Phi\Psi^{n}\,d\sigma \end{gathered} \tag{1}$$

FEniCS uses UFL - unified form assembly language, which is able to take a (nearly verbatim mathematically formatted) variational form, and convert this into a matrix system and solve automatically. The only adjustment that needs to be made is to the boundary integrals. To enforce the integration take place only on Γ_{out}, we use

$$\int_{\Gamma_{\text{out}}} \Phi\Psi\,d\sigma = \int_{\partial\Omega} \Phi\mathbb{1}(\mathbf{x}\in\Gamma_{\text{out}})\Psi\,d\sigma.$$