Finite Element Method for Quantum Mechanics

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What are We Going to do?

- Photonics - building electric circuitry for photons rather than electrons
- Why - photons travel at light speed (electrons are snails)
- Photons don't interact with each other (easier to deal with)
- Can play tricks with resonance to do computations

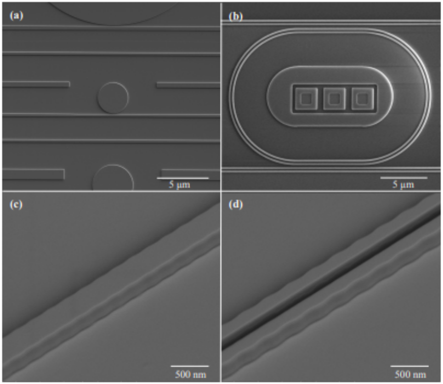


Figure: Figure taken from S. T. Fard et. al.

An Overview of Quantum Mechanics

- **Heisenberg Uncertainty Principle** : " You cannot simultaneously know the position and momentum of a quantum particle"
- Classical rules $\boldsymbol{F} = m\boldsymbol{a}$ are changed to quantum rules: **Schödinger Equation**

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\left[\Psi\right]$$

- $\hbar$ - Planck's Constant (divided by 2π), $\hat{H}$: *Hermitian* operator which produces energy
- QoI: Ψ - wavefunction
- Given operator $\hat{\mathcal{O}}$, giving property ω, the **Probability Density Function** for ω, ρ_ω:

$$\rho_\omega(\boldsymbol{x}, t) = \Psi^*(\boldsymbol{x}, t)\hat{\mathcal{O}}\left[\Psi(\boldsymbol{x}, t)\right]$$

A Simple Case

- Particles interacting with an external potential $V(\boldsymbol{x})$ (time-independent, $\boldsymbol{x} \in \mathbb{R}^2$)
- Particles do not interact with each other (linear PDE)
- Energy: Kinetic + Potential
- Kinetic: $\frac{1}{2m}\hat{p}^2$, mass m, *momentum operator* $\hat{\boldsymbol{p}} = -i\hbar\nabla$
- Schödinger equation for a single particle:

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(\boldsymbol{x})\Psi$$

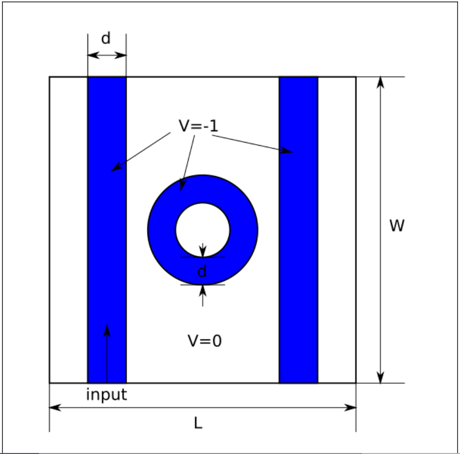
- Nondimensionalize

$$\implies i\frac{\partial \Psi}{\partial t} = -\nabla^2\Psi + \nu V(\boldsymbol{x})\Psi$$

- An interesting question: **Can we understand tunnelling?**

Quantum Tunnelling

- Particle "trapped" (in the classical regime) in a potential well can escape!
- Consider the following example
- Input boundary: Γ_{in}, Other blue boundaries: Γ_{out}, all other boundaries: Γ_D



FEM and Variational Form

- $\Psi \in H^1(\Omega) \times C(\mathbb{R}_+)$
- Inner products (bra-ket notation):

$$\langle \phi | \psi \rangle = \int_\Omega \phi^* \psi \, dx, \quad \langle \phi | \, \mathcal{O} \, | \psi \rangle = \int_\Omega \phi^* \mathcal{O}(\psi) \, dx.$$

- Variational form: $\Phi \in H^1_{D,\mathrm{in}}(\Omega)$ of the Schrödinger equation

$$i \, \langle \Phi | \, \partial_t \, | \Psi \rangle = \langle \nabla \Phi | \nabla \Psi \rangle + \langle \Phi | \, V \, | \Psi \rangle + \int_{\Gamma_{\mathrm{out}}} \Phi^* \frac{\partial \Psi}{\partial n} \, d\sigma$$

- Φ zero on outer boundary and input boundary, nonzero on other (blue boundaries), wave can escape this way
- Enforce open boundary on Γ_{out}:

$$\frac{\partial \Psi}{\partial t} = i \frac{\partial \Psi}{\partial n} \implies \int_{\Gamma_{\mathrm{out}}} \Phi^* \frac{\partial \Psi}{\partial n} \, d\sigma = i \frac{\partial}{\partial t} \int_{\Gamma_{\mathrm{out}}} \Phi^* \Psi \, d\sigma.$$

Finite Dimensional FEM

- Boundary wrapper:

$$B(\Phi, \Psi) = \int_{\Gamma_{\text{out}}} \Phi^* \Psi \, d\sigma.$$

- Build triangulation $\mathcal{T}_h$ on Ω, let $\phi_j(\boldsymbol{x})$ be a set of basis functions for $H^1_{D,\text{in}}(\Omega)$

$$\implies i \sum_{k=1}^{N} \langle \phi_j | \phi_k \rangle \, \lambda_k'(t) = \sum_{k=1}^{N} \left[\langle \nabla \phi_j | \nabla \phi_k \rangle + \langle \phi_j | \, V \, | \phi_k \rangle + B(\phi_j, \phi_k) \right] \lambda_k(t)$$

- ϕ_j are real functions in $H^1(\Omega)$, λ_k are complex functions
- Mass matrix: $\langle \phi_j | \phi_k \rangle$, Stiffness matrix: $\langle \nabla \phi_j | \nabla \phi_k \rangle$, "Potential" matrix: $\langle \phi_j | \, V \, | \phi_k \rangle$, "Boundary" matrix: $B(\phi_j, \phi_k)$

Doing this in FEniCS

Build mesh:

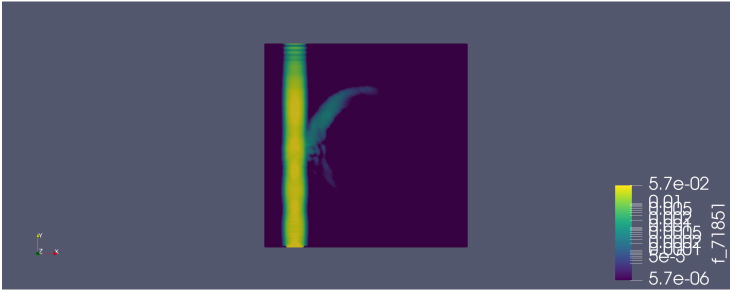
```
origin = Point(0, 0)
farcorner = Point(domainwidth, domainlength)
mesh = RectangleMesh(origin, farcorner, nx, ny)
```

Variational forms

```
H1 = FunctionSpace(mesh, "CG", 1)
Psi = TrialFunction(H1)
Phi = TestFunction(H1)
mass = assemble(Phi * Psi * dx)
stiffness = assemble(
  dot(grad(Phi), grad(Psi)) * dx)
boundary = assemble(Phi * Psi *
  [boundaryindicator] * ds)
potential = assemble(Phi * V * Psi * dx)
```

Time Stepping and Solution

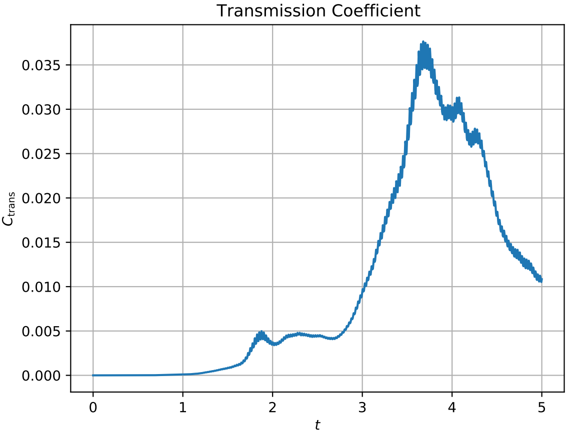
- Crank-Nicolson method used for time stepping
- Domain : $h_{\min} = 0.1$
- $T_{\max} = 5$, $n_t = 1000 \implies \Delta t = 0.005$



Transmission Coefficient

- Computation:

$$C_{\text{trans}} = \frac{\langle \Psi | \, \mathbb{1}_{\Omega_1} \, | \Psi \rangle}{\langle \Psi | \, \mathbb{1}_{\Omega_2} \, | \Psi \rangle}.$$



Future Improvements

- Better boundary condition
- Proper B/C involves fractional derivatives

$$\partial_x \Psi = \sqrt{-i\partial_t - \partial_{yy}}\Psi \quad x \in \Gamma_{\text{out}}.$$

- Test various geometries
- Goal is to get optimal resonance for specified input frequency

$$(\omega_{\text{in}}, R_{\text{ring}}) \mapsto C_{\text{trans}}.$$

- Apply Maxwell equations - photons are electromagnetic wave packets

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