Quantum information and computing

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The goal of this assignment is to simulate and analyze wave propagation in 1D under various physical models and potentials using the FEniCS finite element library.

Part I: Classical Wave Equation

Simulate the classical 1D wave equation:

$$\partial^2 u / \partial t^2 = c^2 \, \partial^2 u / \partial x^2$$

where u(x,t) is the wave field and c is the wave speed.

1. Implement the wave equation in FEniCS.
2. Use an initial Gaussian pulse centered in the domain with zero initial velocity
3. Compare the propagation with and without a spatially varying wave speed c(x) anche check the results with analytical solutions where available.
4. *(Optional) Simulate wave propagation across an interface where has a discontinuity: Define $c(x) = c_1$ for $x < x_0$ and $c(x) = c_2$ for $x > x_0$. Place the initial pulse at $x < x_0$ and observe reflection and transmission. Compare transmitted/reflected waveforms to analytical predictions (e.g., acoustic Fresnel coefficients).*

Part II: Time-Dependent Schrödinger Equation

Simulate the 1D time-dependent Schrödinger equation:

$$i\hbar \, \partial\psi / \partial t = -\hbar^2/(2m) \, \partial^2\psi / \partial x^2 + V(x)\psi$$

(check whether in FEniCS you have to split the complex wavefunction ψ = u + iv into real and imaginary parts and solving a coupled PDE system or not. Compute and plot the probability density $|\psi(x,t)|^2$ and the wave packet width σ(t) and comment on the dynamical regime (ballistic, diffusive/localized, oscillatory).

Scenarios to Simulate

1. Free Particle: V(x) = 0
   - Initial wave packet: Gaussian centered at x_0
   - Observe and quantify ballistic spreading: $\sigma(t) \propto t$
2. Periodic Potential (Kronig-Penney-like):
   - Example: $V(x) = V_0 \cos(2\pi x/a)$
   - Observe slower, sub-ballistic spreading and discuss connection with Bloch waves and effective

mass
3. Linear Electric Field: $V(x) = Fx$
- Observe Bloch oscillations of a localized wave packet and discuss the absence of net drift in the periodic lattice.

4. (optional) Add weak random disorder to the periodic potential to observe Anderson localization.

By the due date please submit the presentation and the code. The final presentation will be **20 minutes** long and it must include the presentation of the problem (i.e., the model, reference paper), the methodology and the obtained results. A final question on the program of the Quantum Information and Computing course will conclude the exam.