50.117 Graphics and Visualization

Final Project Proposal

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§1 Background

Non-relativistic quantum mechanics presents itself as a rich field of study which despite its success, remains strange and unintuitive to even its greatest proponents. The governing equation in quantum mechanics is the famed Schrödinger's equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t) \tag{1}$$

for which this is relevant in the context of 1D systems. Even when constrained to exit along 1D, quantum particles (as represented by the wavefunction $\Psi(x,t)$) exhibit interesting and non-trivial dynamics. Furthermore, the wavefunctions exist over a complex field ($\Psi(x,t) \in \mathbf{C}$), which makes its visualization in spatial dimensions higher than 1 impossible (1 spatial dimension and 2 Argand plane axes already constitute 3 dimensions for visualization).

§2 Project Overview

Our group aims to implement a dynamic visualization of the time-evolution of a wavefunction in 1D. To do so, we adopt Heisenberg's formulation of quantum theory through *matrix mechanics*, but truncate the Hilbert space in order to perform valid computations. In doing so, we Shrödinger equation becomes:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle &= \hat{H}\left|\psi(t)\right\rangle \\ \Rightarrow \quad \left|\psi(t)\right\rangle &= e^{-\frac{i\hat{H}t}{\hbar}}\left|\psi(0)\right\rangle \end{aligned} \tag{2}$$

In the above equation, $\hat{H}$ (*Hamiltonian*) is now a matrix with elements $[\hat{H}]_{ij} = \langle\psi_i|\,\hat{H}\,|\psi_j\rangle$ where $\left|\psi\right\rangle_i$ and $\left|\psi\right\rangle_j$ are eigenstates of the position basis (one-hot vectors). For more information of Dirac notation ($\left|\psi\right\rangle, \left\langle\psi\right|$), refer to this link. What our visualization will then show is the wavefunction across a given slice of space (some segment of the x-axis) and its evolution over time given changes to the Hamiltonian. The users will be allowed to change the potential ($V(x)$) term and thus the Hamiltonian in the Schrödinger's equation, which will cause changes to the wavefunction's form and dynamics.