Solving the Schrödinger Equation for a System with a Disordered Potential

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Introduction

A disordered system is a system that lacks uniformity in its structure. A system with a disordered structure has a randomized potential energy; this potential varies depending on a particle's location within the system. Nature contains many disordered systems such as inorganic crystals and cold atom systems. Knowing how these systems behave over time allows for further use, analysis, and exploitation of their characteristics. The system used in this project was the infinite square well. This system was analyzed using the Schrödinger Equation. This partial differential equation can be solved to approximate the position, momentum, or other measurable factors of a system. This differential equation was numerically solved using the crank-nicolson method.

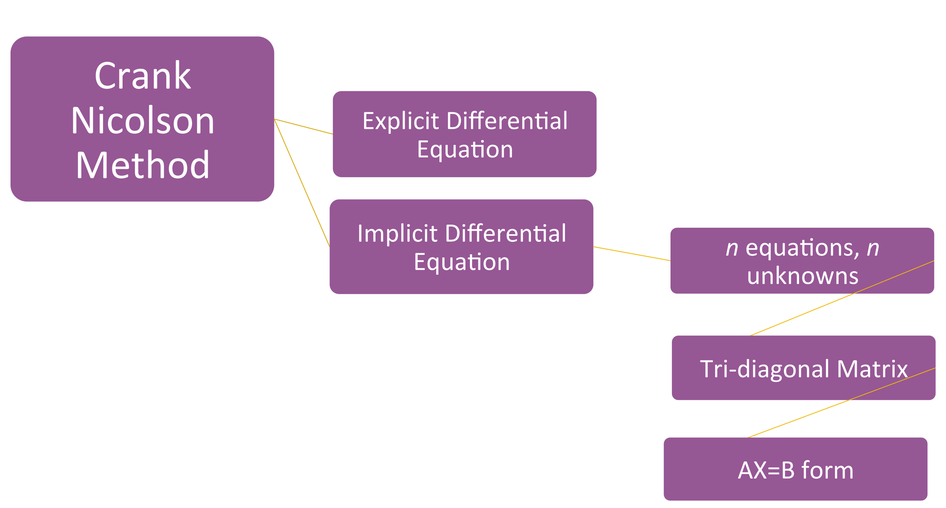
Time-Dependent Schrödinger Equation

$$i\hbar(\partial/\partial t)\psi=H\psi$$

The time-independent Schrödinger equation is a differential equation that when solved, gives the wave function, ψ, of a disordered system. The wave function identifies the relative probability of a particle's position at any given location, so long as certain parameters are met. For the infinite square well, the position of the particle inside this well was measured various times, with and without a potential. The amplitude of the wave function was not expected to change in the ground state. It was, however, expected to change after a disordered potential was added.

Crank-Nicolson Method

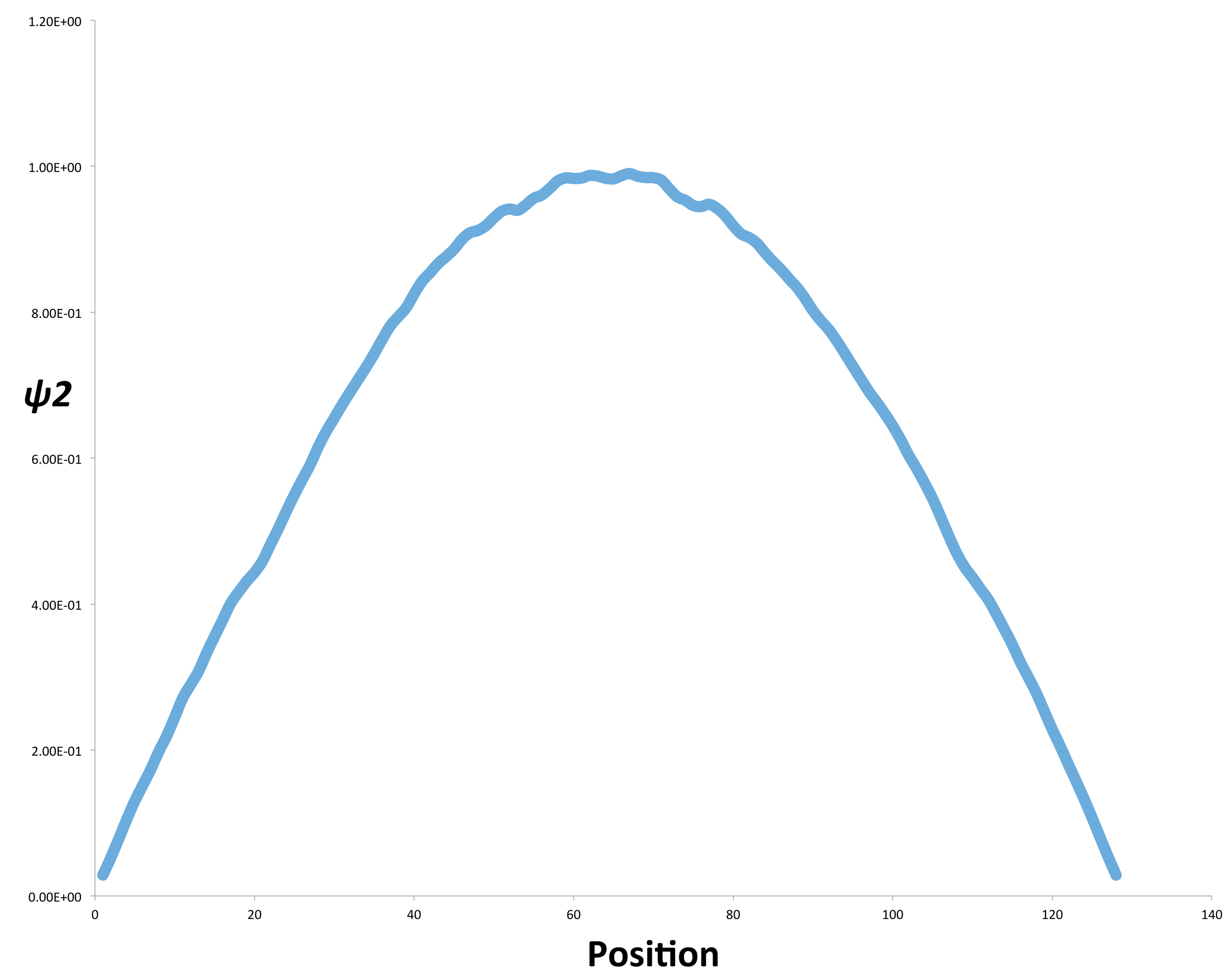
This method numerically solves for the wave function:



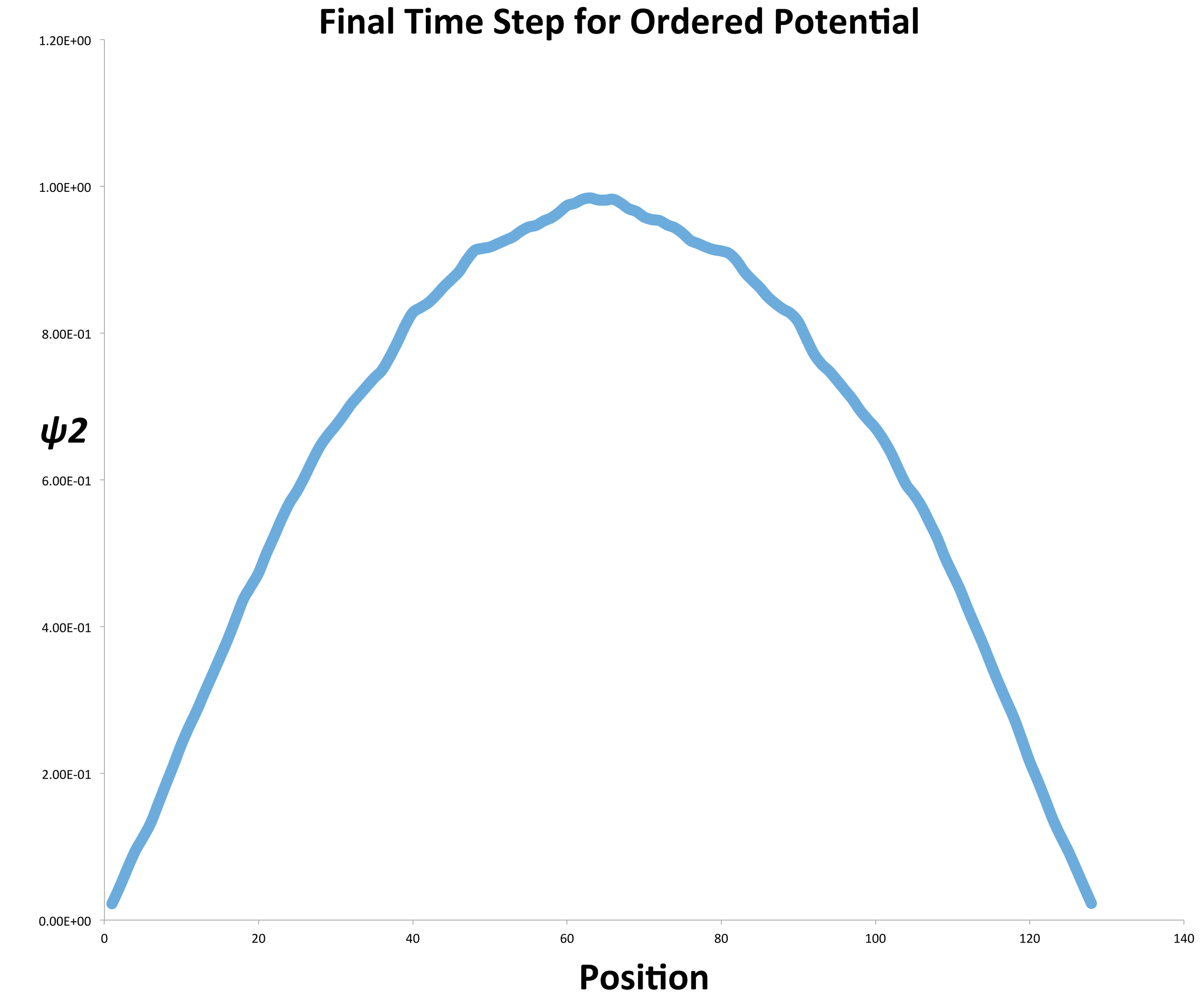
Results

The wave function for the ground state of the infinite square well:

Initial Time-Step for Ordered Potential

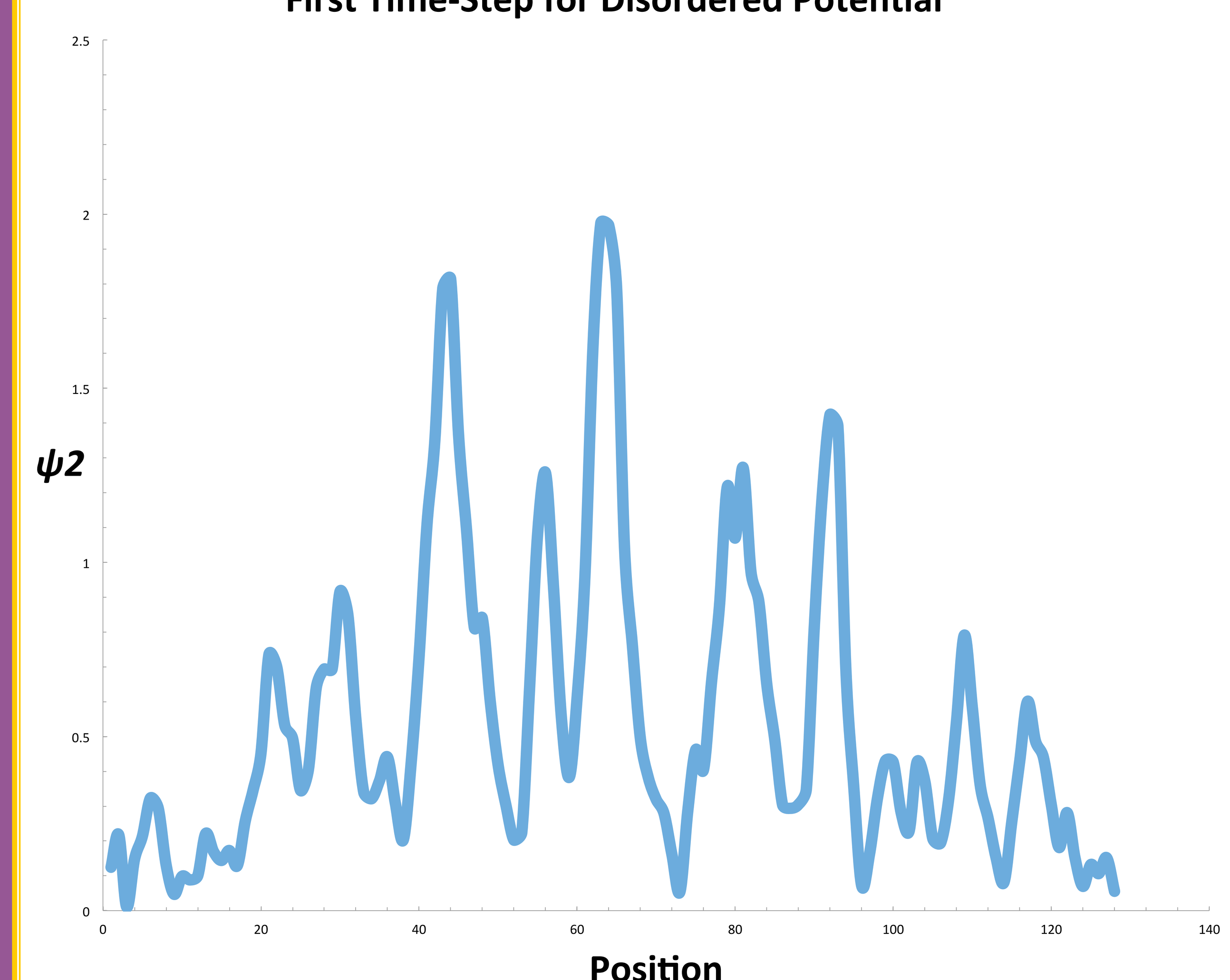


Final Time Step for Ordered Potential

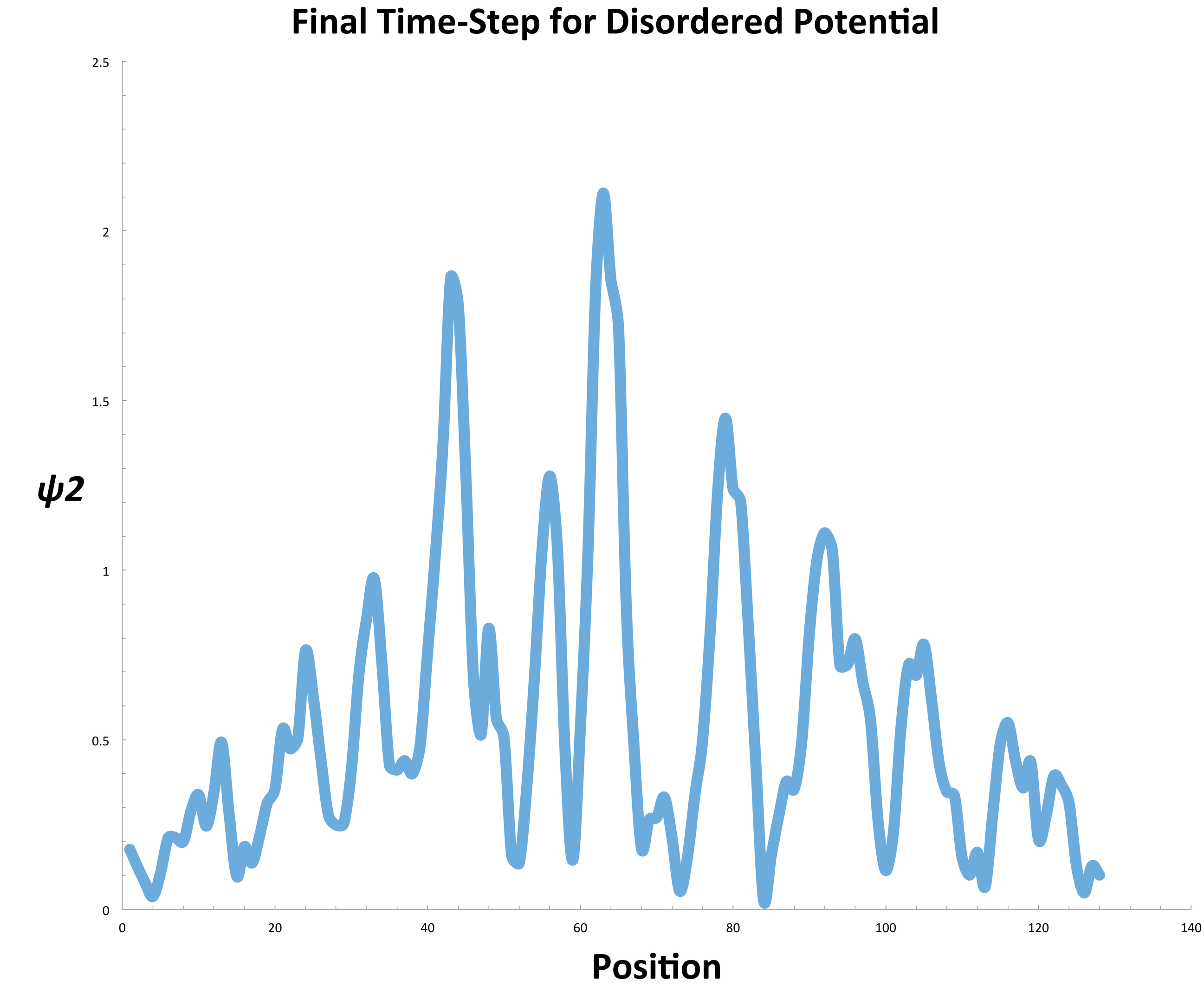


The wave function for the infinite square well after disorder was added to the system:

First Time-Step for Disordered Potential



Final Time-Step for Disordered Potential



Discussion

The first two graphs for the infinite square well before the disorder was added to the system resemble a parabolic shape as expected. The minimum difference between the shapes of the graphs indicate that the simulation was run correctly because the system was still in the ground state. Major alterations were not expected. After the disorder was added, however, the graphs significantly changed from ordered to disordered as well as from initial to final measurements. This indicated that adding disordered properly altered the wave function.

Conclusions

In conclusion, the wave function for the infinite square well was successfully obtained using the Crank-Nicolson method to solve for the Schrödinger equation. The graphs showed the difference between the wave functions for a system with and without a disordered potential. In the future, this simulation can be applied to more complex systems with disordered potentials because the algorithm created can be used on various systems with similar parameters.

References

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