Introduction

The Schrödinger equation, the fundamental equation of quantum mechanics, describes the evolution of the quantum state of a physical system over time. Here we solve the time-dependent Schrödinger equation to follow the evolution of an initially localized two-electron state in the presence of disorder. We study numerically the effects of variable Hubbard interactions and lattice sizes on the spread of the wave function.

Methods

We use the fourth-order Runge-Kutta method to approximate the solutions for the differential equation

$$\frac{df(n_1, n_2)}{dt} = \frac{J(n_1)f(n_1, n_2) + J(n_1 - 1)f(n_1 - 1, n_2) + J(n_2)f(n_1, n_2 + 1) + J(n_2 - 1)f(n_1, n_2 - 1) + \delta_{n_1, n_2} U f(n_1, n_2)}{\delta_{n_1, n_2}}$$

where \(f\) is the wave function, \(n\) is the position operator, \(J\) is the hopping amplitude, and \(U\) is the Hubbard interaction.

We measure the spread of the wave function

$$\sigma = \sum_{n_1, n_2} |f(n_1, n_2)|^2 \sqrt{(n_1 - \langle n_1 \rangle)^2 + (n_2 - \langle n_2 \rangle)^2}$$

where we define

$$\langle n_1 \rangle = \sum_{n_1, n_2} n_1 |f(n_1, n_2)|^2 \quad \text{and} \quad \langle n_2 \rangle = \sum_{n_1, n_2} n_2 |f(n_1, n_2)|^2 .$$

Results

**Right:** The average spread over time of wave functions in systems with two initially localized interacting electrons in a 100 by 100 lattice with random hopping and Hubble interactions between zero and six.

**Below:** Plots of the time evolution of a typical wave function in a system with two interacting electrons initially localized in the center of a 100 by 100 lattice.

Conclusion

Differing values of the Hubbard interaction have clear effects on the spread of the wave function in long time.

Investigations of different lattice sizes will be necessary to see what further effects are present.

References
