Multidimensional Diffusion in Crystalline Solids

How does diffusion differ in multiple dimensions along a crystal lattice?

Hannah Alperstein • Dr. Matt Caplan
Department of Physics • Illinois State University

Introduction

• Diffusion is a process where particles are allowed to spread freely through a medium. Diffusion is modeled as a random walk, where each particle moves in random steps.

• While diffusion is generally considered in a liquid or gaseous phase, diffusion also occurs as a much slower process in solids. Diffusion in solids is slower because particles are trapped by neighboring particles and they are also constricted to specific directions along a crystalline plane.

• In a diffusive process, the displacement grows with the square root of the number of steps because the square of the average distance from origin after each step grows proportionally with time.

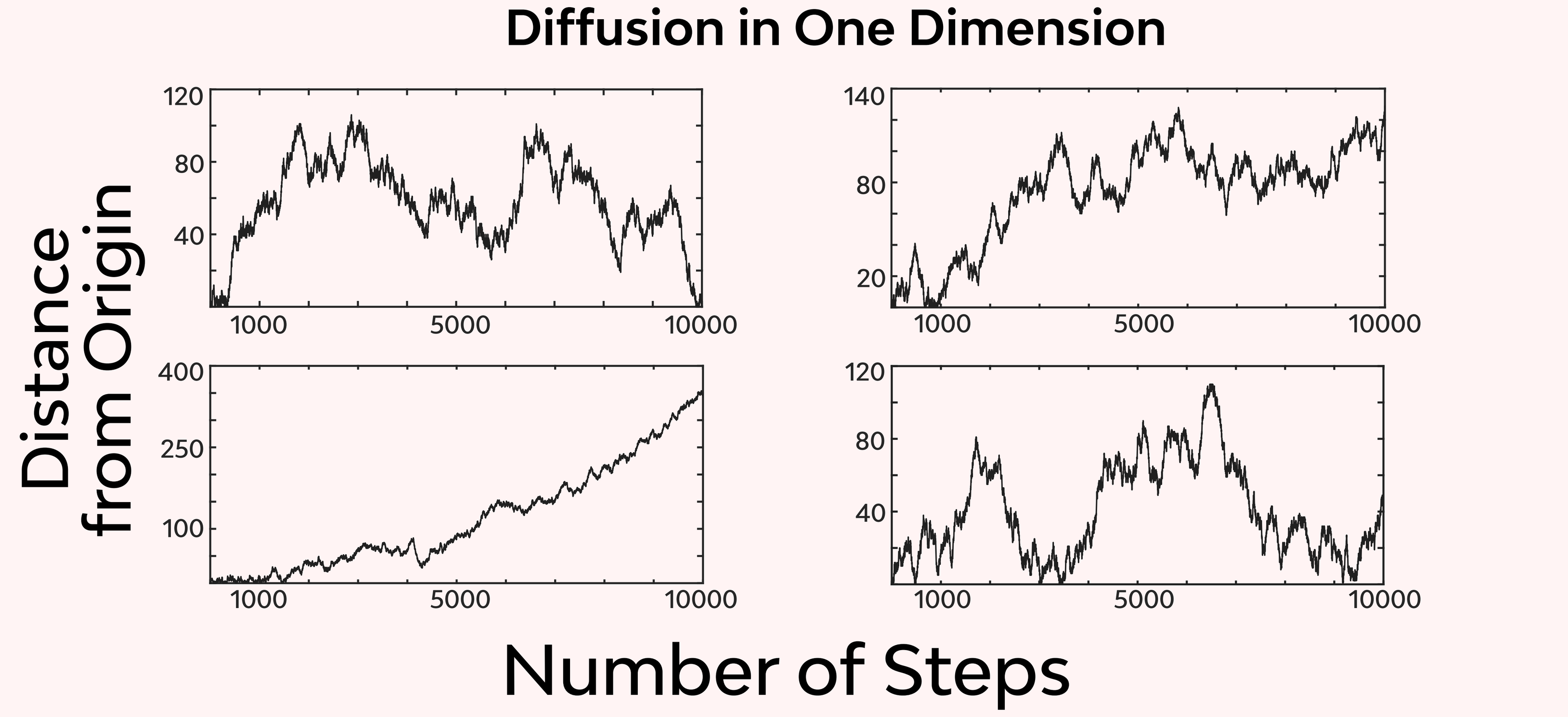


Fig. 1 • Four example trajectories of single particle diffusion in one dimension where the particle has an equal probability of moving in either direction along the x-axis for each step.

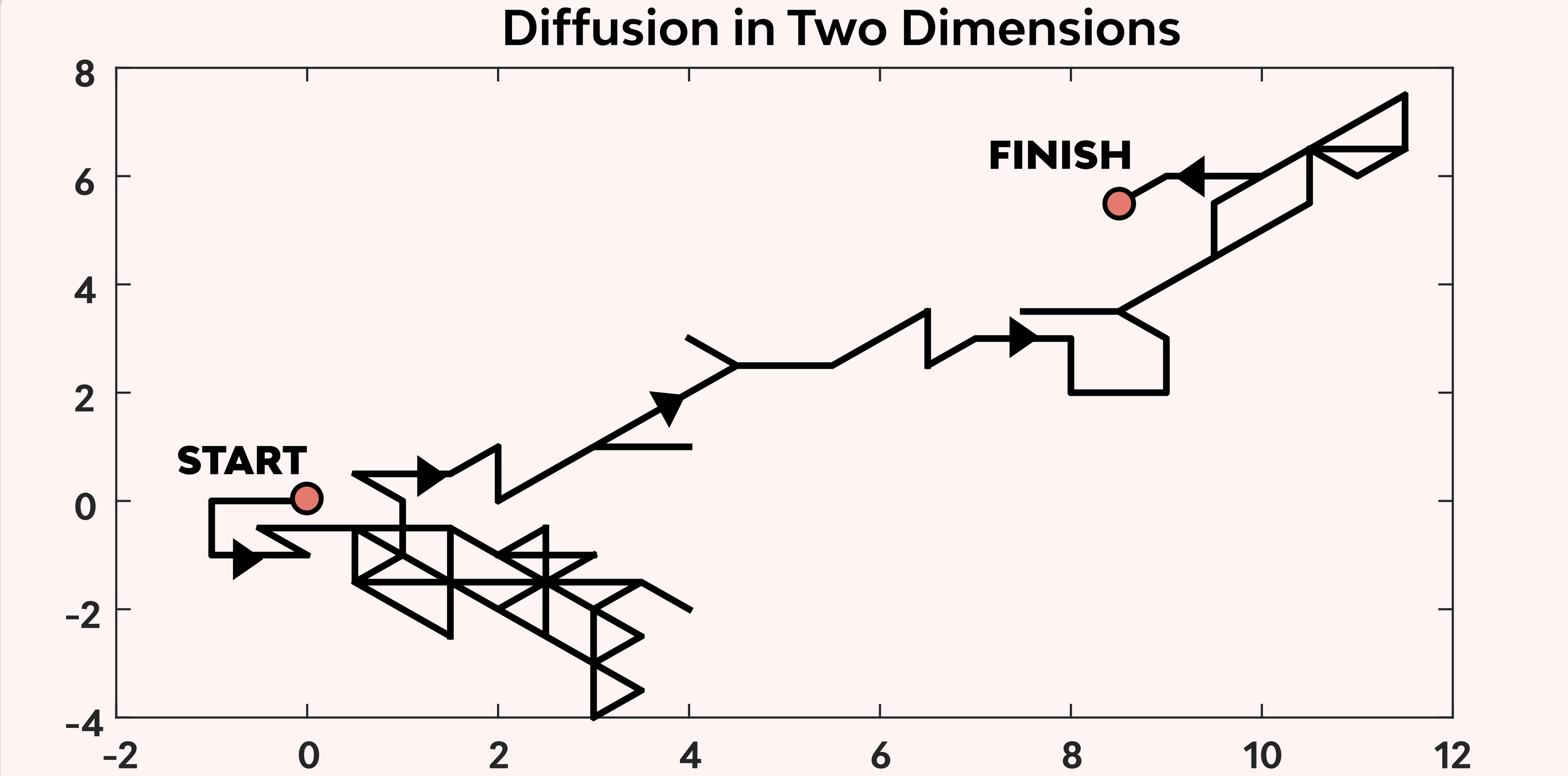


Fig. 2 • An example of a random walk trajectory in two dimensions for 100 steps. The particle has an equal probability of moving along the x/y axis or moving diagonally.

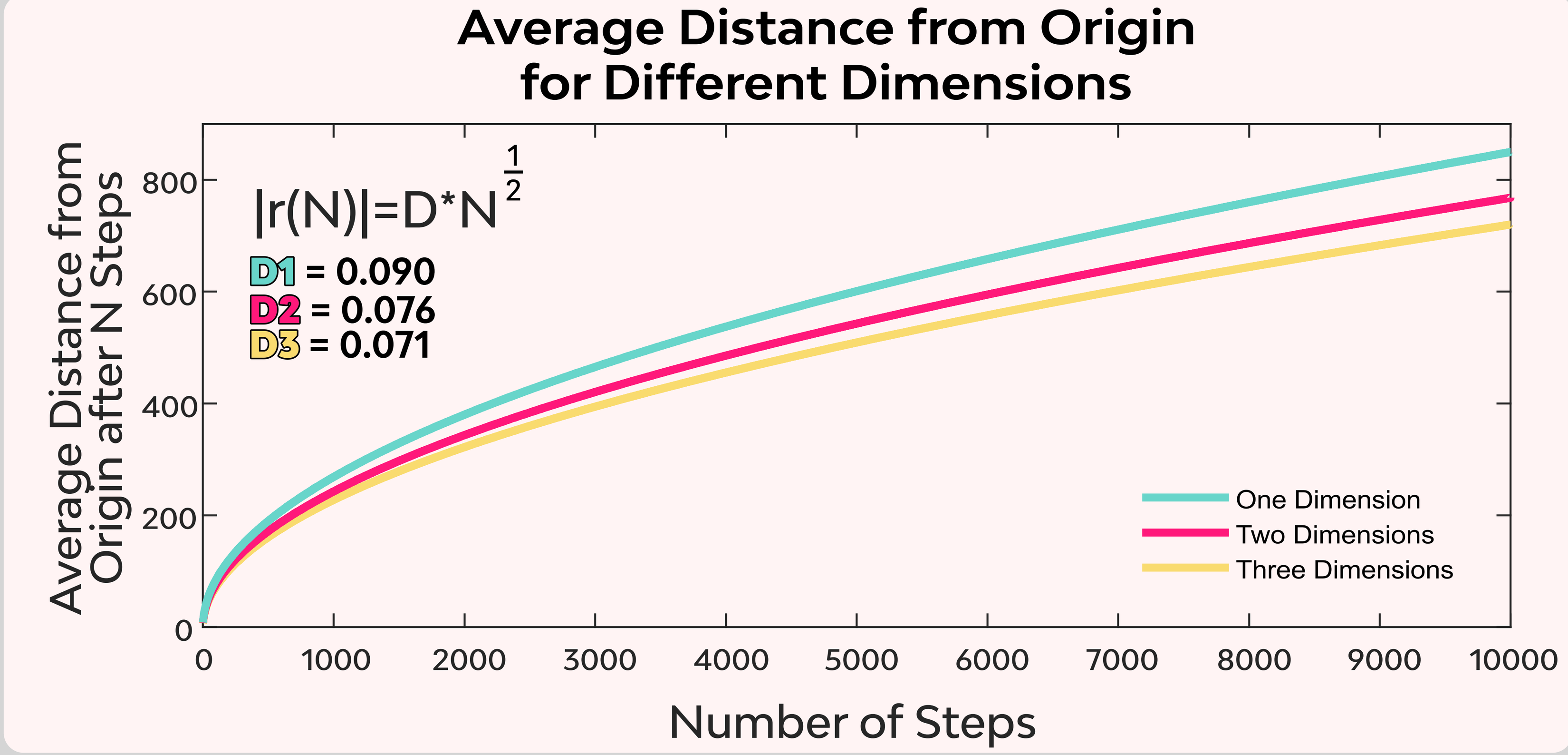
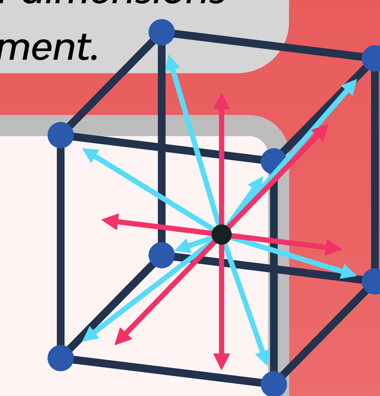
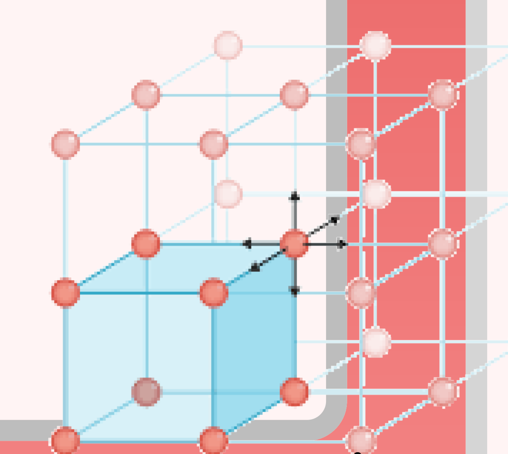


Fig. 3 • Demonstrates how a particle's average distance from origin changes after each step for various dimensions, where "D" is the diffusion coefficient that fits the plot in each dimension and "N" is the number of steps. Diffusion occurs slower in higher dimensions when there is an equal probability between axis and diagonal movement.

• Probability of nearest neighbor versus second nearest neighbor lattice site hops
  — Nearest neighbor= **diagonal movement**
  — Second nearest neighbor= **axis movement**

• Probability **(P)** = probability of a nearest neighbor jump, **1-P**=probability of a second nearest neighbor jump
•**P=0.0:** Nearest neighbor hops forbidden (particle only moves along **axis**)
• **P=0.5:** equal probability of nearest or second nearest neighbor movement
• **P=1.0:** Second nearest neighbor hops forbidden (particle only moves **diagonally**)





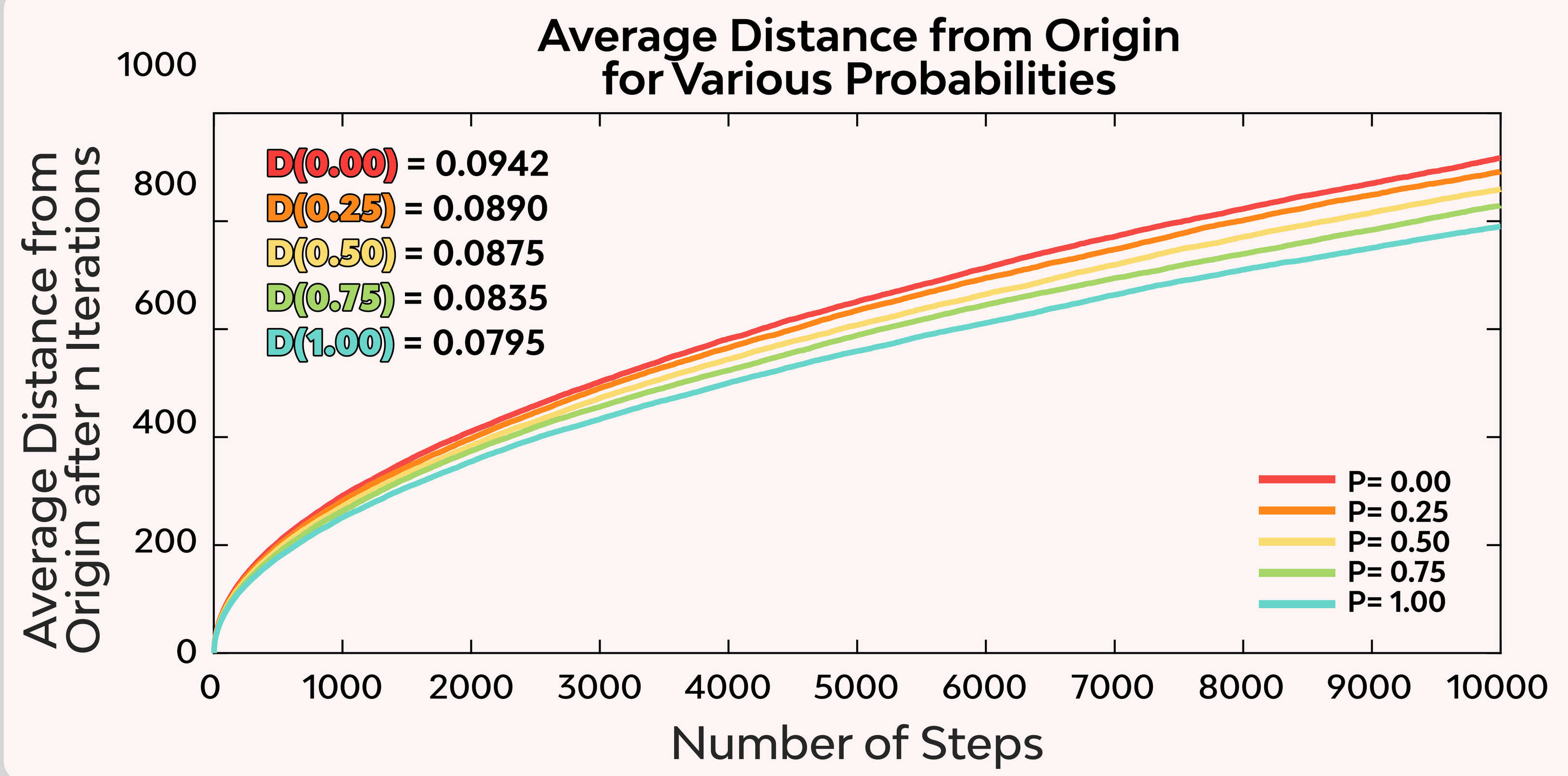


Fig. 4 • When diffusion is biased towards the second nearest neighbor jumps, the process occurs faster because the particle is moving a larger distance for each hop.

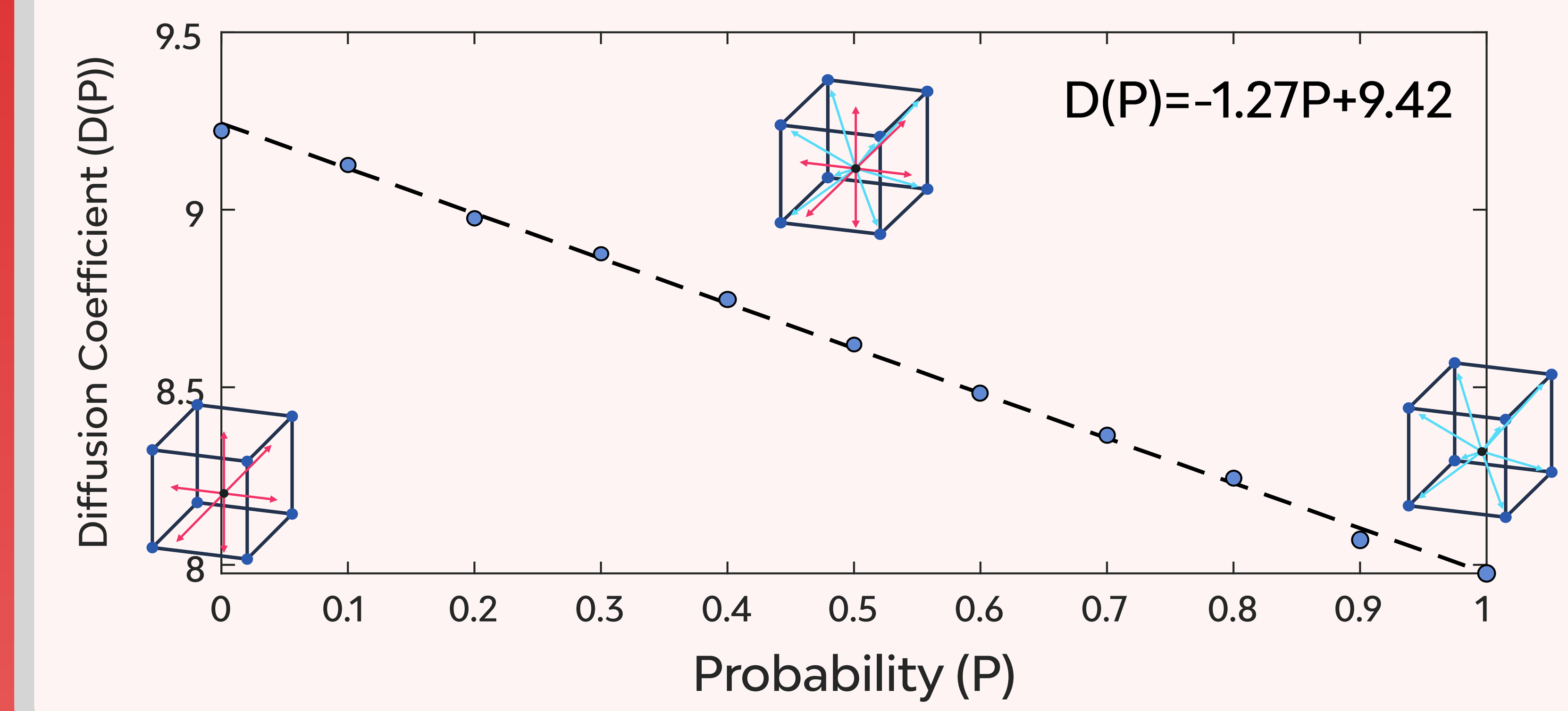


Fig. 5 • Diffusion Coefficient that best fits the diffusive growth shown in Fig. 4 for various nearest neighbor or second nearest neighbor biases.

Results

• Particle displacement in one dimension grows faster resulting in a larger average final distance from origin because the particle can only move directly towards or away from the previous position. Figure 3 shows that diffusion will occur more quickly in a lower dimension if there is an equal rate of lattice site hops.

• Diffusion of particles on a lattice is biased towards certain directions where the probability of a nearest neighbor (diagonal) versus second nearest neighbor (axis) hop affects the diffusion rate. Diffusion occurs quicker when the bias is in favor of second nearest neighbor hops because the particle will move a farther distance on the lattice which will result in a larger final average distance from the origin.

•Fig. 5 demonstrates a linear relationship because it describes the diffusion coefficient for a diffusive process with various probabilities. Diffusion acts as a Poisson Process and since each hop is independent of the previous hop, the sum of the independent Poisson Processes is linearly modeled as a Poisson Process."

Acknowledgements & References

We would like to acknowledge the National Science Foundation and the Noyce Scholarship Program. This project was funded in part by NSF Award #1540591.

Kittel, Charles, and Herbert Kroemer. "Thermal physics." (1998): 164-167.