ISOLATING DIFFUSION COEFFICIENTS OF LATTICE DEFECTS IN COULOMB CRYSTALS

Levi Webb[1] (he/him), Dany Yaacoub[1] (he/him), Matt Caplan[1] (he/him)

[1] Department of Physics, Illinois State University, Normal 61761, USA

Stellar Plasmas

- Exist in the hot, dense regions of white dwarf cores and neutron star crusts
- Do not have a “state of matter” but can behave as solids, liquids, or gases depending on their pressures and temperatures
- **Coulomb crystal**: Coulomb forces hold plasma particles together as though they are in a solid

Molecular Dynamics (MD) - LAMMPS

- LAMMPS [1] is a classical MD code that simulates a evolves a system of particles in time.
- We insert or remove particles to introduce defects into the plasma crystals

Defects

- Interstitials: particles inhabiting spaces between lattice grid points (inserted particles)
- Vacancies: uninhabited grid spaces (removed particles)
- Often form in pairs and ‘annihilate’ when they meet

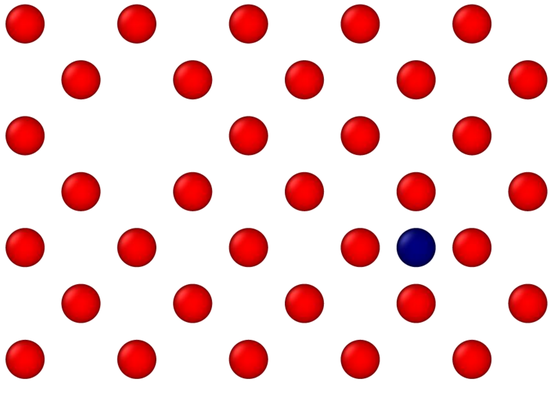

Fig 1. Examples of an interstitial and vacancy in a lattice.

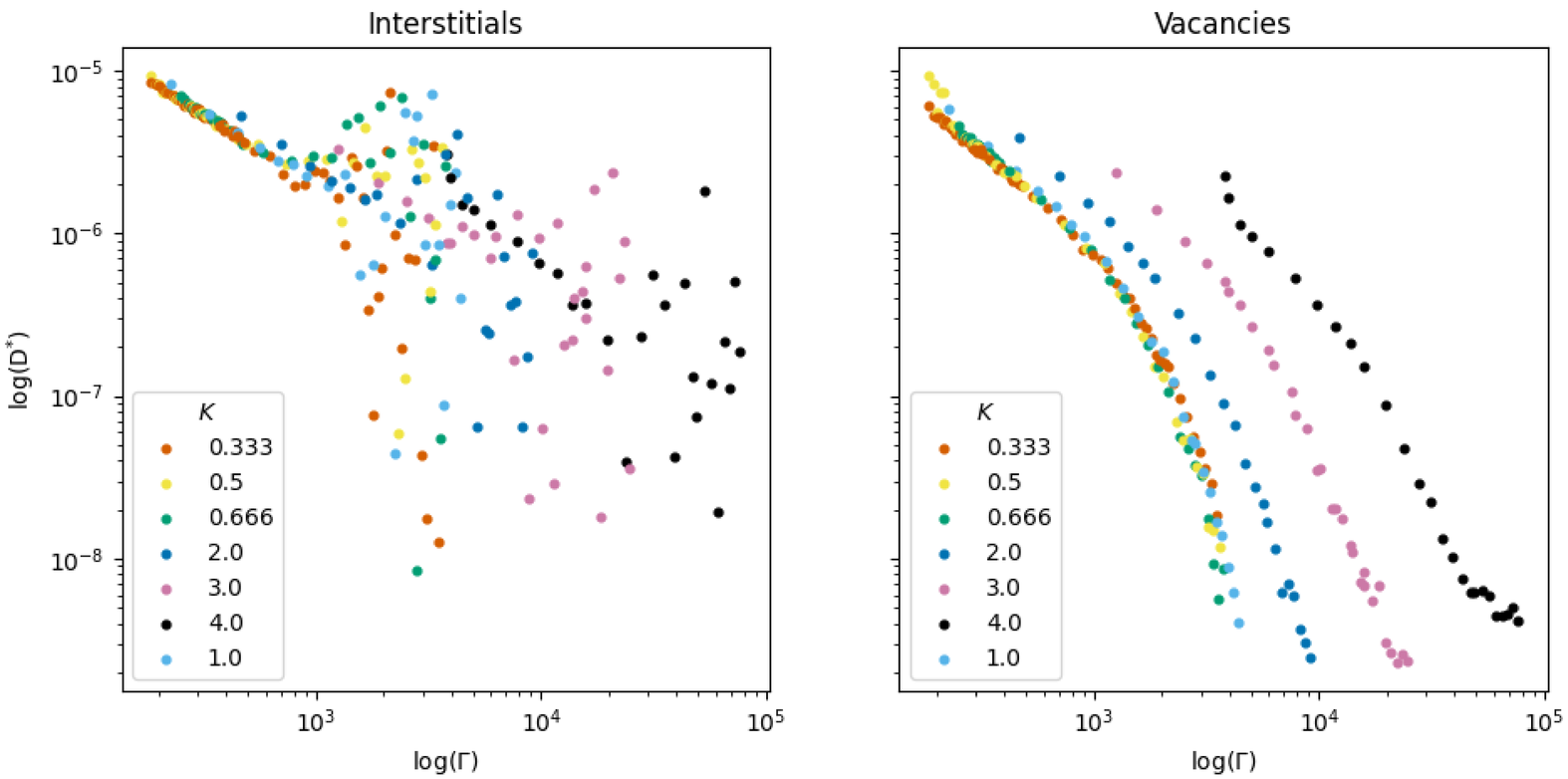

Fig 2. Diffusion coefficient plots at different screening lengths with respect to inverse temperature.

Simulations

- We want to find how the defect propagates, which is called its diffusion coefficient.
- LAMMPS parameters:
  - Small lattice (less likely to form defect pairs)
  - One component plasma (OCP; homogenous)
  - Temperature (variable)
  - Screening length (variable)
  - Potential cutoff = 8 spaces (maximum distance at which interactions between particles is considered)
- We plot the last value of the diffusion coefficient for each run rather than averaging.

Preliminary Results

- Interstitials and vacancies freeze into the crystal at different temperatures. At this point, they are doing a 1D random walk along a column of the lattice.
- Next steps:
  - Verify that our coefficients are for single defects
  - Track how the defect turns via vector analysis

References

[1] Thompson et al. 2022, Computer Physics Comms., 271, 108171

[2] Caplan & Yaacoub, 2024, PRL, 133, 13, 135301

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