Resolving Extended Space and Time Correlations in Molecular Dynamics Simulations of Strongly Magnetized Plasmas

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Research Results and Motivation

- Computed diffusion coefficients in a strongly magnetized one component plasma system using molecular dynamics (MD) simulations
- Significantly reduced particles required to obtain diffusion coefficients by using an elongated domain
- Examples of strongly magnetized plasmas include trapped antimatter, ultracold neutral plasmas, and magnetized dusty plasmas

Molecular Dynamics Simulations Are Used to Compute Diffusion Coefficients

- Periodic boundaries are used to simulate an infinite plasma
- Using a randomly selected subset of the simulation particles, the velocity auto correlation function is calculated
- From the velocity auto correlation function, the self diffusion is calculated using the Green-Kubo relations for a magnetized plasma

\[ D = \lim_{t \to \infty} \langle (r(t) - r(0))^2 \rangle = 6 \int_0^\infty (1 - \frac{s}{t}) Z(s) \, ds \]

- The diffusion coefficient can be found by approximating \( \lim_{t \to \infty} \) as the point which the mean squared displacement plot becomes linear on a log-log scale

Strong Magnetization Leads to Increased Temporal and Spatial Correlations Associated with Coulomb Collisions

- Magnetized one component plasma is characterized by the magnetization strength (\( \beta \)) and coupling strength (\( \Gamma \))

\[ \Gamma = \frac{q^2 / \alpha}{4 \pi \epsilon_0 k_B T} \quad \beta = \frac{\omega_e}{\omega_p} \]

- Additional boxes are added along the magnetic field direction to capture the long-range correlations
- This significantly reduces the number of particles required as compared to using the cubic domain
- Computational cost is decreased with decreasing number of particles required

Elongated Boxes Can Capture the These Increased Correlations With Lesser Number of Particles

- The initial box size is set by the number of particles required for unmagnetized plasma of the same coupling strength

Convergence When Elongating the Domain in the Direction of the Magnetic Field

- Gyroaveraged plot of parallel and perpendicular self diffusion with respect to time in a one component plasma
- Convergence with increasing number of box lengths (rlz) where N is the number of particles in the initial cube, and the domain is stretched by adding additional cubes

With elongated domain, \( \Gamma = 0.1, \beta = 4 \) required 11,000 particles, corresponding to a significant reduction in the number of particles required

Future Work

- Obtain diffusion coefficients using an elongated domain, continuing to explore the parameter space of \( \beta \) and \( \Gamma \), particularly in strongly magnetized and weakly coupled regimes

References


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