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(POS-50) Molecular Dynamics Simulation of Bubble Formation in Liquid Scintillators

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Bubble chambers have been used in the search for dark matter in the form of Weakly Interacting Massive Particles (WIMPs), as well as in the search for neutrinoless double beta decay. The Scintillating Bubble Chamber (SBC) is one such detector which uses an active volume of xenon-doped liquid argon (LAr), a scintillator which allows for the rejection of different classes of background events. In this study, a custom molecular dynamics simulation was written using HOOMD-blue to study the effects of energy deposited through scintillation on bubble formation thresholds in the detector. The simulation uses the parameterized Lennard-Jones potential to model intermolecular forces, common in other molecular dynamics simulations using software like LAMMPS. However, it modifies the standard Seitz "heat spike" model of bubble formation to permit more detailed modeling of atomic recoils and introduce a time-delayed release of energy as scintillation occurs. Preliminary results suggest that most scintillation energy is released on too slow a time scale to be consequential to bubble nucleation. Additionally, bubbles formed using this modified heat spike seem to exhibit the distinct "stages" of proto-bubble formation and rapid expansion before settling into stable growth or contraction, consistent with what has been observed in other molecular dynamics simulations.

Keyword-1

Molecular Dynamics

Keyword-2

Simulation

Keyword-3

WIMP Detection

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