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The effect of kinetic degrees of freedom in the study of microcanonical phase transitions SERGIO DAVIS, Grupo de Nanomateriales, Departamento de Fisica, Facultad de Ciencias, Universidad de Chile, JOAQUIN PERALTA, Departamento de Ciencias Fisicas, Universidad Andres Bello — The methodology for the study of phase transitions in macroscopic systems is well established, as the thermodynamical properties in these systems are ensemble-independent. However, for systems of hundreds of atoms or less, this does not hold, and phase transitions are most commonly studied in the microcanonical ensemble. Microcanonical Monte Carlo (MMC) simulations are not straightforward to perform with both coordinates and momenta, however marginalization of the kinetic degrees of freedom leads to a tractable distribution which can be sampled via MMC methods. Uses of these techniques had been presented in the literature for equilibrium properties but scarcely for the study of phase transitions. In this work, we present a study of microcanonical phase transitions without the use of kinetic degrees of freedom. We generate configurations according to the MMC procedure, which are processed in the framework of the Z-method in order to determine the transition point. We show that the results agree with the standard molecular dynamics implementation of the method for melting. This suggest that the kinetic degrees of freedom (and therefore the microscopic dynamics) are irrelevant for the determination of the transition point, being only dependent on the potential energy landscape.

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