The Mathematics of Microcanonical Car-Parrinello Simulations

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We survey the mathematical aspects of microcanonical Car-Parrinello simulations in ab-initio molecular dynamics. This method replaces the explicit minimization of energy potentials in a time-dependent Born-Oppenheimer approximation on-the-fly by a fictitious Newtonian dynamics. To this end, an artificial mass parameter μ is introduced that controls the electronic motion. Error bounds and their implications for an adaptive control of the mass parameter are discussed.

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