Physics > Computational Physics

Colored-noise thermostats à la carte

Michele Ceriotti, Giovanni Bussi, Michele Parrinello

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Recently, we have shown how a colored-noise Langevin equation can be used in the context of molecular dynamics as a tool to obtain dynamical trajectories whose properties are tailored to display desired sampling features. In the present paper, after having reviewed some analytical results for the stochastic differential equations forming the basis of our approach, we describe in detail the implementation of the generalized Langevin equation thermostat and the fitting procedure used to obtain optimal parameters. We discuss in detail the simulation of nuclear quantum effects, and demonstrate that, by carefully choosing parameters, one can successfully model strongly anharmonic solids such as neon. For the reader's convenience, a library of thermostat parameters and some demonstrative code can be downloaded from an on-line repository.

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