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(G*) POS-H77 – Brownian motion on a stochastic oscillator chain

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Molecular dynamics simulations are, in principle, numerically exact, but severely restricted with respect to the accessible time- and length-scale of the system studied. Stochastic simulations offer an alternative modeling method that overcomes these limitations. Unfortunately, the relation between the properties of the original system and the parameters used in stochastic modeling is not always clear. We address this problem by studying the diffusion of a Brownian particle along a chain of coupled stochastic oscillators. We show that stochastic simulations of the Brownian particle alone may be in quantitative as well as in qualitative disagreement with the result of the full-scale molecular dynamics simulations. As a remedy, we propose to simulate a small part of the chain together with the Brownian particle, which now becomes "dressed". We introduce a recipe to perform the stochastic simulations of the part of the chain. We show that the diffusion coefficient of the Brownian particle in this type of stochastic modeling is practically the same as in the molecular dynamics simulations in a broad parameter range.

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