High order path integrals made easy

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The precise description of quantum nuclear fluctuations in atomistic modelling is possible by employing path integral techniques, which involve a considerable computational overhead due to the need of simulating multiple replicas of the system. Many approaches have been suggested to reduce the required number of replicas. Among these, high-order factorizations of the Boltzmann operator are particularly attractive for high-precision and low-temperature scenarios. Unfortunately, to date, several technical challenges have prevented a widespread use of these approaches to study the nuclear quantum effects in condensed-phase systems. Here we introduce an inexpensive molecular dynamics scheme [1] that overcomes these limitations, thus making it possible to exploit the improved convergence of high-order path integrals without having to sacrifice the stability, convenience, and flexibility of conventional second-order techniques.

[1] V. Kapil, J. Behler, M. Ceriotti, J. Chem. Phys. **145**, 234103 (2016).