Constant-Uncertainty Molecular Dynamics. A Practical Method for Approximating Quantum Dynamics?

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Constant-uncertainty molecular dynamics [1] (CUMD) has been proposed as a "simple and efficient" method in which quantum effects can be incorporated into classical molecular dynamics simulations. The method has been shown to give better agreement with exact quantum mechanical results compared to ring-polymer molecular dynamics [2] (RPMD) for one-dimensional test systems. The method uses RPMD to set up an ensemble of classical particles and then evolves them subject to a constraint between the positions and momenta of the particles (based on the uncertainty principle). We find that the constraint cannot be integrated as it contains terms which are non-linear with respect to momenta; this results in the method using an ad-hoc fix, causing it to be inefficient and algorithmically unstable. As a result, it is unlikely that CUMD can be extended to larger, more realistic systems. However, we use the first step in the method (momenta rescaling of the RPMD beads) as a method in its own right and test it on further 1D and 2D systems.

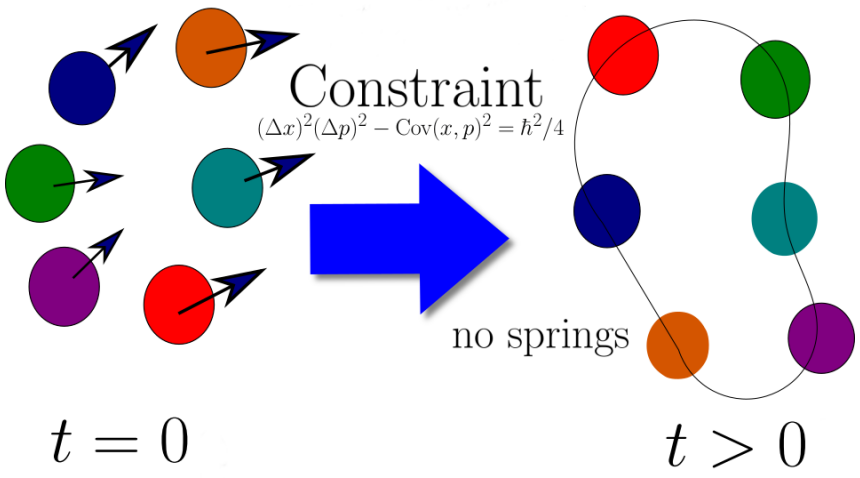

Figure 1: *Idea behind constant-uncertainty molecular dynamcis.*

References

1. T. Hasegawa, *J. Chem. Phys.*, **145**, 171101 (2016).
2. I. R. Craig and D. E. Manolopoulos, *J. Chem. Phys.*, **121**, 3368 (2004).