# Path Integral Molecular Dynamics for Bosons

Barak Hirshberg[a,b], Valerio Rizzi[a,b] and Michele Parrinello[a,b,c]

[a] *Department of Chemistry and Applied Biosciences, ETH Zurich, 8092 Zurich, Switzerland.*
[b] *Institute of Computational Sciences, Università della Svizzera italiana, via G. Buffi 13, 6900 Lugano, Switzerland.*
[c] *Italian Institute of Technology, Via Morego 30, 16163 Genova, Italy.*
barakh@ethz.ch

Cold trapped atoms are fascinating systems, exhibiting fundamental physical phenomena and also potentially useful in emerging quantum technologies. We present a new method for simulating such systems using path integral molecular dynamics. The main difficulty in performing these simulations is enumerating all ring-polymer configurations that arise due to permutations of identical particles. For Bosons, we show that the potential and forces at each time step can be evaluated using a recurrence relation that avoids enumerating all permutations, while providing the correct thermal expectation values. The resulting algorithm scales cubically with system size. The method is tested and applied to Bosons in a 2D trap and agrees with analytical results and numerical diagonalization of the many-body Hamiltonian. An analysis of the role of exchange effects at different temperatures, through the relative probability of different ring-polymer configurations, is also presented.

**References**

1. B. Hirshberg, V. Rizzi and M. Parrinello, arXiv:1905.09053.