

VISTA Seminar

Seminar 20

June 30, 2021

9:30 – 11:00 am EDT / 1:30 – 3:00 pm GMT / 3:30 pm – 5:00 pm Paris

TOC:

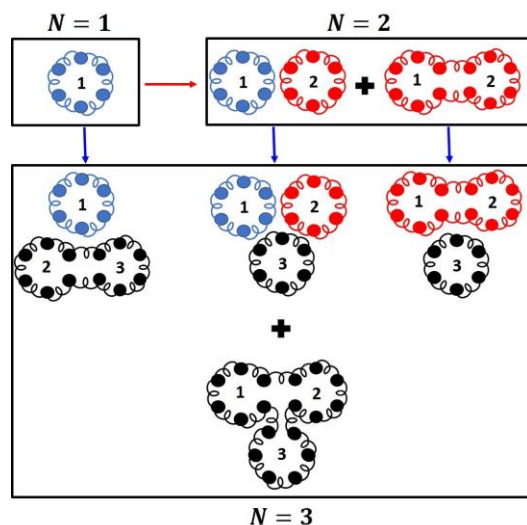
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Path integral molecular dynamics for indistinguishable particles

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Whether particles are bosons or fermions is a most fundamental property of quantum-mechanical systems. It is particularly important for accurately describing systems of ultracold trapped atoms, electrons in quantum dots, ortho- and parahydrogen and others. Path integral molecular dynamics (PIMD) simulations are widely used to study quantum effects in chemistry and physics. However, they completely neglect this property assuming the particles are distinguishable.

We present a new method for simulating indistinguishable particles using PIMD. For bosons, the main difficulty is enumerating all particle permutations, which scales exponentially with system size. We show that the potential and forces 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 allowing the first application of PIMD to large bosonic systems [1].

For fermions, the infamous sign problem presents an additional formidable challenge limiting applications to moderate temperatures and strongly interacting systems. By harnessing the power of free-energy methods, we can alleviate the sign problem and study weakly interacting systems at low temperatures [2-3].

Applications ranging from models of ultracold trapped atoms and electrons in two-dimensional quantum dots to simulations of deuterium under high-pressure and low temperature will be discussed. We will also present an analysis of the role of exchange effects at different temperatures, through the relative probability of different ring-polymer configurations.

References

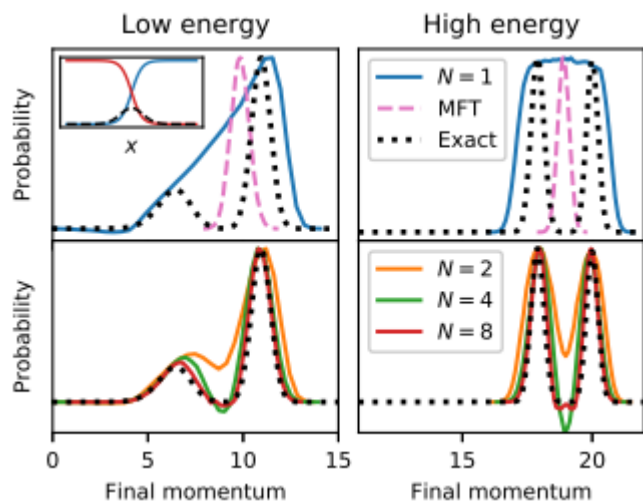
1. B. Hirshberg, V. Rizzi and M. Parrinello, Proc. Natl. Acad. Sci. USA (2019) 116 21445-21449.
2. B. Hirshberg, M. Invernizzi and M. Parrinello, J. Chem. Phys. (2020) 152, 171102.
3. T. Dornheim, M. Invernizzi, J. Vorberger and B. Hirshberg, J. Chem. Phys. (2020) 153, 234104.

Quantum entanglement from uncoupled classical trajectories

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A long-standing challenge in mixed quantum-classical trajectory simulations is the treatment of decoherence and, more generally, entanglement between the classical and the quantal degrees of freedom. Mean-field approaches like Ehrenfest neglect entanglement and therefore fail to describe effects such as wavepacket branching in a nonadiabatic scattering problem. Known remedies include stochastic hops, coupled trajectories or interference between path histories, but a fully classical simulation seems, at first sight, to be impossible. However, we have developed a novel approach which describes the emergence of entangled states entirely in terms of uncoupled and deterministic Ehrenfest-like trajectories. This is derived for a two-level system by mapping the quantum system onto a path-integral representation of a spin-1/2 [1], which is an extension of our previous linearized spin-mapping approach [2, 3].

We demonstrate that the method correctly accounts for coherence and decoherence and thus reproduces the splitting of a wavepacket in Tully's seminal scattering problems (see figure) as the number of discretization steps, N , increases. In contrast to many alternative methods, the path-integral approach can properly treat system with multiple crossings. This discovery opens up a new class of simulations as an alternative to stochastic surface-hopping or coupled-trajectory approaches.

References

- [1] J. E. Runeson and J. O. Richardson, "Quantum entanglement from classical trajectories," *submitted*, arXiv:2105.02075 (2021).
- [2] J. E. Runeson and J. O. Richardson, "Spin-mapping approach for nonadiabatic molecular dynamics," *J. Chem. Phys.*, **151**, 044119 (2019).
- [3] J. E. Runeson and J. O. Richardson, "Generalized spin mapping for quantum-classical dynamics," *J. Chem. Phys.*, **152**, 084110 (2020).

How to connect

Alexey Akimov is inviting you to a scheduled Zoom meeting.

Topic: VISTA, Seminar 20

Time: Jun 30, 2021 09:30 AM Eastern Time (US and Canada)

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