



SEMINAR

Monday, 20/01/2020, 12:00 am

Building 211, seminar room

SPEAKER:

Dr. Barak Hirshberg

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TOPIC:

**Path integral molecular dynamics for bosons
and fermions: From ultracold atoms to
quantum dots**

Abstract:

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 para-hydrogen 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 adding an auxiliary repulsive potential and correcting the results using a variational principle for the free energy, we are able to alleviate the sign problem and study weakly-interacting systems at low temperatures.

The method is tested and applied to ultracold atoms and agrees with analytical and numerically-exact results. Results for few-electron quantum dots will also be discussed as well as an analysis of the role of exchange effects at different temperatures, through the relative probability of different ring-polymer configurations.

[1] B. Hirshberg, V. Rizzi and M. Parrinello, Proc. Natl. Acad. Sci. USA (2019) 116 21445-21449.