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Quantum simulation of conical intersections using trapped ions

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Conical intersections (CIs) are an ever-present phenomenon in chemistry and molecular physics that mark the crossing of energy levels on an adiabatic potential energy surface (PES). Around such intersections, the Born-Oppenheimer approximation breaks down and the coupling between electronic and nuclear coordinates becomes important. Thus, efficiently simulating the dynamics in the vicinity of CIs is an important and open problem. Another notable phenomenon is the geometric phase that accumulates when a wave function loops around CIs on a PES. Such a phase depends only the direction of travel and the solid angle encompassed by the loop with respect to the CI and can have non-trivial effects on the dynamics of the molecule. Meanwhile, trapped atomic ions have proven to be a robust platform for performing quantum simulations of molecules. Manipulation of the internal states and the motion is made possible by light-matter interactions using lasers. These can be mapped to the internal states and nuclear parameters of simple molecules. With this tool, we present a scheme for engineering a CI in trapped ions systems and demonstrating controllable geometric phase interference by using an appropriate initial state and adiabatic evolution. The final state will have a characteristic shape marked by interference between parts of the wave function that took different paths around the CI. Finally, we will present experimental measurements of the spatial distribution and compare the results to numerical calculations.

See paper preprint:

Whitlow, Jacob, et al. "Simulating conical intersections with trapped ions." arXiv preprint arXiv:2211.07319 (2022).

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