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Engineering tunable anharmonic potentials with light-atom interaction for chemical dynamics simulations

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Trapped-ion platforms have emerged as a powerful architecture for quantum simulation, offering high-fidelity universal control over both internal atomic states (spins) and bosonic motional modes. This makes them particularly well-suited for simulating molecular dynamics, where a natural analogy allows a molecule's electronic configuration to be mapped onto the ion's spin, and its vibrational structure onto the ion's motion.

This approach has enabled pioneering studies of time-resolved vibrational spectroscopy [1], geometric phase effects at conical intersections [2, 3], and open-system chemical dynamics of real molecules [4]. To date, however, these implementations have been restricted to harmonic oscillator models, failing to encapsulate the crucial anharmonicity present in most molecular potentials.

Here, we overcome this limitation by implementing anharmonic dynamics in a trapped-ion system using coherent, programmable quantum control with light-atom interactions. We present a flexible scheme that leverages state-dependent forces and qubit rotations to engineer widely tuneable anharmonic potentials. As a key demonstration, we realize a double-well potential of the form $V(x) = \delta x^2 + \epsilon \cos\ (\eta x)$. This allows us to access rich, nonlinear dynamics, most notably observing quantum tunnelling of a wavepacket between the two wells. These results establish a pathway for simulating chemically relevant potentials on a programmable quantum platform.

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