Path integral methods for reaction rates

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In this talk, I will review both the ring polymer molecular dynamics (RPMD) rate theory approximation to adiabatic (Born-Oppenheimer) reaction rates [1-7], and the Wolynes theory approximation to non-adiabatic (Fermi Golden Rule) reaction rates [8,9]. Both of these theories are based on imaginary time path integrals, both provide an excellent description of quantum mechanical zero point energy and tunnelling effects, and both are readily applicable to chemical reactions in arbitrarily complex (anharmonic and multi-dimensional) systems. My review will serve as an introduction to Joseph Lawrence's talk later in the same session, in which he will show how the RPMD rate theory approximation to the Born-Oppenheimer rate and the Wolynes theory approximation to the Golden Rule rate can be combined to give a highly accurate path integral description of electron transfer rates across the full range of electronic couplings from the non-adiabatic to the adiabatic regime [10].

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