Equation-of-motion coupled-cluster method for electron-molecule shape resonance and inter-atomic coulombic decay

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In this talk, a novel complex absorbing potential (CAP) based equation-of-motion coupled-cluster method will be presented for describing electron-molecule shape resonace as well as inter-atomic coulombic decay problems. Both these involve meta-stable states and inclusion of complex absorbing potential to the Hamiltonian makes the wave function square-integrable allowing bound state methods to be applied. Resonance energy and width are identified from real and imaginary parts of energy. We also compare with earlier CAP based multi-reference variants of coupled-cluster method. Numerical results are presented for proto-type cases.