Semiclassical computational methods for quantum dynamics with band-crossing and uncertainty

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Abstract: Band-crossing is a quantum dynamical behavior that contributes to important physics and chemistry phenomena such as quantum tunneling, Berry connection, chemical reaction etc. In this talk, we will discuss some recent works in developing semiclassical methods for band-crossing in surface hopping. For such systems we will also introduce an "asymptotic-preserving" method that is accurate uniformly for all wave numbers, including the problem with random uncertain band gaps.