

A periodic orbit formula for quantum reactions through transition states

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Transition State Theory forms the basis of computing reaction rates in chemical and other systems. Recently it has been shown how transition state theory can rigorously be realized in phase space using an explicit algorithm. The quantization has been demonstrated to lead to an efficient procedure to compute cumulative reaction probabilities and the associated Gamov-Siegert resonances. In this letter these results are used to express the cumulative reaction probability as an absolutely convergent sum over periodic orbits contained in the transition state.

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