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Semiclassical Scattering on Conical Intersections ANDREI PIRYATINSKI, Theoretical Division, Center for Nonlinear Studies, Los Alamos National Laboratory, MISHA STEPANOV, SERGEI TRETIAK, VLADIMIR CHERNYAK, Department of Chemistry, Wayne State University, 1 COLLABORATION — The problem of nonadiabatic vibrational dynamics in the vicinity of the electronic energy surface crossing is a key to understanding of variety of fundamental processes in photochemistry including radiativeless energy relaxation and photoisomerization in (bio)molecules. To address the problem, advanced theoretical methods have been developed and implemented as numerical techniques. In this contribution we focus on the photoexcited wavepacket scattering problem in the vicinity of conical intersection, and demonstrate that simple analytical expressions for the scattering matrix can be obtained in the semiclassical approximation. Simplicity of the latter expressions allow us to develop a clear quantitative picture of the photochemical processes taking place near the level crossing surface. This picture is verified using the numerical simulations, and good agreement is found for the realistic set of parameters. Therefore, it is now feasible to implement our computational method into the large scale molecular dynamics simulations significantly reducing the computational costs.

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