TIME EVOLUTION OF PENDULAR STATES OF ASYMMETRIC-TOP MOLECULES

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Molecular rotation can be transformed by the interaction with a strong electric field into a pendular motion [1] in which the molecular axis is oriented or aligned. Usually, two electrodes are used to apply a dc electric field to the molecules [2]. Due to the border effects of the conducting plates the field does not zero suddenly but it extends far from the plates. Therefore, molecules traveling in a beam experience a varying electric field when they approach the Stark plates. Here, we investigate the adiabaticity of the population transfer for molecular ensembles from the field-free region to the static-field region. Rotational-eigenvalue trajectories as a function of electric field strength can present many avoided crossings for asymmetric-top molecules. These crossings will be transversed diabatically or adiabatically depending on the ratio between the variation of the field and the size of the avoided crossings. In the ideal case of every crossing being avoided, the population distribution of the ensemble in the field will be the same of the field-free molecular ensemble.
We solve the time-dependent Schödinger equation by using a propagator based on a modified split-operator technique combined with the Riemann integral product method. The high efficiency of this method allows us the propagation of rotational wavefunctions for very long times, which is needed for going from the field-free region to the static-field region. Examples for several molecules will be presented.

[1]. B. Friedrich and D. R. Herschbach, Nature **353**, 412 (1991).
[2]. D. T. Moore, L. Oudejans, and R. E. Miller, J. Chem. Phys., **110**, 197 (1999), and refs. therein.