MOLECULAR DYNAMICS AND A SIMPLIFIED MASTER EQUATION FOR SPECTRAL LINE SHAPES

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Borrowing heavily from the literature, we develop a transport relaxation equation for the off-diagonal elements of the density matrix. It is applicable to a large range of topics in laser theory, nonlinear optics and spectral line shapes, etc. Applying this single equation to the case of infrared electric dipole transitions, permits us to recover, quickly and simply all of the well known spectral line shapes found in the literature. It also offers further insight into the process of line mixing, particularly in the weak mixing limit. An outline of a new treatment of Dicke narrowing and other speed dependent contributions to spectral profiles is also given in terms of the transport relaxation equation. The new treatment also provides a numerical method for including the effects of statistical correlation between the evolution of the internal and translational degrees of freedom.