MOTIONAL DYNAMICS BY ESR AND THE STOCHASTIC LIOUVILLE EQUATION

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Over the last several decades, a powerful and successful theoretical methodology, based upon the Stochastic Liouville Equation (SLE), has been developed to analyze ESR spectra in terms of motional dynamics. This methodology will be described in some detail. This will include the structure of the spin Hamiltonian; transformations between lab and molecular frames, which are necessarily fluctuating in time; the spin-density matrix; models of rotational diffusion including MOMD and SRLS; the structure of the SLE and how it enters into the lineshape function; methods of numerically solving the SLE, including the Lanczos Algorithm for its fast diagonalization; and the extensions to Two-Dimensional, Fourier Transform ESR.