



# Innsbruck Physics Colloquium

## Master equations for spin dynamics

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In a typical photochemical scheme for the formation and recombination of a charge-separated radical pair, the photo-excitation of a donor-bridge-acceptor (D-B-A) molecule is followed by a rapid electron transfer along the bridge to produce the charge-separated radical pair in its singlet electronic state,  $^1[D^+-B-A^-]$ . This then undergoes coherent intersystem crossing to the triplet state,  $^3[D^+-B-A^-]$ . For organic radicals  $D^+$  and  $A^-$ , this intersystem crossing is typically mediated by weak magnetic (hyperfine) interactions, and is sensitive to a magnetic field. During the intersystem crossing, the singlet radical pair decays to the ground state  $^1D-B-A$  molecule with a first order rate constant  $k_S$ , and the triplet radical pair decays to the excited  $^3D-B-A^*$  molecule with a rate constant  $k_T$ .

I will introduce the Nakajima-Zwanzig (NZ) equation, and then describe three applications of this equation to the radical pair problem. In the first, the NZ equation is used to derive a master equation for the spin density operator of the radical pair which correctly includes both the coherent intersystem crossing and incoherent recombination processes. In the second application, the NZ equation is used to analyse when it is valid to work with a simple kinetic model [2]. And in the third application, the NZ equation is shown to provide a more accurate framework than Redfield theory for including electron spin relaxation effects in radical pairs [3]. All three of these applications will be illustrated with example calculations, primarily of spin-dependent charge recombination along molecular wires.

**Colloquium: Tuesday, 14.01.2020**

**17:15 h in lecture hall C**

**DK-ALM Pre-Talk: 16:30 h**

**Matthias Kondrak**

**Quantitative Spectroscopy of Red Supergiants**

Snacks will be provided in between the pre-talk and the colloquium.