Quantum and semiclassical methods for radical pair spin dynamics

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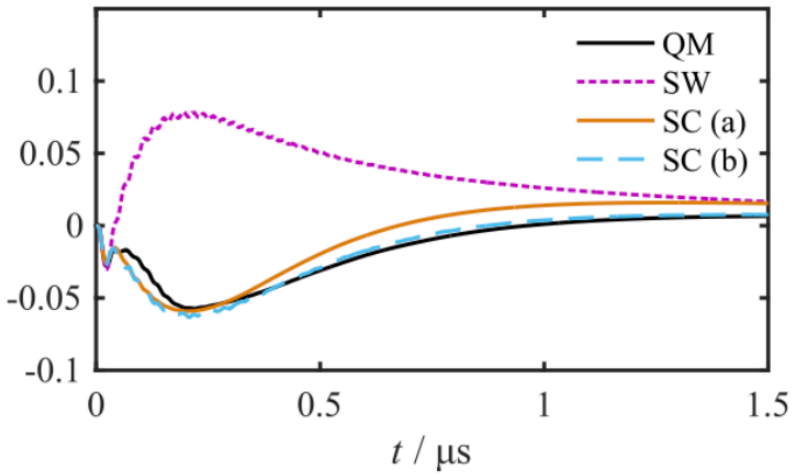
Peter Hore introduced us to the spin dynamics of radical pairs almost a decade ago. Since then, we have developed new semiclassical [1,2] and quantum mechanical [3-5] methods for simulating this spin dynamics, and applied them to a variety of interesting problems. For example we have recently calculated the exact quantum mechanical spin dynamics of a photo-excited carotenoid-porphyrin-fullerene (CPF) radical pair containing 45 hyperfine-coupled nuclear spins [6]. This was quite an achievement because the 2^{47} coupled states in the Hilbert space would have made a standard quantum mechanical calculation quite impractical. We have also shown that an appropriate semiclassical approximation reproduces our quantum mechanical results for the CPF radical pair at a small fraction of the computational cost [6]. This talk will review these developments and use them to argue that the problem of simulating the spin dynamics of even rather complicated radical pairs has now been solved.



Magnetic field effect on the survival probability of a $C^{+}PF^{-}$ radical pair from exact quantum mechanical (QM), Schulten-Wolynes (SW), and improved semiclassical (SC) calculations [6].

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