

Developing an anisotropic extension of spin dynamics for quantum biosensing

Institution	The University of Wollongong
Project details	Magnetic fields can influence the behaviour of molecules through their interaction with electron spins. In some proteins, these electron spins evolve through different paired quantum states via the coupling of the nuclear magnetic moment with the electrons magnetic moment. Understanding this interaction these spin dynamics is vital to the development of quantum biosensors. Recent experiments have demonstrated control of these states through application of a resonant radio-frequency in conjunction with a weak magnetic field^{1,2}. Transitions between these states depend not only on the strength of the magnetic field (mediated by the Zeeman effect³), but also on its direction relative to the molecule (anisotropy). We have recently developed a theoretical model to calculate this spin evolution isotropically^{4,5}, that is direction-averaged, to simplify the physical description. An isotropic approach is often a reasonable approximation for molecules undergoing rapid rotational motion, like in proteins in solution, however controlling the spin evolution no longer becomes possible when direction is averaged. For this internship project, we will extend our existing theoretical framework to include anisotropic spin evolution, setting the stage for publishable scientific works. In this role, we will be trained in quantum chemical modelling techniques and magnetic field effects. The source code for the original code will be provided as a guide. You will then work with me to develop and code the math required to describe anisotropic spin evolution, then we will apply it to a real system. 1. Abrahams, <i>et al.</i>; Nature, 2026; 649, 1172-1179. 2. Burd, <i>et al.</i>; Nature, 2026; 651, 940-945. 3. Drummond, <i>et al.</i>; Nature Communications, 2021; 12, 4532. 4. Manian, <i>et al.</i>; The Journal of Chemical Physics, 2026; 164, 18, 184103. 5. Manian, <i>et al.</i>; ChemRxiv:10.26434/chemrxiv.15000458
Who can apply	A background in physics, chemistry, mathematics, or a related discipline would be advantageous. No previous experience with quantum chemistry or spin dynamics is required. Enthusiasm and curiosity are important.
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