Theoretical magneto-optical spectroscopy for solid state defect quantum bits

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We live in the era of second quantum revolution in which solid state defect quantum bits play a significant role. An exemplary solid state defect quantum bit is the nitrogen-vacancy center in diamond which can be effectively initialized and readout at room temperature. We show how theoretical magneto-optical spectroscopy on nitrogen-vacancy center explained its optical spin polarization loop which is the key mechanism in the initialization and readout. To this end, methods to calculate highly correlated electronic states and levels embedded in the itinerant solid state electron system with thousands of electrons has been developed [1] which is often called "quantum embedding" method or can be viewed as a multiscale method where the itinerant electron system is treated by density functional theory whereas the Coulomb-interaction between the strongly interacting orbitals in the system is directly calculated, i.e., so called configurational interaction theory. To our knowledge, there is no rigorous theory about the interface of the two approaches, i.e., the double counting term, therefore, we have recently started to use density matrix renormalization group wavefunction methods based on density functional theory ground state calculations which produce promising results for defect spins in hexagonal boron nitride [2,3]. We show that understanding the optical spin polarization loop requires the exploitation of dynamical effects due to the enhanced electron-phonon interaction. In this regard, we show the power of Jahn-Teller theorem when combined with density functional theory calculations of few thousands of electrons system [4,5]. In particular, we show the extension of Herzberg-Teller theorem from the optical transition to intersystem crossing [6] which is the key of quantum bit operation of nitrogen-vacancy center and related quantum systems. We briefly touch the importance of *ab initio* spin-related coupling tensors in the description of defect qubits, such as hyperfine tensors, in understanding the qubit's spin dephasing and spin coherence times [7].

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