M. J. Rodríguez

E. A. Rodríguez-Mena, Y. M. Niquet

Univ. Grenoble Alpes, CEA, IRIG-MEM-L_Sim, 17 Av. des Martyrs, 38000, Grenoble, France

mauricio-javier.rodriguezgarcia@cea.fr

We introduce a computational method, derived from configuration interaction, which enables efficient calculations of the spectrum of two-particle problems in very realistic geometries. We apply this method to a double hole spin qubit in a Germanium heterostructure. We analyze the nature and physics of the exchange interaction, J, between such two qubits. We highlight the role played by the Coulomb correlations and the importance of the couplings with the excited states (See Fig. 1). We also discuss the mixing of the singlet (S) and triplet (T) states by spin-orbit coupling, difference including the of a-factors the between the dots and Rashba interactions while tunneling. The S-T₀ mixing is particularly relevant for two-qubit gates and the S-T- mixing for singlet-triplet qubits and for readout [1]. We show, in particular, that inhomogeneous cool-down strains can make a significant contribution to these mixings. We then analyze the dependence of J and the S-T₋ gap on the orientation of the magnetic field while keeping the detuning between the dots fixed. This reveals that the S-T- mixing is maximal for inplane magnetic fields and most sensitive to the orientation in this plane. The magnitude of the calculated S-T-splittings is consistent with the available experimental data [2]. Finally, we show that we can achieve timedependent two-particule simulations with our methodology and compute the fidelities of the initialization and readout of a singlettriplet qubit as an illustration.

References

- Jirovec, D. et al. A singlet-triplet hole spin qubit in planar Ge. Nat. Mater. 20, 1106–1112 (2021).
- [2] Fang, Y., Philippopoulos, P., Culcer, D., Coish, W. A. & Chesi, S. Recent advances in hole/spin qubits. Mater. Quantum. Technol. 3, 012003 (2023).

Figures



Figure 1: Band structure of the system as a function of the detuning between the dots for a full configuration interaction (CI) calculation and our proposed dressed basis approach.