Complete TCAD study of a 3C-SiC based Q-simulator

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Abstract: The complete numerical investigation of processes and protocols to produce and characterize a quantum simulator is discussed. As a case of study, we consider interacting spin states of divacancies and H functionalized surfaces in 3C-SiC.

A complete quantum (Q-) technology computer aided design (Q-TCAD) analysis for reproducing "in-silico" the fabrication steps and the ODMR based protocols [1,2] necessary to realize and control a q-simulators is here presented. The q-simulator system under study is based on electronic spin states residing in open volume defects (namely, V_C-V_{Si} di-vacancies) which interact through hyper-fine coupling with the S=1/2 nuclear spins of H atoms chemisorbed on (100) or (111) reconstructed 3C-SiC surfaces. From bulk to near-to-surface defects configurations are considered to gradually achieve hyper-fine coupling intensity which potentially exceeds locally the dipole-dipole coupling. We demonstrate that linked chain of atomistic process and quantum-device simulations is a key-tool to understanding the realistic atomic structure of the quantum simulator devices and their eventual deviations with respect to the ideal operational conditions. A particular example of this complete analysis, which will be discussed in a paper in the preparation stage, is shown in the attached figure where the impact of the real di-vacancy position in the close-to ground state adiabatic preparation protocol is studied.

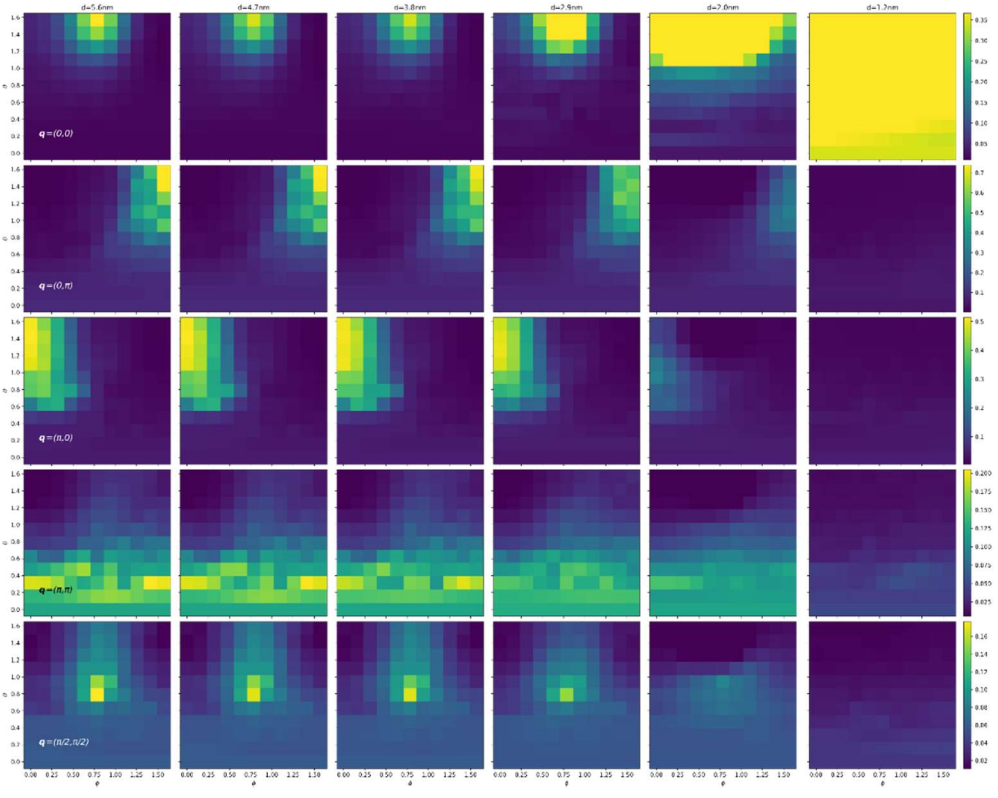

Figure Maps, as a function of the external magnetic **B** field direction in polar coordinates (B,Θ,ϕ) of the structure factors S(**q**) calculated for the modified and quantum simulated XXZ model after an the adiabatic quenching protocol for the interacting H nuclear and di-vacancies electron spins on (100) 3C-SiC surface for the 5 different spin $\mathbf{q} \equiv (q_x, q_y)$ waves indicated for each row in the panels. In the columnar sequence maps at different distance of the defect position and the plan where the H nuclei resides are reported.

References

[1] Tommaso Fazio, Ioannis Deretzis, Giuseppe Fisicaro, Elisabetta Paladino and Antonino La Magna "First-Principles Investigation of Near-Surface Divacancies in Silicon Carbide" Physical Review A 109, 022603 (2024).

[2] Philip Kitson,Tobias Haug, Antonino La Magna, Oliver Morsch and Luigi Amico"Rydberg atomtronic devices" Physical Review 110, 043304 (2024).