Circles: Quantum Dots and Single Atoms
Simulation and experimental characterization of electron spin qubits in solid-state devices

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Although semiconductor-enabled classical electronics and computer science, based on classical physics, have met the requirements of an ever-inflating number of pervasive applications for several decades thanks to astonishing technological progress, some hard problems still remain beyond the capabilities of classical computers. The emergence of quantum technologies, stemming from quantum physics, is not just an innovation in this field but a fundamental paradigm shift that, by exploiting properties such as superposition and entanglement, offers the potential to accelerate approaches to solving complex problems and enhancing the security of data transmission between distant terminals. The new quantum era, which is at its dawn, is anticipated to have an unprecedented social impact, enabling the research of tomorrow across several pivotal fields.

These perspectives necessitate a physical system capable of encoding, processing, and retaining quantum information for a sufficiently long amount of time. Nowadays, quantum hardware belongs to the category of Noisy Intermediate Scale Quantum (NISQ) computers, i.e., available quantum computers are small and susceptible to several non-ideal phenomena, such as quantum coherence loss and randomization of quantum information [24]. Since the beginning of the 21$^{\text{st}}$ century, the research on the physical implementation of quantum hardware has explored several approaches: magnetic nuclei in diamagnetic molecules controlled via nuclear magnetic resonance (NMR) [27], superconductive qubits [14], molecular nanomagnets [11], trapped ions [6], photons [13], topological qubits [15], defects and dopants in solid-state materials, and quantum dots in semiconductors [7].

The legacy of classical electronics, which resulted in high-yield highly reproducible reliable CMOS processes, has propelled the exploration of CMOS-compatible semiconductor-based structures for next-generation quantum computers, driven by their promise of scalability and the opportunity to leverage well-established technological processes [29, 18], thereby easing the integration of quantum and classical computing systems [16].

The widespread interest in semiconductor quantum devices has been fuelled by significant experimental advancements in charge control, gate fidelities, and coherence times observed in both quantum dots and single dopants in semiconductor materials. Notable advantages include the small qubit footprint, typically on the order of tens of nanometers, and the fast gate-controlled manipulation and read-out procedures [28]. Furthermore, semiconductor quantum devices can be controlled through electric (metal gates) and magnetic (integrated micromagnets) fields, a crucial feature for envisioning possible control schemes of a dense array of several qubits together [30]. In this context, quantum dots have demonstrated promising scalability attributes. Conversely, this remains a challenge for dopant-based systems, which, on the other hand, are distinguished by remarkably long coherence times [26, 23, 22].

The work discussed in this essay focuses on solid-state technologies as viable platforms for future quantum computers, and can be divided into three main parts:

- Development and validation of a multi-level simulation infrastructure for quantum dots in semiconductor heterostructures.
- Methods for cryogenic device-level simulations of semiconductor heterostructures.
- Experimental characterization of single-dopant devices for quantum applications, focusing on ^{209}Bi implanted devices.

1 Modelling spin-based quantum devices

The optimal engineering of currently available quantum computers, which are small and flawed by several non-ideal phenomena, requires an efficacious methodology for exploring the design space. There is an unmet need for the development of reliable hardware-aware simulation infrastructures able to efficiently emulate the behaviour of quantum hardware that commits to looking for innovative systematic ways, with a bottom-up approach starting from the physical level, moving to the device level and up to the system level. Currently available classical simulators of quantum computers mainly belong to two well-established families: physically accurate but CPU-intensive simulators based on the direct solution of Schrödinger and Lindblad equations [5, 4, 12] and fast high-level ideal simulators [1] developed for handling many qubit systems. The research presented in the first part of this work stands between the two families. It is oriented towards the development of a multi-technology simulation infrastructure of noisy quantum computers — based on the definition of CPU-and-memory friendly hardware-aware *compact models* — that aims to fulfil two objectives. The first one is the emulation of the execution of the same quantum circuit on different hardware platforms under a reasonable set of approximations. The second one is the analysis, for every technology, of the performance dependence on both physical parameters and control degrees of freedom, thus enabling their optimisation according to some fiducial parameters.

The quantum simulation toolchain envisioned in this work is hoped to be a first step towards the development of a design infrastructure that, leveraging existing physical simulators and novel compact models, could mimic the well-established multi-level design procedure routinely employed in classical electronics. The relevant physical parameters — such as Zeeman splittings, coherence time constants, J-couplings and many-body singlet-triplet splitting, g-factors, chemical shieldings, and several others — can be extracted from the experimental characterisation of the quantum devices or exploiting finite-element method (FEM) and ab-initio simulators. The downstream *intermediate-level* simulation infrastructure is provided with the extracted device parameters and with several technology-dependent control parameters — such as the static magnetic field, the MW/RF electromagnetic fields and the phase and duration of quantum gates. The input quantum circuit, described in OpenQASM 2.0 [9] — standard de facto for quantum algorithms —, is handled by a technology-aware compilation utility presented in [25] and not discussed in this thesis. Then, the noisy-compact model infrastructure carries out an ideal and a noisy simulation and delivers in the output the probability distribution of the eigenstates and some performance metrics, such as the fidelity. A similar approach for the emulation of quantum-key distribution (QKD) circuits is outlined in [8] but falls outside the scope of this thesis.

Since homonuclear Nuclear Magnetic Resonance (NMR) quantum computers [27] represent an iconic example of a spin-based system affected by non-ideal phenomena, this work initially discusses modelling approaches for this technology. These non-ideal phenomena can be efficaciously simulated by the developed compact models — based on the density matrix formalism — without requiring the direct integration of the Lindblad equation. Among the others, one can mention:

- Randomization of the quantum information caused by the joint effect of relaxation and decoherence.
- Residual unwanted coupling: NMR is a *fully-connected* technology, meaning that every nucleus is always interacting with all other nuclei of the same molecule. Ad-hoc refocusing schemes can be applied exclusively during the execution of two-qubit gates and not for single-qubit ones. Therefore, the latter are affected by residual unwanted coupling effects.
- Off-resonance: in homonuclear quantum registers, the single-qubit addressability relies on faint local variations of the static magnetic field (chemical shielding). Hence, when addressing a qubit with a resonant field, the other nuclei are also partially affected.
- Trade-off between soft and hard pulses: a hard (short) pulse implies a broad Fourier spectrum, thus leading to relevant off-resonance and negligible residual coupling; vice-versa for a soft (long) pulse.

Afterwards, the methodology developed for NMR is inherited and expanded to semiconductor quantum dots with some modifications that reflect the peculiarities of this technology — such as the dependence on the detuning, on the many-body exchange interaction and on the on-site Coulomb repulsion —

starting from an approximation of the many-body second-quantization Fermi–Hubbard model through a Schrieffer–Wolff transformation.

2 Cryogenic simulation of quantum devices

The multi-level simulation infrastructure introduced above necessitates several input physical parameters, which can be acquired through either experimental data or existing physical simulators, usually Poisson-Schrödinger FEM solvers. The simulations of quantum algorithms reported in this work employ a hybrid approach: some physical parameters are derived from simulations performed with two Poisson-Schrödinfer FEM solvers (NextNano [5] and QTCAD [4]), while others — currently beyond the capabilities of available simulators — are extracted from experimental data documented in the scientific literature. However, the simulation of nano-electronic devices at cryogenic temperatures presents several challenges, mainly associated with the steep behaviour of the Fermi–Dirac integrals. The carrier populations exhibit an exponential dependence on the temperature T, which results in rapid variations of carrier densities over extremely short length scales, particularly near locations where the conduction or valence band edge intersects the Fermi level. Consequently, solving the Poisson equation at cryogenic temperatures (below 100 K) is well-known to be an involved task [4]. Even a small change in conduction or valence band energies between successive iterations of the Poisson solution can lead to significant variations in carrier populations, causing numerical instabilities. Overcoming this challenge requires careful engineering of the mesh. The second part of this thesis elaborates on the methodology employed to simulate some semiconductor heterostructures adopted for quantum computation applications.

3 Experimental characterization of single bismuth donors in nanoelectronic devices

Among the numerous semiconductor qubit hardware platforms, single group-V donors in ^{28}Si have excellent properties considered essential for high-fidelity quantum computation. Scientific efforts on ^{31}P donors have yielded remarkable achievements [19], including extended coherence times [26, 23, 22], high single-shot spin readout fidelity [20, 23], and notable gate fidelities for both single-qubit and two-qubit operations [10, 21, 17], all achieved with implanted nanoelectronic devices fabricated with CMOS-compatible processes.

However, despite the advancements achieved with ^{31}P donors, limitations persisted in the types of experiments that could be conducted due to their small nuclear spin number. To explore larger Hilbert spaces, recent research has broadened its scope to include heavier group-V donors characterized by larger nuclear spin numbers [2, 3].

Following this path, the last part of this work focuses on the experimental characterization of the heaviest group-V donor: ^{209}Bi. Silicon-bismuth defect systems are characterized by uncommon properties, such as strong hyperfine constant and large nuclear spin number, which constitute a strong rationale for studying the possibility of encoding quantum information on single bismuth donors.

The investigation and experimental characterization of these systems necessitate the fabrication of nanoelectronic devices, where single donors can be implanted, and their properties can be measured, and an advanced experimental setup for cryogenic electronic measurements, which is analysed in this work.

Finally, the experimental characterization of nanoelectronic devices with implanted ^{209}Bi donors is discussed, from initial tuning to the observations of signatures of single-shot readout. To the best of the author's knowledge, no prior published studies have addressed single-bismuth donors in silicon. Thus, the work discussed in this chapter represents an initial step towards characterizing these systems.

References

[1] Gadi Aleksandrowicz et al. *Qiskit: An Open-source Framework for Quantum Computing*. Jan. 2019. DOI: 10.5281/zenodo.2562111. URL: https://zenodo.org/records/2562111 (visited on 01/11/2024).

[2] Serwan Asaad. *Electrical Control and Quantum Chaos with a High-Spin Nucleus in Silicon*. Springer Theses. Cham: Springer International Publishing, 2021. ISBN: 978-3-030-83472-2 978-3-030-83473-9. DOI: 10.1007/978-3-030-83473-9. (Visited on 09/17/2023).

[3] Serwan Asaad et al. "Coherent electrical control of a single high-spin nucleus in silicon". In: *Nature* 579.7798 (Mar. 2020), pp. 205–209. ISSN: 1476-4687. DOI: 10.1038/s41586-020-2057-7. (Visited on 02/21/2024).

[4] Félix Beaudoin et al. "Robust Technology Computer-Aided Design of Gated Quantum Dots at Cryogenic Temperature". In: *Applied Physics Letters* 120.26 (June 27, 2022), p. 264001. DOI: 10.1063/5.0097202. (Visited on 09/17/2023).

[5] S. Birner et al. "Nextnano: General Purpose 3-D Simulations". In: *IEEE Transactions on Electron Devices* 54.9 (Sept. 2007), pp. 2137–2142. DOI: 10.1109/TED.2007.902871. (Visited on 09/17/2023).

[6] Colin D. Bruzewicz et al. "Trapped-ion quantum computing: Progress and challenges". In: *Applied Physics Reviews* 6.2 (June 2019), p. 021314. ISSN: 1931-9401. DOI: 10.1063/1.5088164. (Visited on 04/05/2024).

[7] Guido Burkard et al. "Semiconductor Spin Qubits". In: *Reviews of Modern Physics* 95.2 (June 14, 2023), p. 025003. DOI: 10.1103/RevModPhys.95.025003. arXiv: 2112.08863 [cond-mat, physics:physics, physics:quant-ph]. (Visited on 09/17/2023).

[8] Carlo Caputo et al. "A simulator of optical coherent-state evolution in quantum key distribution systems". In: *Optical and Quantum Electronics* 54.11 (Sept. 2022), p. 689. ISSN: 1572-817X. DOI: 10.1007/s11082-022-04041-8. (Visited on 04/24/2024).

[9] Andrew W. Cross et al. *Open Quantum Assembly Language*. July 13, 2017. arXiv: 1707.03429 [quant-ph]. URL: http://arxiv.org/abs/1707.03429 (visited on 09/17/2023). preprint.

[10] Juan P Dehollain et al. "Optimization of a solid-state electron spin qubit using gate set tomography". In: *New Journal of Physics* 18.10 (Oct. 2016), p. 103018. ISSN: 1367-2630. DOI: 10.1088/1367-2630/18/10/103018. (Visited on 02/21/2024).

[11] A. Gaita-Ariño et al. "Molecular spins for quantum computation". In: *Nature Chemistry* 11.4 (Apr. 2019), pp. 301–309. ISSN: 1755-4330, 1755-4349. DOI: 10.1038/s41557-019-0232-y. (Visited on 04/05/2024).

[12] J Robert Johansson, Paul D Nation, and Franco Nori. "QuTiP: An open-source Python framework for the dynamics of open quantum systems". In: *Computer Physics Communications* 183.8 (2012). https://doi.org/10.1016/j.cpc.2012.02.021, pp. 1760–1772. DOI: 10.1016/j.cpc.2012.02.021.

[13] Pieter Kok and Brendon W. Lovett. *Introduction to Optical Quantum Information Processing*. 1st ed. Cambridge University Press, Apr. 2010. DOI: 10.1017/CBO9781139193658. (Visited on 04/05/2024).

[14] P. Krantz et al. "A quantum engineer's guide to superconducting qubits". In: *Applied Physics Reviews* 6.2 (June 2019), p. 021318. ISSN: 1931-9401. DOI: 10.1063/1.5089550. (Visited on 04/05/2024).

[15] Ville Lahtinen and Jiannis K. Pachos. "A Short Introduction to Topological Quantum Computation". In: *SciPost Physics* 3.3 (Sept. 2017). arXiv:1705.04103 [cond-mat, physics:quant-ph], p. 021. ISSN: 2542-4653. DOI: 10.21468/SciPostPhys.3.3.021. (Visited on 04/05/2024).

[16] Ruoyu Li et al. "A Crossbar Network for Silicon Quantum Dot Qubits". In: *Science Advances* 4.7 (July 6, 2018), eaar3960. DOI: 10.1126/sciadv.aar3960. (Visited on 09/17/2023).

[17] Mateusz T. Madzik et al. "Precision Tomography of a Three-Qubit Donor Quantum Processor in Silicon". In: *Nature* 601.7893 (Jan. 20, 2022), pp. 348–353. DOI: 10.1038/s41586-021-04292-7. (Visited on 09/17/2023).

[18] Marco De Michielis et al. "Silicon spin qubits from laboratory to industry". In: *Journal of Physics D: Applied Physics* 56.36 (June 2023), p. 363001. DOI: 10.1088/1361-6463/acd8c7.

[19] Andrea Morello et al. “Donor Spins in Silicon for Quantum Technologies”. In: *Advanced Quantum Technologies* 3.11 (Nov. 2020), p. 2000005. DOI: 10.1002/qute.202000005. (Visited on 09/17/2023).

[20] Andrea Morello et al. “Single-Shot Readout of an Electron Spin in Silicon”. In: *Nature* 467.7316 (Oct. 2010), pp. 687–691. DOI: 10.1038/nature09392. (Visited on 09/17/2023).

[21] J T Muhonen et al. “Quantifying the quantum gate fidelity of single-atom spin qubits in silicon by randomized benchmarking”. In: *Journal of Physics: Condensed Matter* 27.15 (Apr. 2015), p. 154205. ISSN: 0953-8984, 1361-648X. DOI: 10.1088/0953-8984/27/15/154205. (Visited on 02/21/2024).

[22] Juha T. Muhonen et al. “Storing quantum information for 30 seconds in a nanoelectronic device”. In: *Nature Nanotechnology* 9.12 (Dec. 2014), pp. 986–991. ISSN: 1748-3395. DOI: 10.1038/nnano.2014.211. (Visited on 02/21/2024).

[23] Jarryd J. Pla et al. “High-fidelity readout and control of a nuclear spin qubit in silicon”. In: *Nature* 496.7445 (Apr. 2013), pp. 334–338. ISSN: 1476-4687. DOI: 10.1038/nature12011. (Visited on 02/20/2024).

[24] John Preskill. “Quantum Computing in the NISQ era and beyond”. In: *Quantum* 2 (Aug. 2018), p. 79. DOI: 10.22331/q-2018-08-06-79. (Visited on 04/05/2024).

[25] Andrea Russo et al. “Exploring the Advantages of Layout Procedure with Fully-Connected Quantum Computing Technologies”. In: *Advanced Quantum Technologies* 7.1 (Jan. 2024), p. 2300128. ISSN: 2511-9044, 2511-9044. DOI: 10.1002/qute.202300128. URL: https://onlinelibrary.wiley.com/doi/10.1002/qute.202300128 (visited on 04/09/2024).

[26] Stefanie B. Tenberg et al. “Electron Spin Relaxation of Single Phosphorus Donors in Metal-Oxide-Semiconductor Nanoscale Devices”. In: *Physical Review B* 99.20 (May 14, 2019), p. 205306. DOI: 10.1103/PhysRevB.99.205306. (Visited on 09/17/2023).

[27] L. M. K. Vandersypen and I. L. Chuang. “NMR Techniques for Quantum Control and Computation”. In: *Reviews of Modern Physics* 76.4 (Jan. 12, 2005), pp. 1037–1069. DOI: 10.1103/RevModPhys.76.1037. (Visited on 09/17/2023).

[28] Lieven MK Vandersypen and Mark A Eriksson. “Quantum computing with semiconductor spins”. In: *Physics Today* 72 (2019), pp. 8–38. DOI: 10.1063/PT.3.4270.

[29] LMK Vandersypen et al. “Interfacing spin qubits in quantum dots and donors—hot, dense, and coherent”. In: *npj Quantum Information* 3.1 (2017), p. 34. DOI: 10.1038/s41534-017-0038-y.

[30] M Veldhorst et al. “Silicon CMOS architecture for a spin-based quantum computer”. In: *Nature communications* 8.1 (2017), pp. 1–8. DOI: 10.1038/s41467-017-01905-6.