DI

TN

MP

BI

DESIGNING QUANTUM LOGIC GATES ON SILICON CHIPS WITH LARGE-SCALE MULTIPHYSICS SIMULATIONS

Allocation: Innovation and Exploration/221.4 Knh
PI: Rajib Rahman[1]
Collaborator: Andrew S. Dzurak[2]

[1]Purdue University
[2]University of New South Wales

EXECUTIVE SUMMARY

Quantum computing is a revolutionary method of information processing that takes advantage of the quantum mechanical principles of superposition and entanglement. It is theoretically proven to provide a massive improvement of the complexity of certain algorithms used in cryptography, database search, and modeling correlated quantum systems such as atoms, molecules, and superconductors.

One of the most scalable designs of quantum information processing chips is based on the interactions between a few electrons trapped in silicon chips under metallic electrodes. These trapped electrons can be selectively manipulated in a crystal containing hundreds of millions of other electrons and nuclei, defects, magnetic and electrical noise, and mechanical vibrations [1]. In this project, the research team developed a method for computing the interactions between the trapped electrons in a realistic environment and studied the effect of variations in the environment on the interactions. This study will help in accelerating the experimental and chip design processes of quantum computing systems.

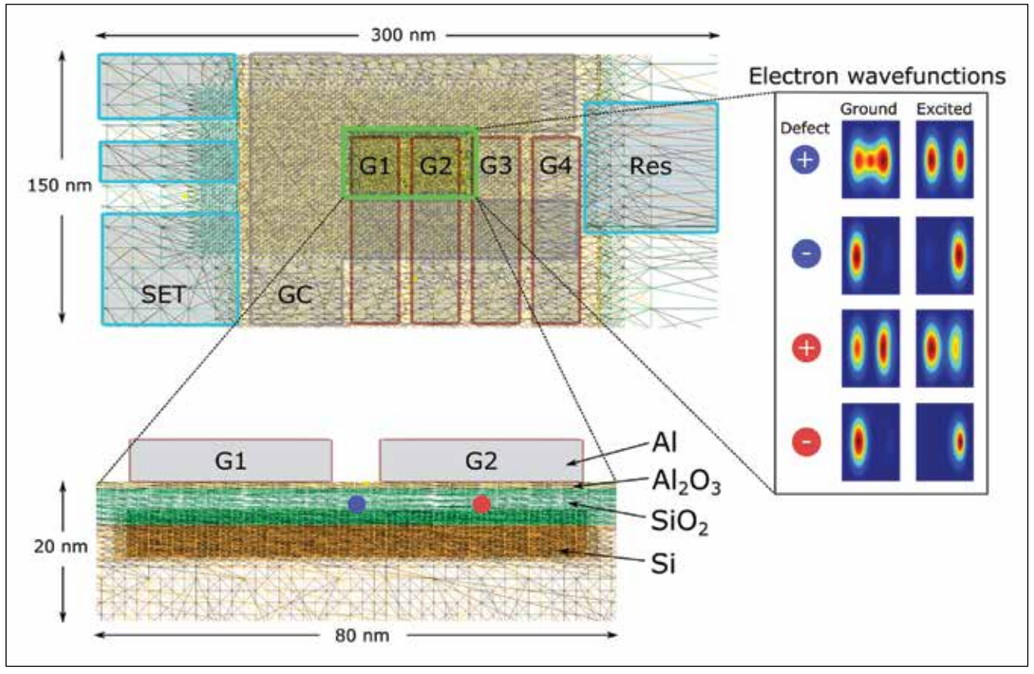

Figure 1: Top and side views of a multiqubit silicon device showing gate electrodes (G), a single-electron transistor (SET), a charge reservoir region, dielectrics (Al_2O_3 and SiO_2), and nonideal charge traps. Mixed inhomogeneous meshing was used to solve for the quantum electronic density of trapped electrons in continuum self-consistently. Atomistic quantum dot wave functions formed under electrodes G1 and G2 are shown for different defect locations and charges.

RESEARCH CHALLENGE

The team computed the interaction between two electrons trapped under positively charged electrodes occupying an area of 25 nanometers (nm) x 25 nm and separated by 10 nm. The efficient working of these chips requires the interaction strength to be designed accurately. The interaction strength depends on multiple factors such as device geometry, electrode voltages, neighboring crystal atoms, proximity to other charged defects, electrical noise, and crystal strain. The biggest challenge is to efficiently address the impact of all these factors to provide insight and guidance into the design of quantum logic gates.

METHODS & CODES

The factors that determine interaction strength can be grouped by the physics that efficiently describe them, *i.e.*, continuum, atomistic, and correlated. The team has developed three different modeling tools to address each of these: (1) finite-element method-based software for continuum physics, (2) large-scale atomistic tight binding software for atomic and solid-state physics, and (3) full configuration interaction method-based software for correlated physics. The tools consecutively process data to arrive at the final results. The methods are embedded in the NEMO package.

RESULTS & IMPACT

The research team has shown the impact of gate lengths, gate spacings, and voltages on the quantum mechanical interaction strength between two qubits (the basic unit of quantum information). This "exchange" interaction has been shown to be sensitive to the design. The researchers have proposed the use of a special "exchange gate" for efficient control of two qubits. They also have shown that nonideal factors such as defects and strain can cause electrical distortions in the device. However, in most cases electrical tuning of gate voltages can be used to overcome nonideal behavior.

WHY BLUE WATERS

All three methods used in this project require large processing power, memory, and storage facilities. Furthermore, the methods are often run sequentially with data being translated from one form to another. Blue Waters provided all the needed resources. Access to a large number of nodes and storage disks was particularly critical. Furthermore, the support staff constantly monitored the system and helped with libraries and compilation, which enabled the research team to focus on the science.

PUBLICATIONS & DATA SETS

H. Sahasrabudhe and R. Rahman, "Computational modeling of exchange splitting in Si/SiO2 based double quantum dots," presented at the Amer. Phys. Soc. March Meeting, Boston, MA, U.S.A., March 4–8, 2019, id.E35.004.