New study uses machine learning to bridge the reality gap in quantum devices

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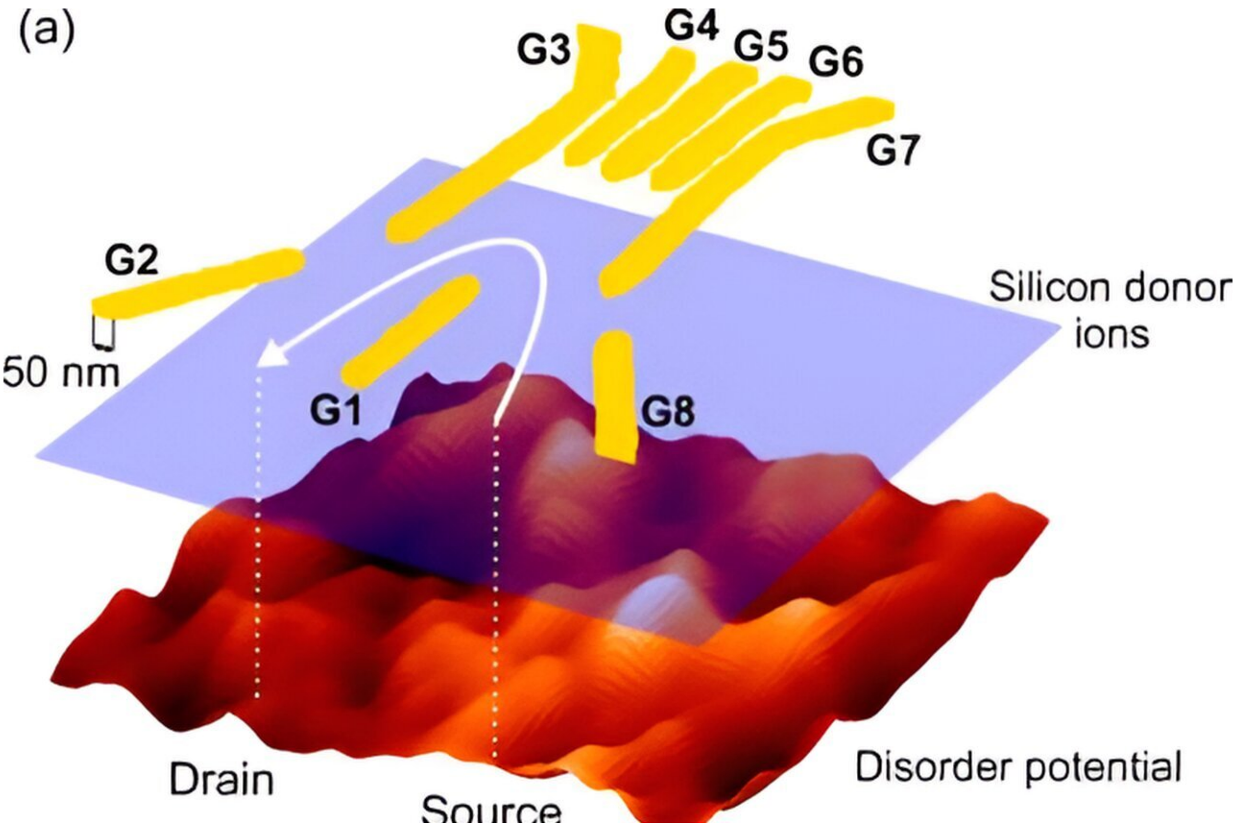

(a) Device geometry including the gate electrodes (labeled G1–G8), donor ion plane, and an example disorder potential experienced by confined electrons. Typical flow of current from source to drain is indicated by the white arrow. (b) Schematic of the disorder inference process. Colors indicate the following: red for experimentally controllable variables, green for quantities relevant to the electrostatic model, blue for experimental device, and yellow for machine learning methods. Dashed arrows represent the process of generating training data for the deep learning approximation and are not part of the disorder inference process. Credit: *Physical Review X* (2024). DOI: 10.1103/PhysRevX.14.011001

A study led by the University of Oxford has used the power of machine learning to overcome a key challenge affecting quantum devices. For the first time, the findings reveal a way to close the "reality gap": the difference between predicted and observed behavior from quantum devices. The results have been published in *Physical Review X*.

Quantum computing could supercharge a wealth of applications, from climate modeling and financial forecasting to drug discovery and artificial intelligence. But this will require effective ways to scale and combine individual quantum devices (also called qubits). A major barrier against this is inherent variability, where even apparently identical units exhibit different behaviors.

Functional variability is presumed to be caused by nanoscale imperfections in the materials from which quantum devices are made. Since there is no way to measure these directly, this internal disorder cannot be captured in simulations, leading to the gap in predicted and observed outcomes.

To address this, the research group used a "physics-informed" machine learning approach to infer these disorder characteristics indirectly. This was based on how the internal disorder affected the flow of electrons through the device.

Lead researcher Associate Professor Natalia Ares (Department of Engineering Science, University of Oxford) said, "As an analogy when we play 'crazy golf,' the ball may enter a tunnel and exit with a speed or direction that doesn't match our predictions. But with a few more shots, a crazy golf simulator, and some machine learning, we might get better at predicting the ball's movements and narrow the reality gap."

The researchers measured the output current across an individual quantum dot device for different voltage settings. The data was input into a simulation, which calculated the difference between the measured current and the theoretical current if no internal disorder was present.

By measuring the current at many different voltage settings, the simulation was constrained to find an arrangement of internal disorder that could explain the measurements at all voltage settings. This approach combined mathematical and statistical approaches coupled with deep learning.

Associate Professor Ares added, "In the crazy golf analogy, it would be equivalent to placing a series of sensors along the tunnel, so that we could take measurements of the ball's speed at different points. Although we still can't see inside the tunnel, we can use the data to inform better predictions of how the ball will behave when we take the shot."

Not only did the new model find suitable internal disorder profiles to describe the measured current values, but it could also accurately predict voltage settings required for specific device operating regimes.

The model provides a new method to quantify the variability between quantum devices. This could enable more accurate predictions of how devices will perform and help engineer optimum materials for quantum devices. It could inform compensation approaches to mitigate the unwanted effects of material imperfections in quantum devices.

Co-author David Craig, a Ph.D. student at the Department of Materials, University of Oxford, added, "Similar to how we cannot observe black holes directly but we infer their presence from their effect on surrounding matter, we have used simple measurements as a proxy for the internal variability of nanoscale quantum devices."

"Although the real device still has greater complexity than the model can capture, our study has demonstrated the utility of using physics-aware machine learning to narrow the reality gap."

More information: D. L. Craig et al, Bridging the Reality Gap in Quantum Devices with Physics-Aware Machine Learning, *Physical Review X* (2024). DOI: 10.1103/PhysRevX.14.011001

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