



Engineering high-fidelity gates in silicon quantum processors

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Therapeutic drug design for COVID-19



J. Phys. Chem. B 2020, 124, 8201-8208

npj Quantum Information 7.1 (2021): 1-5.

Increase computational space with different encodingsBits = deterministicQubits = probabilistic $\hat{z} = |0\rangle$





Increase computational space combining multiple qubits



4 computational states from 2 qubit **→** 4 states for each qubit pair

Encoding information in correlations



'spooky action at a distance' → *entanglement*

$$\psi_1 \otimes |\psi_2 = (c_1^1 |0\rangle_1 + c_2^1 |1\rangle_1) \otimes (c_1^2 |0\rangle_2 + c_2^1 |1\rangle_2)$$

Information is stored in the correlation between states \rightarrow exponentially increased computational space

- N = 30 (IonQ machine) $\rightarrow \sim 1$ GB classical transistors

- N = 50 (Google machine) $\rightarrow \sim 8,000$ TB classical transistors

- $N=800 \rightarrow$ > number of atoms in the universe to encode information !!

 $|\psi\rangle = (|0\rangle + |1\rangle)^{\otimes N}$

 $N \rightarrow$ number of physical qubits

Entanglement encoding for drug design and other applications



Protein folding *Quantum simulation*

Classical algorithm (HF): $\mathcal{O}(2^N)$

Quantum algorithm (VQE): $\mathcal{O}(N^3)$

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Optimization Search algorithms

Classical algorithm (MTZ): $\mathcal{O}(2^N)$

Quantum algorithm (Grover): $\mathcal{O}(\sqrt{N})$



FactoringQuantum Fourier transformClassical algorithm (NFS): $\mathcal{O}(2^N)$

Quantum algorithm (Shor's):

 $\mathcal{O}(\log N)$ or $\mathcal{O}(N^3)$

https://quantum-computing.ibm.com/composer/docs/iqx/guide/shorsalgorithm

Encoding quantum information in a physical system: small magnets



Trapping single spins in semiconductors



Trapping single spins in semiconductors



Voltage gates modify 2DEG potential \rightarrow trap electrons with high precision

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A zoo of quantum computing architectures

Qubit	Superconducting	Silicon Spin Qubits	Ions/Atoms	Photons
Number Qubits Demonstrated	72 (Bristlecone) 53 (Sycamore) 50 IBM	4	32	~70
Gate Fidelities (2 QB)	99.9%	>99.5%	>99.9%	>99.5
One qubit gate fidelity	99.95%	>99.95%	>99.99%	>99.5
Challenges in qubit scalability	Qubit crosstalk dominates, decoherence, too big	Low 2-qubit fidelities, too many wires , too cold	Bulky vacuum systems, soft potential (weak interaction)	Cannot reliably produce photons, difficult to mediate interaction

Images from: Martinis Group/Google, IonQ, PsiQuantum

Towards an intermediate scale silicon quantum computer

Challenges	Proposed solution		
 Low-connectivity Spins limited to nearest-neighbor interactions Difficult to form large cluster states 	Quantum random accesss memory		
 Complexity Each qubit requires multiple wires connected to bond pads Simultaneous voltage + MW control 	Overlapping gate architecture → all qubits share same barrier voltage		
Qubit infidelity -Decoherence induced → spin-spin interactions lead to information loss - Noise induced → charge noise leading to fluctuations in exchange interactions	Pulse engineering for noise induced infidelity. Res-Sqrt(SWAP) gates for decoherence induced.		

Infidelity in silicon spin-qubit systems: decoherence + noise



Nakajima, Takashi, et al. Physical Review X 10.1 (2020): 011060.

Charge noise induced infidelity



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Charge noise induced infidelity (cont'd))



Controlling spins with microwaves

- Apply magnetic field orthogonal to *B*
- Needs to be resonant with spins rotating frame
- Microwave frequencies
- Axis of rotation = phase



Shaping pulses for noise robustness

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http://mriphysics.github.io/teaching-rf-pulses.html

Systematic pulse engineering for single qubit gates



Yang, C. H., et al. (2019): 151-158.

Pulse time (µs)

 Ω_{v}

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Pulse engineering protocol: gradient based optimization

$$\mathcal{H} = \Omega_{drift} \Omega_{ESR} (\Omega_x \sigma_x + \Omega_y \sigma_y) + (f_{ESR} + \epsilon_z) \sigma_z$$

noise from phase flips

Randomize e_ (1)

 ϵ_z

- Calculate $\frac{\delta\Psi}{\delta\Omega}$ for all Ω pointwise, with the current Hamiltonian H Update $\Omega \xrightarrow{\delta\Omega} \Omega + \eta \frac{\delta\Psi}{\delta\Omega}$ (2)
- (3)
- Filter Ω for smoothness and bound condition $\Omega_{max}^2 \ge \Omega_x^2 + \Omega_y^2$ (4)





Extension to 2-qubit gates: CNOT gate

Operator	Gate(s)		Matrix
Pauli-X (X)	- x -		$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	- Y -		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	- Z -		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	$-\mathbf{H}$	$rac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$	
Phase (S, P)	- S -		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8~(\mathrm{T})$	- T -		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP	\supset	_*_ _*_	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}$



If control = 1, flip target!

Pulse shaping for CNOT gate





Pulse shaping for CNOT gate (cont'd)



Outlook: towards therapeutic drug design using quantum



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Will need hundreds of qubits!

Acknowledgments







ESE PhD Association!

Prof. Anthony Sigillito

Dr. Seong Oh