Method for efficient simulation of driven quantum information systems

Spenser Talkington, University of California, Los Angeles (UCLA)

The advent of computers has revolutionized the way we conduct our lives. Computers help us to solve problems and perform tasks quickly and efficiently. They do this by translating commands into binary logic. Whether we need to save a document, download an image, or crunch numbers, all these tasks are transformed through software into an equivalent series of binary arithmetical and logical operations.

This binary logic is particularly efficient for tasks like multiplying integers, but is very inefficient for other tasks like factoring integers. Because of this inefficiency, information, such as online credit card transactions, can be protected with encryption. In encryption, data is scrambled in accordance with a large integer, and unscrambling requires factoring that integer.

While this method of encryption protects scrambled information from binary computers, it does not protect it from large quantum computers. This is because quantum computers are based on a different logical system where factoring integers is easy [1]. Quantum computers also provide a method to realize a new, unbreakable encryption.

In quantum computing, information is stored in qubits, where information is the superposition of two obervable states which collapses into one state when measured:

$$|\psi\rangle = c_0|0\rangle + c_1|1\rangle \;\Rightarrow\; \begin{cases} |0\rangle \text{ with } |c_0|^2 \text{ chance} \\ |1\rangle \text{ with } |c_1|^2 \text{ chance} \end{cases}$$

No one has yet created a quantum computer that is large enough to threaten classical encryption. One key to building such a large quantum computer is understanding how information that is stored in real qubits evolves with time. In general this is computationally expensive, and requires solving the Schrödinger Equation numerically:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

Solid state quantum dot qubits are particularly appealing to use in a quantum computer because they leverage existing materials science technologies, and should be more easily scalable to create large quantum computers than other types of qubits [2].

Yet, the parameter spaces of solid state qubits are usually very large and this makes their simulation challenging. For example, in a charge-based quantum dot qubit in silicon, even after discarding the spin and lattice degrees of freedom, there are six valley states for each quantum dot [2]. Considering the lowest two of these states turns simulation of a qubit into that of a four-state system with ten degrees of freedom.

In the field of quantum information, these simulations have traditionally been completed by numerically solving the von Neumann Equation for density matrices (equivalent to the Schrödinger Equation). While density matrix methods are extensible to systems with relaxation and coupling to environment, they are so slow that:

$$t_{\text{simulation}} \sim t_{\text{experiment}}$$

This is acceptable if one wants to explain the results of an experiment where the relevant parameters are known and have been measured. On the contrary, density matrix evolution is not very useful if we want to:

- Predict the results of an experiment
- Explain unexpected experimental results where the relevant physical parameters are unknown
- Identify the structures and parameters best-suited to realizing robust qubits

To address the problem of quickly simulating real qubit systems, I considered simulating qubits in the limit of short times, following discussions with graduate students Nicholas Penthorn, John Rooney, and Tim Wilson, and with the guidance of Professor HongWen Jiang.

For short times, energy is conserved in the system (approximating the system as isolated) and particle number is conserved (approximating state relaxation as negligible). If in addition, one assumes that Hamiltonians at different times commute[1], then one can evolve $|\psi\rangle$ with a unitary time-evolution operator $\mathscr{U}$, where $\mathscr{U}^\dagger\mathscr{U} = \mathbf{1}$:

$$|\psi(t)\rangle = \mathscr{U}(t)|\psi(0)\rangle$$

For a Hamiltonian $H(t)$, the energy basis is the set of eigenvectors $\{|a_j\rangle\}$ corresponding to eigenvalues $\{E_j\}$, as determined by diagonalizing H. Using this basis, the time evolution of state $|\psi\rangle$ for small times Δt is:

$$|\psi(t+\Delta t)\rangle = \sum\nolimits_j e^{-iE_j\Delta t/\hbar}|a_j\rangle\langle a_j|\psi(t)\rangle$$

This generalizes to finite times by letting:

$$\mathscr{U}(t) \approx \prod_{n=1}^{N}\sum_{j=1}^{\dim} e^{-iE_j^{(n)}(t_n-t_{n-1})/\hbar}|a_j^{(n)}\rangle\langle a_j^{(n)}|$$

Where the product is matrix multiplication, and $\{E_j^{(n)}\}$/$\{|a_j^{(n)}\rangle\}$ are the corresponding eigenvalues/vectors of $H(t_n)$ for some well-chosen list of times $\{t_n\}$.[2]

Simulation Method for Trapezoidal Driving

(1) Declare initial state and driving

(2) Compute rise and fall unitaries

(3) For each specified readout time

- (a) Compute plateau unitary
- (b) Evolve state
- (c) Readout state

I identified three methods for choosing lists of times $\{t_n\}$ for experimental time-dependent drivings of $H(t)$ that ensure fast and accurate computations:

1. Evaluate constant driving in one step
2. Extend previous computations
3. Store unitaries for repeated drivings

For example, one common manipulation of a qubit is with “trapezoidal driving”, where one state starts with an energy much lower than the other state for encoding, rises linearly, plateaus at a new energy splitting for interference, and then falls linearly to return to the initial splitting for readout. This evolution can be simulated efficiently using the methods I have developed by following the schematic above.

I then computationally implemented this “optimized unitary” evolution method, and compared the accuracy of its results against the corresponding density matrix method implemented in the popular quantum simulation software QuTiP [4], for three realistic qubit systems with time-dependent driving [5,6,7]. I found that the optimized unitary method found the same results as the QuTiP method to within 2%, see Fig. 1.

[1] Which is experimentally justified as on-site potentials vary but tunnelings remain constant, see [8].

[2] The times $\{t_n\}$ are ‘well-chosen’ if the approximation of $\mathscr{U}$ is ‘close,’ and the computation is ‘fast.’

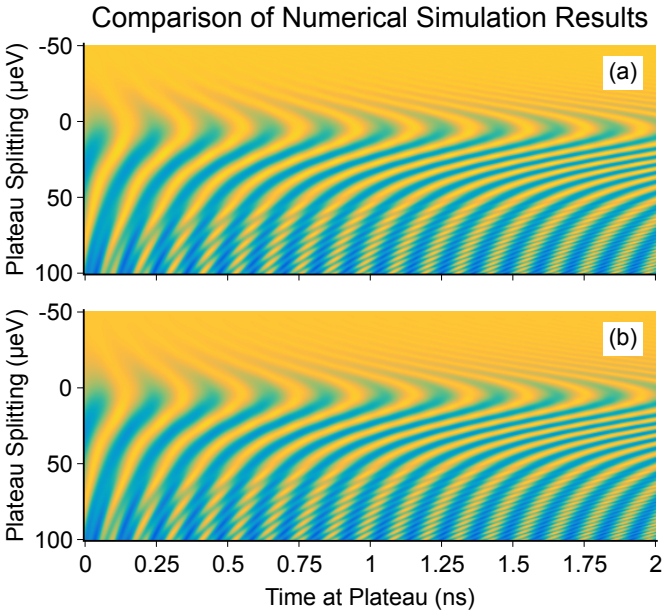

FIG. 1. Images of the time evolution of a quantum dot qubit driven by a trapezoidal pulse using the Hamiltonian from Shi, *et al*. [5]. The optimized unitary method is 395 times faster than the QuTiP method. (a) Density matrix methods using QuTiP took 5.92 hr to determine this image. (b) The optimized unitary method took 54 sec to determine this image.

In addition, I compared the duration of the simulation in the optimized unitary method with the QuTiP method and found that the new method was over two order of magnitude faster for all images, see Fig. 2.

These results indicate that for short times, unitary evolution with optimization for experimental driving is a way to quickly simulate real qubit systems:

$$t_{\text{simulation}} \ll t_{\text{experiment}}$$

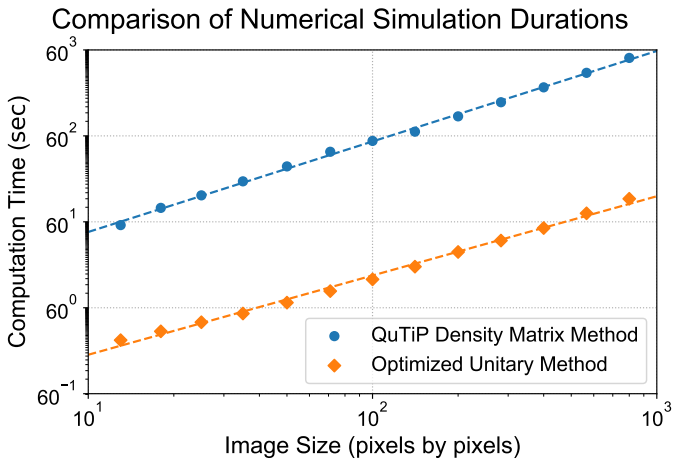

FIG. 2. Computational times for determining images of the time evolution of a quantum dot qubit driven by a trapezoidal pulse using the Hamiltonian from Schoenfield, *et al.* [6]. For 100 by 100 images, the optimized unitary methods for a trapezoidal driving pulse is 732 times faster than the QuTiP method.

With these new simulation techniques, it is now possible to explore the parameter spaces of real qubits to explain experimental results more quickly and to predict the structures and parameters most favorable to realizing robust qubits.

This in turn makes developing the large quantum computers capable of factoring large numbers and breaking classical encryption a step closer to realization.

I have submitted a paper describing these methods to Physical Review B, posted it on arXiv [8], and have presented the results at the APS Far West Conference.

References:

[1] P.W. Shor. Proc. IEEE FOCS **35**, 124 (1994).
[2] F.A. Zwanenburg, *et al.*, Rev. Mod. Phys **85**, 961 (2013).
[3] J.J. Sakurai, *et al.*, *Modern Quantum Mechanics* (Cambridge University Press, 2017).
[4] J.R. Johansson, *et al.*, Comput. Phys. Commun. **183**, 1760 (2012).
[5] Z. Shi, *et al.*, Nat. Commun. **5**, 3020 (2014).
[6] J.S. Schoenfield, *et al.*, Nat. Commun. **8**, 64 (2017).
[7] N.E. Penthorn, *et al.*, npj Quantum Inf. **5**, 1 (2019).
[8] S.M. Talkington and H.W. Jiang, Under review at Phys. Rev. B. arXiv:1909.02532.