Scaling Issues in Ensemble Quantum Algorithms

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Abstract

Ensembles of quantum systems, such as liquid state NMR, have been proposed as possibilities for implementing quantum algorithms. For such implementations, projective measurement outcomes are replaced by expectation values. Although these are apparently deterministic, we point out that real implementations involve ensembles of finite size, giving probabilistic approximations to expectation values. The performance of such algorithms must be compared to their classical probabilistic counterparts. We discuss proposed scalable ensemble versions of the Deutsch-Jozsa algorithm in this context and show that their performance is worse than the classical probabilistic algorithm.

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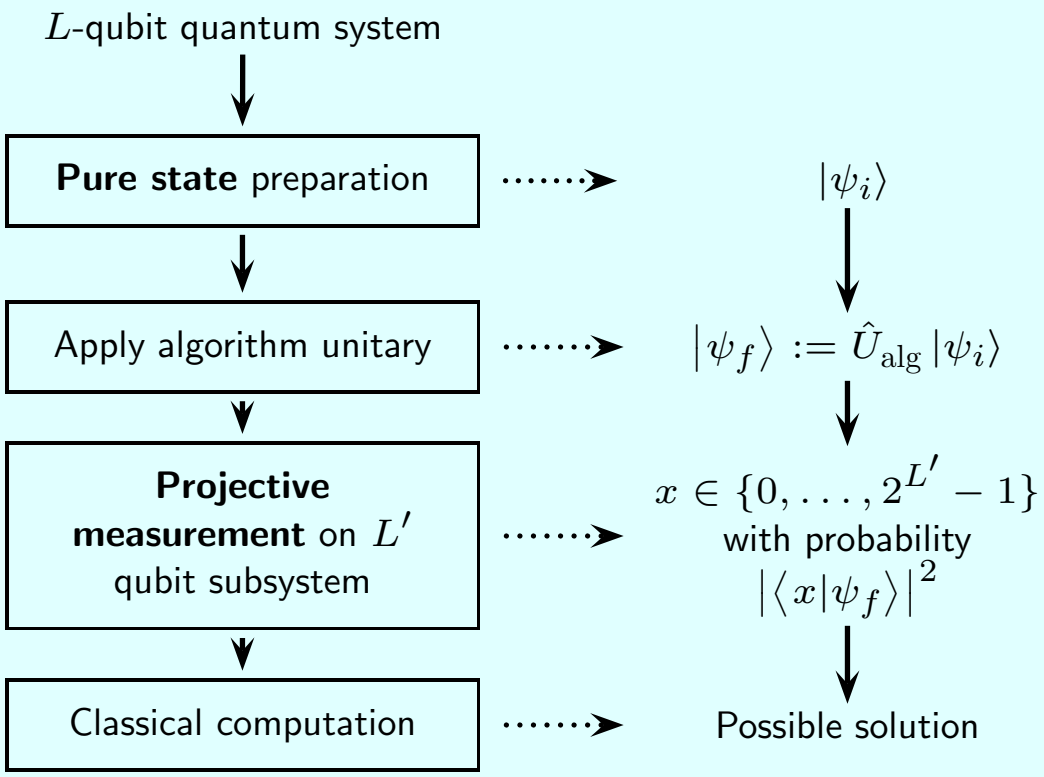
"Standard" Quantum Computing

Implementations on a **single quantum system amenable to projective measurements.**



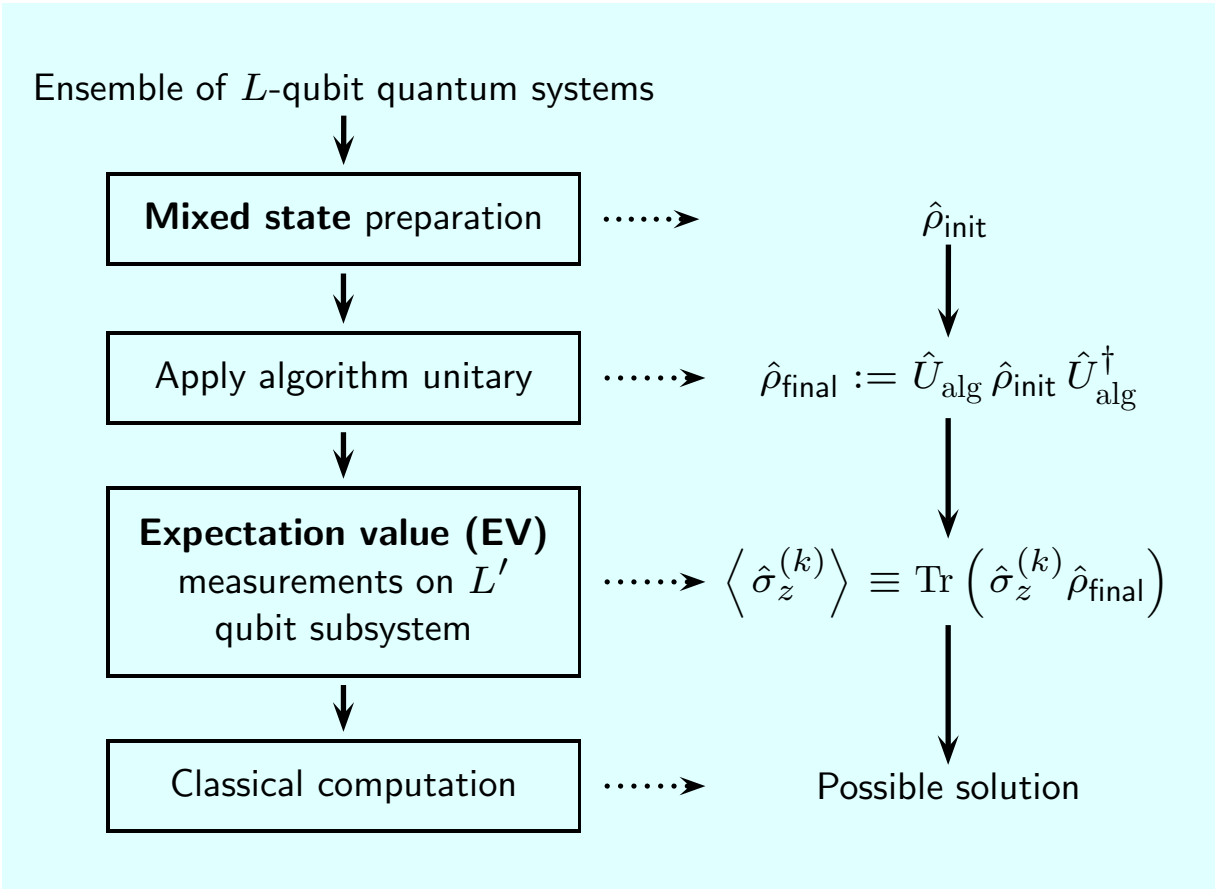
- For useful algorithms the probability of returning x corresponding to trivial or incorrect solutions is small.
- Typically a decomposition

$$\hat{U}_{\rm alg} = \hat{U}_m \ldots \hat{U}_1$$

into simple unitary operations facilitates algorithm implementation.

Expectation Value Quantum Computing

Implementations using an **ensemble of identical, non-interacting quantum systems.**

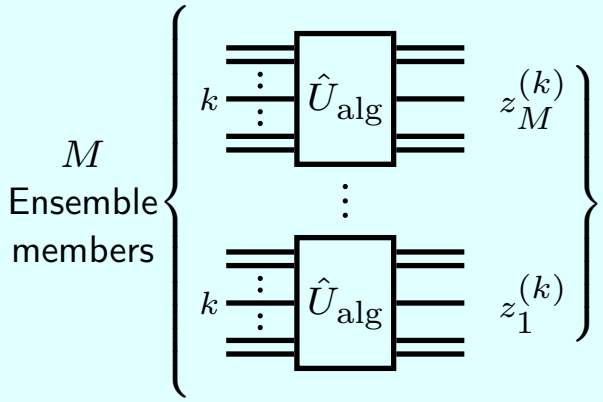


- The ensemble is in a mixed state and it is impossible to extract projective measurement outcomes from any single ensemble member. The "standard" versions of quantum algorithms must be modified accordingly.
- **Idealized NMR implementations** of quantum algorithms follow this scheme.

Idealized EV implementations extract the problem solution from the **expectation values (EVs)**, $\left\langle \hat{\sigma}_z^{(k)} \right\rangle$, for qubits $k = 1, \ldots, L$. These implementations are **deterministic.**

Expectation-Value Quantum Computing: Real vs. Idealized Implementations.

Real EV implementations use ensembles with a **finite number of members**. The ensemble **approximates expectation values via sample averages** of projective measurement outcomes on individual ensemble members. Fluctuations in the sample averages imply **probabilistic outcomes.** **Real NMR implementations** follow this with $M \approx 10^{20}$ ensemble members (sample molecules).



Projective measurement outcomes on ensemble members give sample averages:

$$\overline{z^{(k)}} := \frac{1}{M}\sum_{j=1}^{M} z_j^{(k)}$$

Projective measurement outcomes on qubit k of ensemble member j:

Projector $|0\rangle\langle 0|$ $\leftrightarrow$ $z_j^{(k)} = +1$ with prob $\mathrm{Tr}\left(\hat{\rho}_{\rm final}|0\rangle\langle 0|\right)$

Projector $|1\rangle\langle 1|$ $\leftrightarrow$ $z_j^{(k)} = -1$ with prob $\mathrm{Tr}\left(\hat{\rho}_{\rm final}|1\rangle\langle 1|\right)$

approximate EVs via $\left\langle \hat{\sigma}_z^{(k)} \right\rangle \approx \overline{z^{(k)}}$.

Success rates for real EV implementations must be **compared to those for classical probabilistic algorithms.** The multiplicity of algorithm unitary applications across all ensemble members must be included for a fair comparison.

Mixed State Preparation

Pseudo-pure state preparation schemes allow thermal equilibrium inputs to mimic pure states at the cost of signal strength. Scalable proposals avoid catastrophic signal losses at the cost of algorithm modifications.

- For L spin $1/2$ nuclei the Hamiltonian

$$\hat{H} = \frac{\hbar}{2}\sum_{j=1}^{L}\omega_j\hat{\sigma}_z^{(j)} + \frac{\pi\hbar}{2}\sum_{j\neq k}J_{jk}\hat{\sigma}_z^{(j)}\otimes\hat{\sigma}_z^{(k)}$$

with weak coupling gives the thermal equilibrium density operator

$$\hat{\rho_{\text{th}}} \approx \frac{1}{2^L}\left(\hat{I} - \frac{\hbar}{2}\sum_{j=1}^{L}\omega_j\hat{\sigma}_z^{(j)}\right) \qquad \text{when} \quad \omega_j \gg J_{jk}.$$

- **Pseudo-pure state preparation** schemes accomplish

$$\hat{\rho}_{\text{th}} \rightarrow \hat{\rho}_{\text{init}} = \frac{1-\varepsilon}{2^L}\hat{I} + \varepsilon\left|\psi_i\right\rangle\left\langle\psi_i\right| \qquad \text{with } \varepsilon = \frac{\alpha L}{2^L}$$

where α is independent of L. **Standard algorithm unitaries** can be used but the **signal strength decreases exponentially with the problem size:**

$$\left|\left\langle\hat{\sigma}_z^{(k)}\right\rangle\right| \leq \frac{\alpha L}{2^L}.$$

- **Scalable implementations** use initial states with a fixed number of qubits, k, in a pure state and the remainder in states for which signal strength scales well. Examples are $\hat{\rho}_{\text{th}}$ or

$$\hat{\rho}_{\text{init}} = \frac{1}{2^{L-k}}\hat{I}\otimes\left|\psi_i\right\rangle\left\langle\psi_i\right|$$

Modified algorithm unitaries are required but the **signals scale well** with problem size.

Deutsch-Jozsa Problem

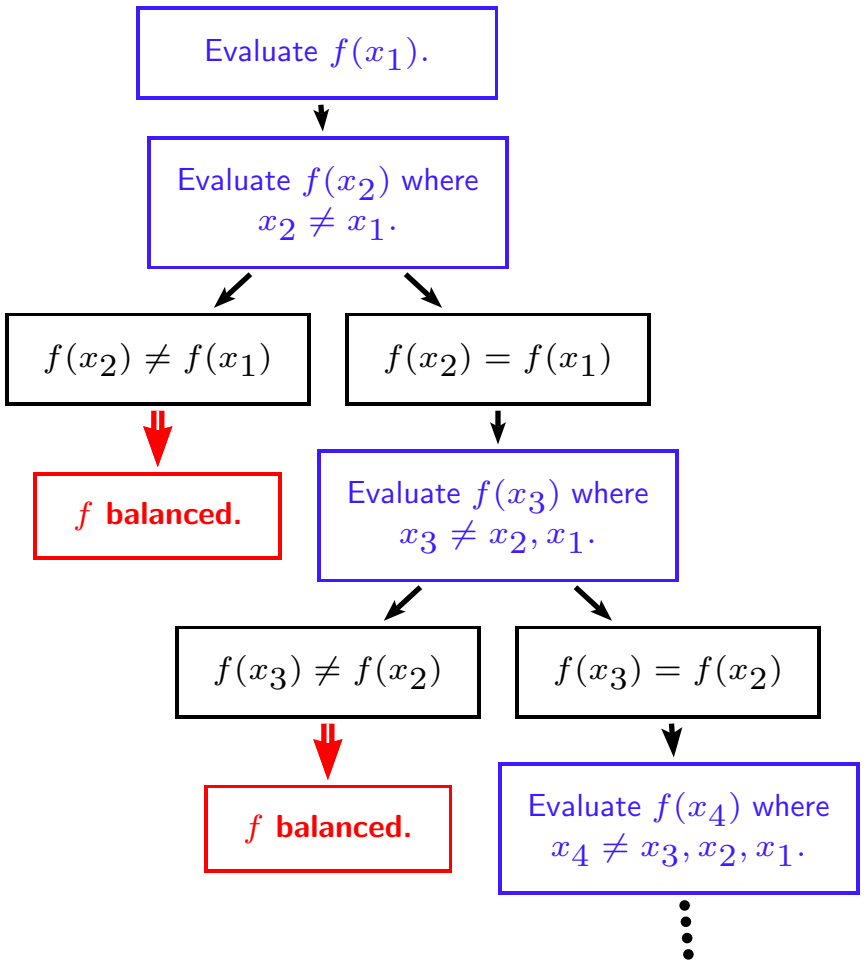
The Deutsch-Jozsa algorithm is a testbed for quantum computing. Do scalable EV versions exist?

- Deutsch-Jozsa problem considers $f : \{0,1\}^N \to \{0,1\}$ satisfying

f is constant	$\Rightarrow$	$f \equiv 0$ or $f \equiv 1$
f is balanced	$\Rightarrow$	$f(x) = 0$ for exactly half the arguments, $f(x) = 1$ for the other half.

  and asks to determine the type given that f is either balanced or constant.

- **Classical algorithm** applies "oracle" f at distinct randomly chosen $x_1, x_2, x_3, \ldots$.



DJ Problem: Classical Solutions

- **Deterministic classical algorithm** solves the problem with certainty by terminating when $f(x_{k+1}) \neq f(x_k)$ (balanced) or $2^N/2 + 1$ oracle invocations which return the same result (constant).

- **Probabilistic classical algorithm** terminates after $M \leq 2^N/2$ oracle invocations on distinct randomly chosen inputs and concludes:

$$\begin{aligned} f(x_1) = f(x_2) = \ldots = f(x_M) \quad &\Rightarrow \quad f \text{ constant.} \\ f(x_k) \neq f(x_j) \text{ for some } j,k = 1,\ldots,M \quad &\Rightarrow \quad f \text{ balanced.} \end{aligned}$$

This never misidentifies a constant function. A balanced function is erroneously identified as constant whenever the first M oracle invocations return the same result. The probability of misidentification is

$$p_{\text{fail}}^{\text{classical}} = 2 \underbrace{\frac{N/2}{N} \frac{N/2-1}{N-1} \cdots \frac{N/2-M+1}{N-M+1}}_{\substack{\text{Probability that oracle always returns } 0 \\ \text{(or always } 1\text{) on } M \text{ distinct inputs.}}}$$

$$\Rightarrow \quad p_{\text{fail}}^{\text{classical}} < 2\frac{1}{2^M}.$$

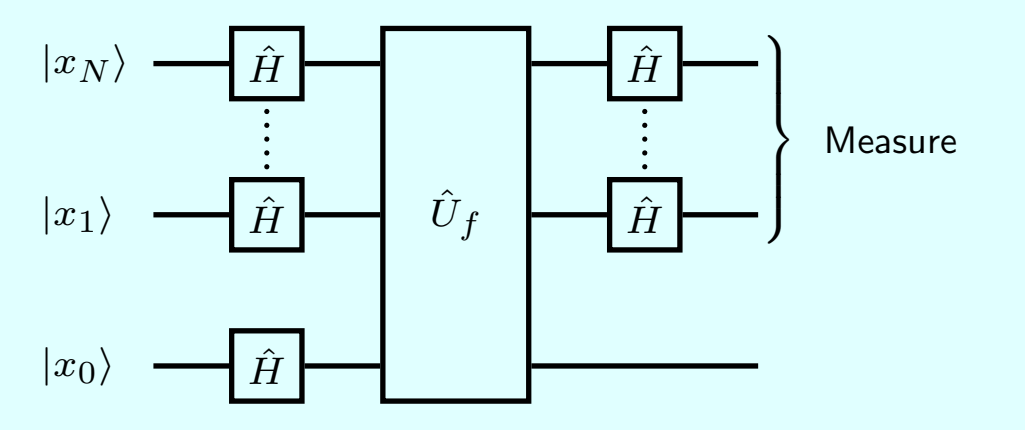
DJ Problem: "Standard" Quantum Solutions

- **"Standard" quantum algorithm** uses a single quantum system having an N qubit argument register, a one qubit function register and the oracle defined on computational basis states via:

$$\hat{U}_f \left|x\right\rangle \left|x_0\right\rangle := \left|x\right\rangle \left|x_0 \oplus f(x)\right\rangle$$

  where $\left|x\right\rangle = \left|x_N\right\rangle \ldots \left|x_1\right\rangle$ and $\left|x_0\right\rangle$ represent function and argument register basis states respectively.

- Applying the following circuit, terminating with a **projective measurement.**



- With initial states $\left|x_N\right\rangle = \ldots = \left|x_1\right\rangle = \left|0\right\rangle$ and $\left|x_0\right\rangle = \left|0\right\rangle$, measurement in the computational basis yields z where

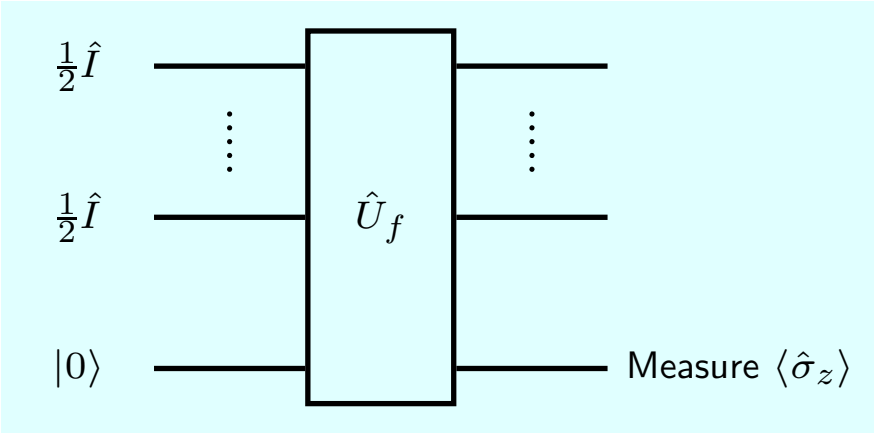
$$\begin{array}{lll} x = 0 & \Rightarrow & f \text{ constant.} \\ x \neq 0 & \Rightarrow & f \text{ balanced.} \end{array}$$

"Standard" quantum algorithm solves DJ problem **with certainty with one oracle invocation.**

DJ Problem: Proposed EV Quantum Solutions

Modified versions of the DJ algorithm for expectation value quantum computers apparently avoid the pseudo-pure state scaling problem [1, 2].

- Maximally mixed states for the argument register, pure state for the function register only!



- Oracle apparently evaluates f at all possible arguments:

$$\hat{\rho}_{\text{init}} = \frac{1}{2^N}\sum_{x=0}^{2^N-1}|x\rangle\langle x|\otimes|0\rangle\langle 0| \xrightarrow{\hat{U}_f} \frac{1}{2^N}\sum_{x=0}^{2^N-1}|x\rangle\langle x|\otimes|f(x)\rangle\langle f(x)|$$

- The expectation values for the function register

$$\langle\hat{\sigma}_z\rangle = \begin{cases} \pm 1 & f \text{ constant} \\ 0 & f \text{ balanced} \end{cases}$$

The idealized EV algorithm solves the problem with one function evaluation with certainty.

DJ Problem: Statistics of EV Quantum Solutions

In a real EV implementation of the proposed ensemble DJ algorithm, fluctuations in the sample averages imply some possibility for misidentifying a balanced function as constant.

- **Constant** f identification

$$\begin{aligned} f \equiv 1 \quad &\Rightarrow \quad z_j^{(0)} = 1 \quad \text{for } j = 1 \ldots M \quad \Rightarrow \quad \overline{z^{(0)}} = 1 \\ f \equiv -1 \quad &\Rightarrow \quad z_1^{(0)} = -1 \quad \text{for } j = 1 \ldots M \quad \Rightarrow \quad \overline{z^{(0)}} = -1 \end{aligned}$$

  leads to the decision criterion

$$\overline{z^{(0)}} = \pm 1 \quad \Rightarrow f \quad \text{constant}$$

- **Balanced** f distinguished from constant f, in the best resolution case, if at least two projective measurement outcomes on individual ensemble members differ, giving

$$-1 + \tfrac{2}{M} \leq \overline{z^{(0)}} \leq 1 - \tfrac{2}{M} \quad \Rightarrow f \quad \text{balanced}$$

- **Balanced** f **misidentified** if all ensemble members give the same projective measurement outcome. The probability that this occurs is the probability of failure for the real EV quantum solution,

$$p_{\text{fail}}^{\text{quantum}} = 2\tfrac{1}{2^M} > p_{\text{fail}}^{\text{classical}}$$

  where the classical failure rate is for the random classical algorithm after M oracle calls (equivalent to 1 oracle call on each of M ensemble members in the EV quantum solution).

The **proposed EV quantum algorithm performs more poorly than it classical counterpart.** In the classical random algorithm f is evaluated on M different inputs; this cannot be guaranteed in the proposed EV quantum versions.

Conclusions

- There is an important distinction between idealized and real expectation value implementations of quantum algorithms. Idealized implementations are deterministic whereas real implementations are probabilistic.
- The success probability for a real expectation value implementation must be compared to classical probabilistic solutions using equivalent resources. The multiplicity of ensemble members must be included in this accounting.
- Certain existing scalable proposals for solving the Deutsch-Jozsa problem have a greater failure probability than the classical probabilistic algorithm using equivalent resources.

References

[1] J. M. Myers, A. F. Fahmy, S. J. Glaser, and R. Marx. Rapid solution of problems by nuclear-magnetic-resonance quantum computation. *Phys. Rev. A*, 63:032302, 2002.

[2] F. M. Woodward and R. Brüschweiler. Solution of the Deutsch-Josza problem by NMR ensemble computing without sensitivity scaling. *arXiv: quant-ph/0006024*, 2000.