Quantum Linear Systems Problem

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U.S. DEPARTMENT OF ENERGY
Office of Science

Quantum Numerical Linear Algebra
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LDRD
innovation for our nation

Main references

In this talk, I will follow these papers:

- “Quantum algorithms for solving linear systems of equations”, AW Harrow, A Hassidim, and S. Lloyd, Phys. Rev. Lett. 15, 150502 (2009).

- “Quantum linear systems algorithm with exponentially improved dependence on precision”, A.M. Childs, R. Kothari, and **R.D. Somma**, SIAM J. Comp. **46**, 1920 (2017).

- “Quantum algorithms for systems of linear equations inspired by adiabatic quantum computing”, Y. Subasi, **R.D. Somma**, and D. Orsucci, Phys. Rev. Lett. 122, 060504 (2019).

- “Quantum state verification in the quantum linear systems problem”, **R.D. Somma** and Y. Subasi, PRX Quantum 2, 010315 (2021)

Linear systems problem (LSP)

Given an $N \times N$ matrix A, an N–dimensional vector $\vec{b}$, and the equation

$$\begin{bmatrix} A_{11} & A_{12} & \dots \\ \vdots & \ddots & \\ A_{N1} & & A_{NN} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_N \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_N \end{bmatrix}$$

equivalently $A\vec{x} = \vec{b}$, solve for $\vec{x} = (x_1, x_2, \dots, x_N)^T$.

- The best general purpose classical algorithm (conjugate gradient) has asymptotic complexity $O(N\sqrt{\kappa})$.
- This is a polynomial dependence in the dimension

Quantum linear systems problem (QLSP)

Given the previous system of linear equations, prepare a quantum state that approximates:

Harrow, Hassidim, Lloyd
PRL 103, 150502 (2009)

$$|x\rangle = \frac{\sum_{i=1}^{N} x_i |i\rangle}{\left(\sum_{i=1}^{N} |x_i|^2\right)^{1/2}}$$

where $A\vec{x} = \vec{b}$, and $\vec{x} = (x_1, x_2, \ldots, x_N)^T$.

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where $A\vec{x} = \vec{b}$, and $\vec{x} = (x_1, x_2, \ldots, x_N)^T$.

Specifically, for a given precision $\epsilon > 0$, the approximate (mixed or pure) quantum state ρ_x satisfies

$$\frac{1}{2}\mathrm{Tr}\,|\rho_x - |x\rangle\langle x|| \leq \epsilon$$

- All known formulations and results for this problem can be described in this form

Why is this problem interesting?

- Linear systems are ubiquitous in science, engineering, and more.
- Quantum computers are known to provide exponential quantum speedups for some problems, so it is natural to understand what they can do in linear algebra problems.
- Beyond linear systems, studying new problems and how to solve them with quantum computers sometimes result in new algorithmic primitives that are used in other quantum algorithms.

Why is this problem interesting?

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- Beyond linear systems, studying new problems and how to solve them with quantum computers sometimes result in new algorithmic primitives that are used in other quantum algorithms.
- This "quantum" version of the problem is, however, only useful for computing expectation values in the solution of the system, but not for obtaining the actual vector. That would take time that is, at least, linear in *N*.
- Are there any interesting applications?

"Read the fine print", S. Aaronson, Nature (2015)

Assumptions and queries in the QLSP

Assumptions on A:

- A is Hermitian and sparse, spectral norm 1, and of dimension NxN, $N=2^n$.
- A is invertible and its condition number, the ratio between the largest and smallest singular values, is $\kappa<\infty$.

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There exists a procedure that computes the matrix elements of A as follows:

$$|j\rangle\,|i\rangle\,|z\rangle \xrightarrow{\mathcal{U}_A} |j\rangle\,|i\rangle\,|z \oplus A_{ji}\rangle \ , \qquad \text{(matrix elements)}$$

$$|j\rangle\,|l\rangle \xrightarrow{\mathcal{U}_A} |j\rangle\,|f(j,l)\rangle \ . \qquad \text{(location of non-zero elements)}$$

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There exists another procedure that prepares the "initial state" as follows:

$$|b\rangle = \mathcal{U}_b|0\rangle \ , \ |b\rangle = \frac{\sum_{i=1}^{N} b_i|i\rangle}{(\sum_{i=1}^{N}|b_i|)^{1/2}}$$

Query complexity in the QLSP

- Both procedures are considered as black boxes. While they eventually need to be implemented using two-qubit gates, we will abstract away their inner workings.

- For simplicity, we will assume that these procedures can be implemented in “constant” time. The number of uses of the procedures determine then query complexity of the algorithm. We will separate the different query complexities when necessary.

- The number of queries also give a hint on what to expect for the gate complexity, e.g., it provides a lower bound.

QLSP results on query complexity: polylog scaling in N

- Harrow, Hasidim, Lloyd (2008): Quantum phase estimation

$$\tilde{O}(\kappa^2 \log(N)/\epsilon)$$

- Ambainis (2012): Variable time amplitude amplification

$$\tilde{O}(\kappa \log(N)/\epsilon^3)$$

- Childs, Kothari, **Somma** (2017): LCU, Chebyshev approx.

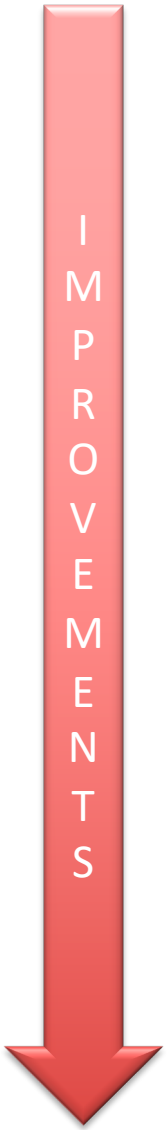
$$\tilde{O}(\kappa \log(N)\ \mathrm{poly}\ \log(1/\epsilon))$$

- Subasi, **Somma**, Orsucci (2018): adiabatic quantum approach

$$\tilde{O}(\kappa \log(N)/\epsilon)$$

- An, Lin (2019): adiabatic quantum approach

$$O(\kappa \log(N)/\epsilon)$$



The rest of this talk

- I will describe the high-level ideas in the HHL and one of our quantum algorithms for the QLSP that exponentially improves the dependence in precision.

- I'll make a quick comment on applications.

- I will present some recent results on the complexity of quantum state verification in the QLSP, which demonstrate that prior quantum algorithms are optimal and that recent variational approaches to this problem won't work.

QLSP: The general idea

$$A\ ,\ \vec{b} \quad \Rightarrow \quad |x\rangle \propto A^{-1}|b\rangle$$

Goal: construct a unitary (quantum circuit) acting on a larger space such that

$$V = \left(\begin{array}{c|c} cA^{-1} & X \\ \hline X & X \end{array}\right)$$

$$V|b\rangle|0\rangle = \underbrace{c'|x\rangle|0\rangle} + |\mathrm{trash}\rangle$$

If you find the ancilla in 0, then you are done

HHL algorithm

- The HHL algorithm implements an approximation of $1/(\kappa A)$ to the initial state using quantum phase estimation (QPE).
- QPE provides an estimate of the eigenvalues of A in a different register. Conditioned on this value, the HHL algorithm performs a rotation on an ancilla qubit so that the amplitude in |0> is almost inverse proportional to the eigenvalue.
- The next step is to perform amplitude amplification to obtain the desired state with large probability.
- The complexity is given by the number of amplitude amplification rounds times the complexity of QPE. In the worst case this is

$$\tilde{O}(\kappa^2 \log(N)/\epsilon)$$

Harrow, Hassidim, Lloyd, PRL 103, 150502 (2009)

LCU Algorithm: Linear combination of unitaries

A Fourier transform approach:

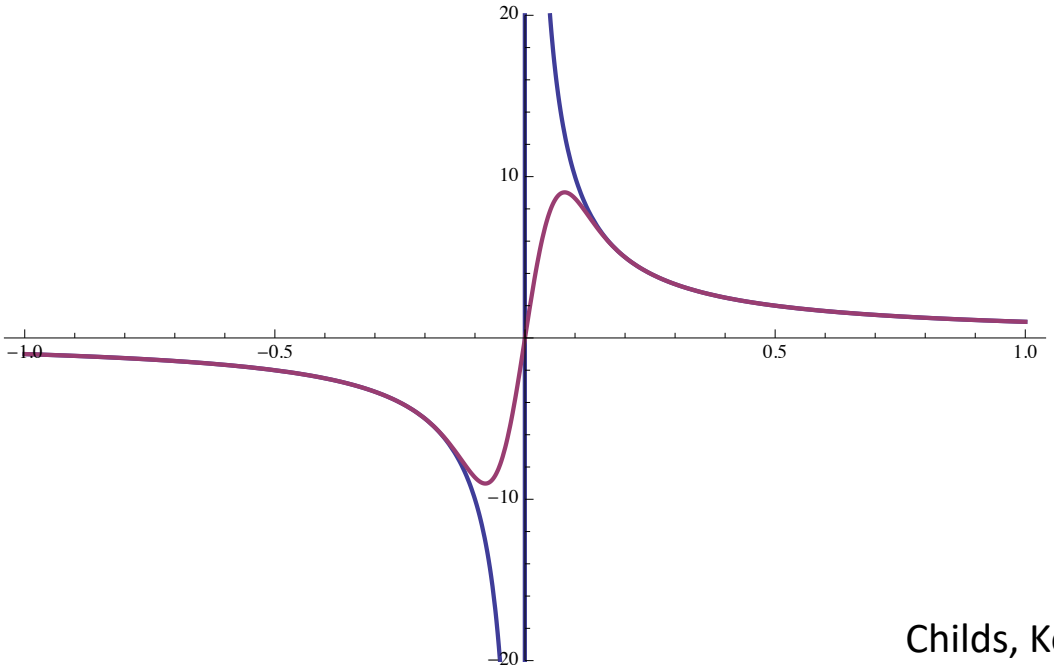
$$\frac{1}{x} = \frac{i}{\sqrt{2\pi}} \int\int dydz\ ze^{-z^2} e^{-ixyz}$$

$$\frac{1}{A} \approx_\varepsilon \frac{i\delta y\ \delta z}{\sqrt{2\pi}} \sum_{j=0}^{J} \sum_{k=-K}^{K} z_k\ e^{-(z_k)^2/2}\ e^{-iA(y_j z_k)}$$

Linear combination of unitaries (LCU)

The maximum evolution time satisfies

$$t_{\max} = O(\kappa \log(\kappa/\epsilon))$$



Childs, Kothari, **Somma**, SIAM J. Comp 46, 1920 (2017)

LCU Framework

$$|\psi\rangle \rightarrow \frac{(\alpha V_1 + \beta V_2)|\psi\rangle}{\|(\alpha V_1 + \beta V_2)|\psi\rangle\|}$$

$$> 0 \ , \ \alpha + \beta = 1$$

Childs, Kothari, **Somma**, SIAM J. Comp 46, 1920 (2017)

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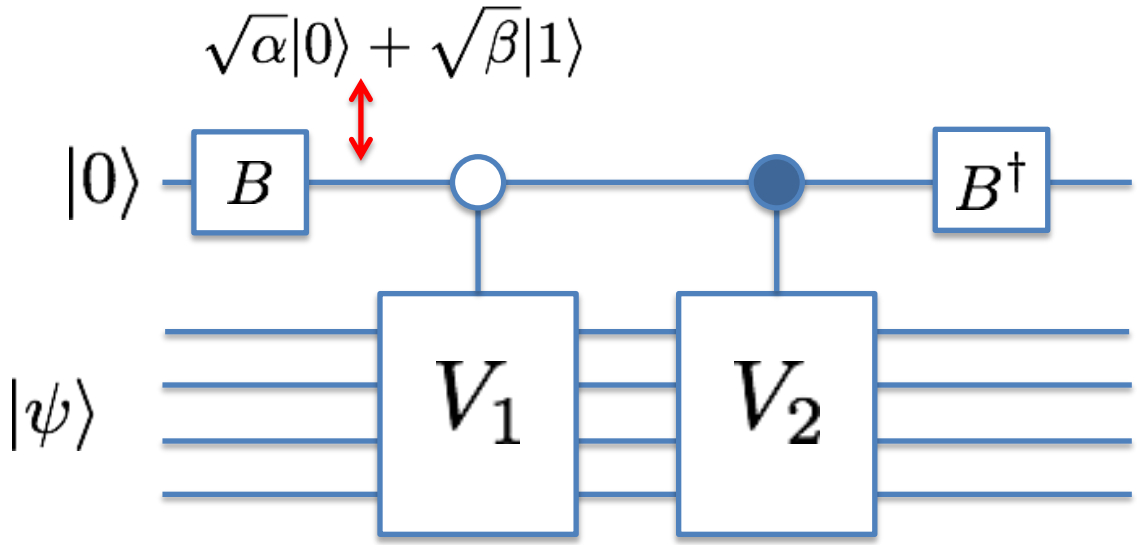

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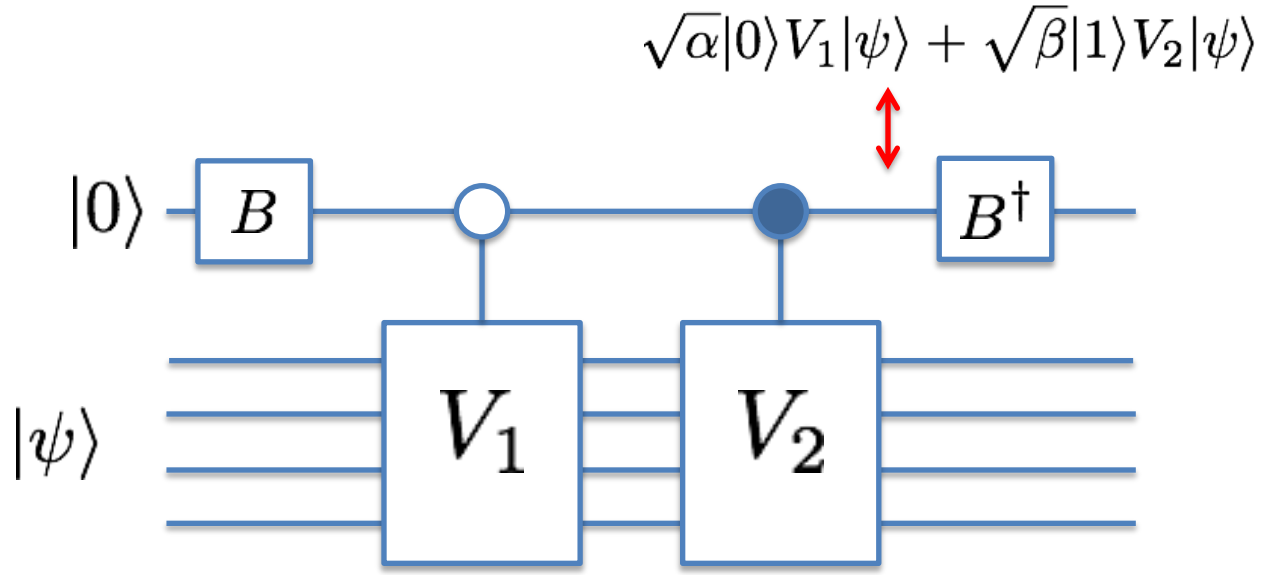

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LCU Framework

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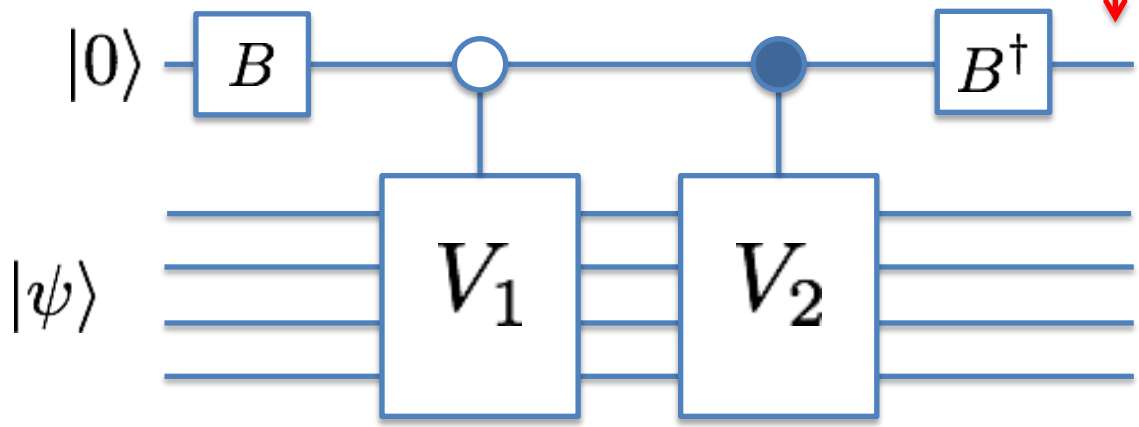
$$|0\rangle(\alpha V_1 + \beta V_2)|\psi\rangle + \sqrt{\alpha\beta}|1\rangle(V_1 - V_2)|\psi\rangle$$



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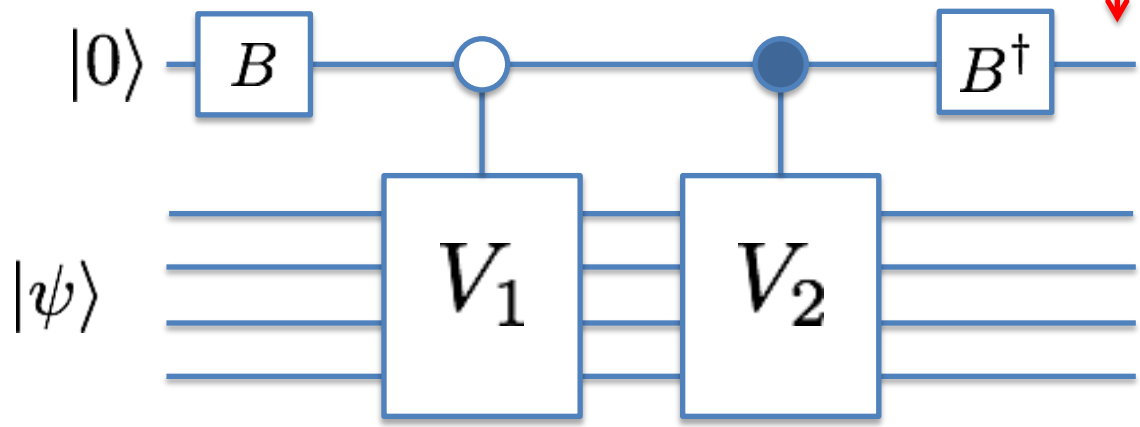


If we measured here, we would obtain the correct state with some probability

$$\Pr(0_{\text{anc}}) = \|(\alpha V_1 + \beta V_2)|\psi\rangle\|^2$$

- Actually, we will increase the desired amplitude using amplitude amplification
- This approach can be generalized to larger LCUs

LCU Algorithm: Complexity (worst case)

- The complexity of the LCU algorithm is mainly given by the number of amplitude amplification rounds times the complexity of implementing the LCU.

- Since the largest eigenvalue is 1 and we are applying $1/(\kappa A)$ to the initial state, we need $\mathcal{O}\left(\|(1/\kappa A)|b\rangle\|^{-1}\right)$ rounds of amplitude amplification. This is linear in κ in the worst case.

- Since the smallest eigenvalue is $1/\kappa$, we need to evolve with A for time that is linear in κ and polylogarithmic in the precision parameter ϵ.

- Putting all together, the worst-case complexity is

$$\tilde{O}(\kappa^2 \ \mathrm{polylog}(1/\epsilon))$$

being an exponential improvement in precision.

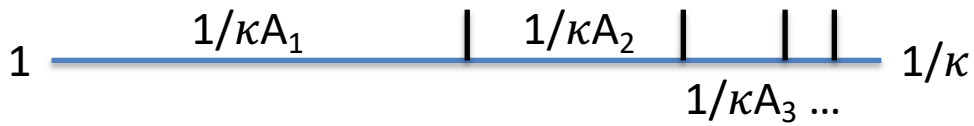
Childs, Kothari, **Somma**, SIAM J. Comp 46, 1920 (2017)

Variable time amplitude amplification

$$\kappa^2 \rightarrow \kappa$$

- The quadratic dependence on κ comes from two worst-case considerations: First, the accurate implementation of the operator $1/(\kappa A)$ is costly if the initial state has support on the eigenspace of small singular values. Second, the number of rounds in amplitude amplification is large if the initial state has support on the eigenspace of large eigenvalues.

- VTAA "solves" the problem in stages. The original idea is to use phase estimation and amplitude amplification in various steps: First, apply $1/A$ for those eigenstates with eigenvalues that are close to 1, then do amplitude amplification, then implement $1/A$ to eigenstates with smaller eigenvalues, amplitude amplification, and so on…



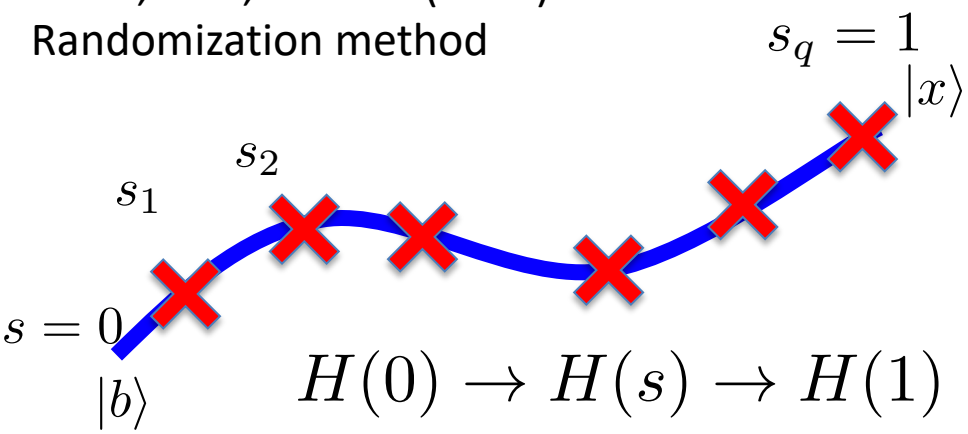
Ambainis, arXiv: 1010.4458 (2010); Childs, Kothari, **Somma**, SIAM J. Comp 46, 1920 (2017)

Adiabatic-inspired algorithm

- The approach based on linear combinations of unitaries requires many ancillary systems and even more if we use VTAA. This can be improved using techniques such as quantum signal processing but still requires many ancillas.

- We resolved this issue by providing a quantum algorithm inspired by adiabatic evolutions. We built a Hamiltonian whose eigenstate is the state we want to prepare and found an interpolating path where the minimum gap scales as $1/\kappa$.

Boixo, Knill, Somma (2009):
Randomization method



- Nearby measurements drive the state to the target one (quantum Zeno effect)

- Measurements are simulated by evolving with the Hamiltonian for random time

Subasi, **Somma**, Orsucci, Phys. Rev. Lett. 122, 060504 (2019)

Adiabatic-Inspired Algorithm

- The basic idea is to build a Hamiltonian whose eigenstate gives the solution to the QLSP

$$\underbrace{(P_b^{\perp} A)}_{B}.\vec{x} = P_b^{\perp}.\vec{b} = 0$$

$$H|x\rangle|1\rangle = 0 \; , H = B^{\dagger} \otimes \sigma^{-} + B \otimes \sigma^{+} = \begin{pmatrix} 0 & B \\ B^{\dagger} & 0 \end{pmatrix}$$

The ancilla can be discarded, but it's needed for the current approach

Interpolating Hamiltonian defined via: $A(s) = (1-s)I + sA \; , \; 0 \leq s \leq 1$

Subasi, **Somma**, Orsucci, Phys. Rev. Lett. 122, 060504 (2019)

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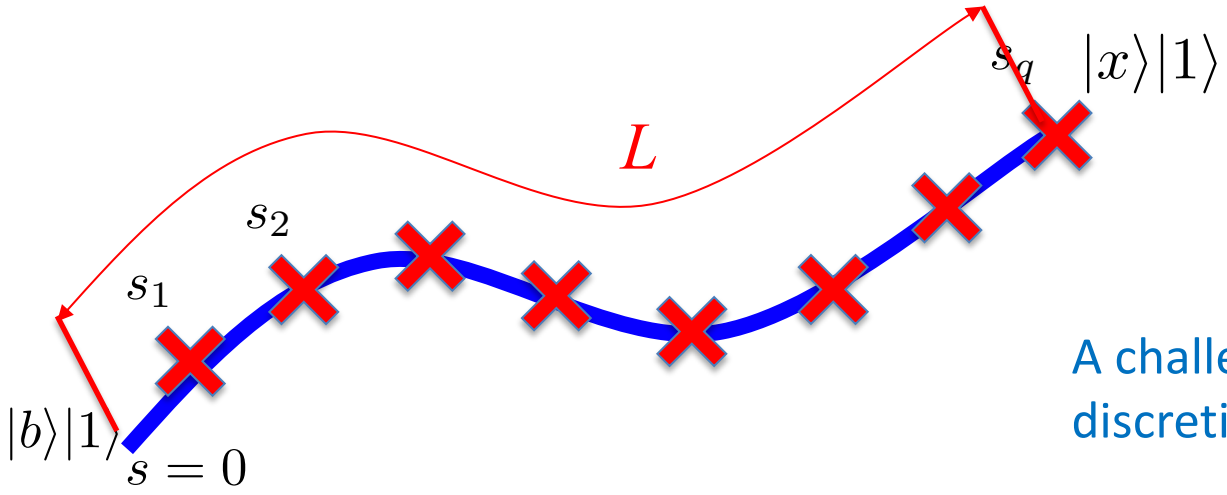
Interpolating Hamiltonian defined via: $A(s) = (1-s)I + sA \;,\; 0 \leq s \leq 1$

Interpolation between a "simple" linear system Ix=b and a complicated one, Ax=b

Adiabatic-Inspired Algorithm: Complexity (worst case)



A challenge: Find the discretization points

- The expected evolution time with the Hamiltonians in the randomization method satisfies

$$T_{RM} = O\left(\frac{L^2}{\epsilon\Delta}\right)$$

L is the path length
Δ is the min gap
ϵ is the error (trace norm)

- The overall complexity is $\tilde{O}(\kappa \log(N)/\epsilon)$

Subasi, **Somma**, Orsucci, Phys. Rev. Lett. 122, 060504 (2019)

Adiabatic-Inspired Algorithm: Complexity

- The complexity is almost optimal, i.e., linear in the condition number
- The algorithm is built upon evolutions with ”simple” Hamiltonians
- Only one ancilla required
- While the complexity is linear in $1/\varepsilon$ it can be made logarithmic in this quantity using a better method to simulate measurements [Boixo, Knill, Somma 2010].

- This algorithm has been derandomized by An, Lin (2019)

Why are these improvements useful?

- We were able to develop optimal algorithms for the QLSP using significantly less resources than previous approaches.

- These improvements allowed us to prove a polynomial quantum speedup for hitting time estimation of a Markov chain (A. Chowdhury, R.D. Somma, QIC 17, 0041 (2017)).

- Having a small complexity dependence on precision is important for, e.g., computing expectation values of observables at the quantum metrology limit.

We claim an exponential speedup, but…

- As mentioned, the QLSP solves a problem related to systems of linear equations by encoding the solution in a quantum state. **It does not output the full vector.**

Applications showing a polynomial/unknown quantum speedup

- In physics, where the goal is to compute the expectation value of the inverse of a matrix. This idea was used in [1] for obtaining the resistance of a network.

- In stat mech, where, e.g., estimating the hitting time of a Markov chain also reduces to computing the expectation value of the inverse of a matrix [2].

- In ML, for solving problems related to least-squares estimation [3], by applying the pseudoinverse.

- For "solving" certain linear differential equations [4].

[1] G. Wang, arXiv:1311.1851 (2013).
[2] A. Chowdhury and R. Somma, QIC 17, 0041 (2017)
[3] N. Wiebe, D. Braun, and S. Lloyd, PRL 109, 050505 (2012).
[4] D. Berry, A. Childs, A. Ostrander, and G. Wang, CMP 356, 1057 (2017)

We claim an exponential speedup, but…

- Finding more applications for quantum algorithms like these is important, especially if we find problems for which an exponential speedup is obtained.

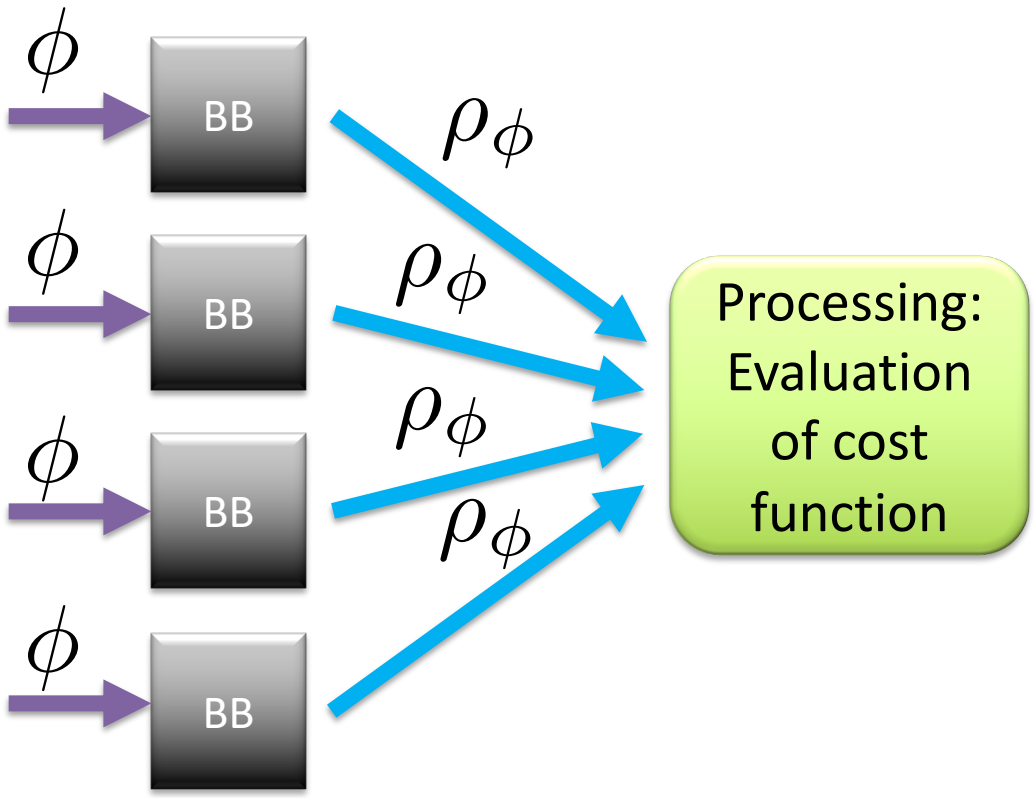
- More recent work on the computation of Green's functions: Tong, An, Wiebe, Lin, "Fast inversion, preconditioned quantum linear system solvers and fast evaluation of matrix functions", Phys. Rev. A 104, 032422 (2021).

QLSP: more recent ideas

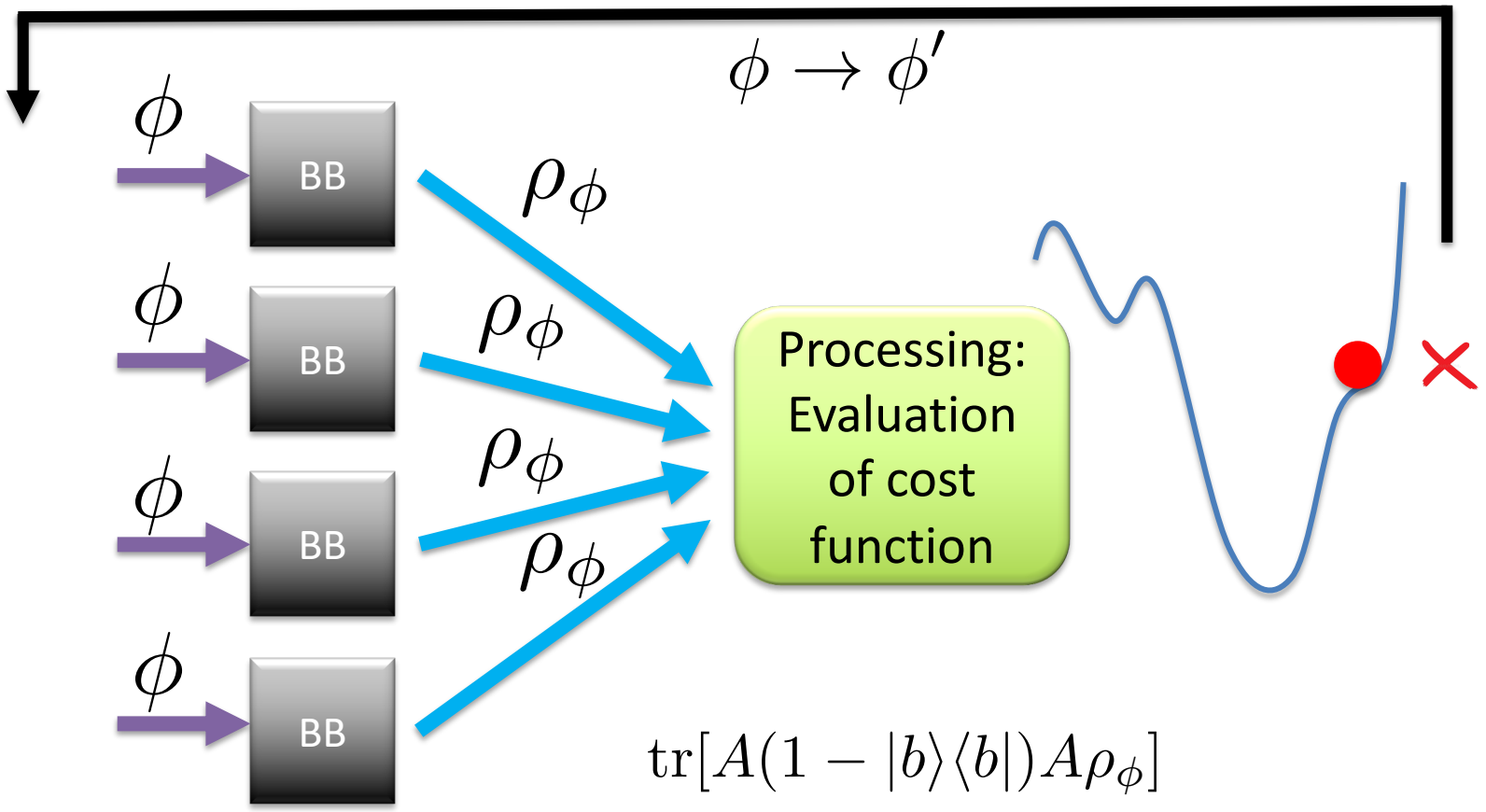
- Proposed variational and related quantum algorithms to this problem.
- Claims: These approaches may be useful for NISQ technologies, may solve the QLSP faster, may not need quantum error correction, etc.
- Nice and simple ideas… do they work?

- D. An and L. Lin, *Quantum Linear System Solver Based on Time-Optimal Adiabatic Quantum Computing and Quantum Approximate Optimization Algorithm*, arXiv:1909.05500 (2019).
- H.-Y. Huang, K. Bharti, and P. Rebentrost, *Near-Term Quantum Algorithms for Linear Systems of Equations*, arXiv:1909.07344 (2019).
- C. Bravo-Prieto, R. LaRose, M. Cerezo, Y. Subasi, L. Cincio, and P. J. Coles, *Variational Quantum Linear Solver: A Hybrid Algorithm for Linear Systems*, arXiv:1909.05820 (2019).
- X. Xu, J. Sun, S. Endo, Y. Li, S. C. Benjamin, and X. Yuan, *Variational Algorithms for Linear Algebra,* arXiv:1909.03898 (2019).

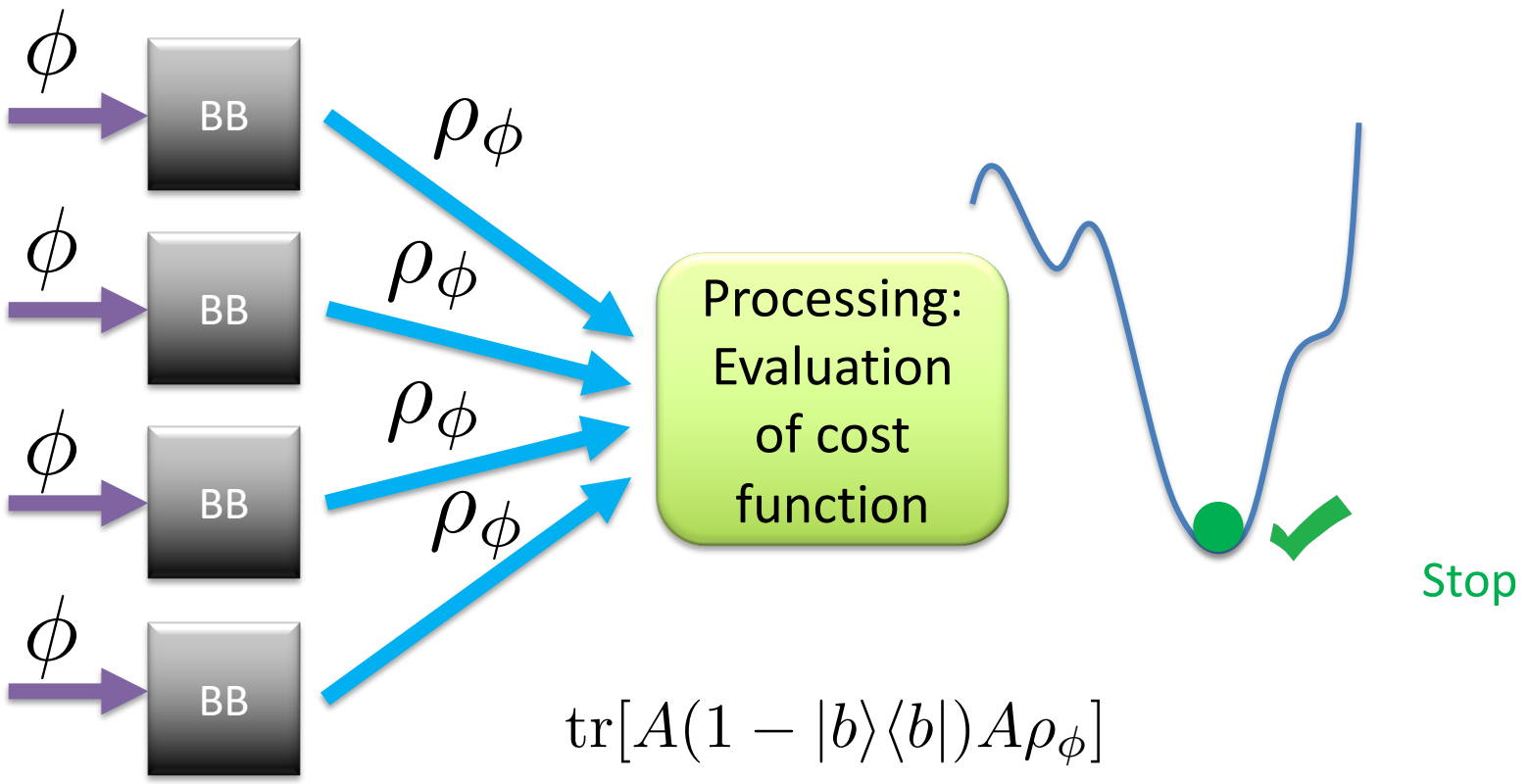
QLSP: Variational approach



QLSP: Variational approach



QLSP: Variational approach



QLSP: more recent ideas

Do these approaches work?

- Do they require a costly optimization loop?
- Do they require computing cost functions within high accuracies?
- What's the running time? How does it compare with other approaches?
- Is it correct to say that no quantum error correction is needed? Why are these approaches suitable for NISQ?

QLSP: more recent ideas

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- What's the running time? How does it compare with other approaches?
- Is it correct to say that no quantum error correction is needed? Why are these approaches suitable for NISQ?

- To analyze these questions, we need to understand first quantum state verification in the QLSP.
- This is only part of the motivation. Regardless of these approaches, the QSV problem is interesting in itself as it may tell us something about the complexity of other quantum methods for other problems.

QLSP: more recent ideas

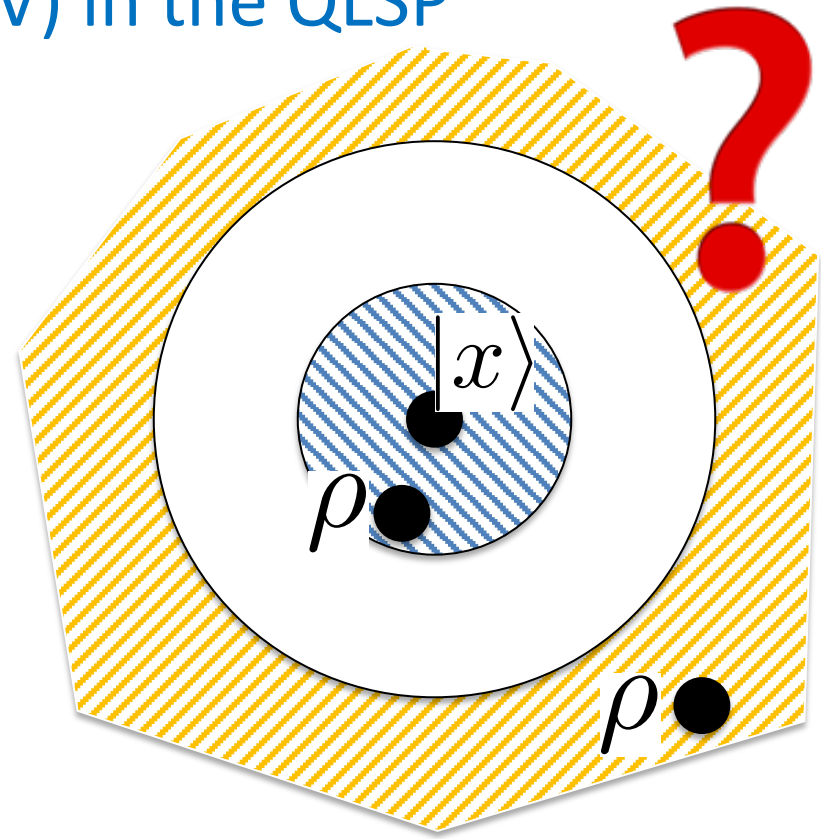
Do these approaches work?

- Do they require a costly optimization loop?
- Do they require computing cost functions within high accuracies?
- W
- I

In the rest of my talk, I will introduce the quantum state verification (QSV) problem and show that, indeed, QSV is expensive. One implication is that these recent ideas result in quantum algorithms with running times significantly larger than previously known quantum algorithms for the QLSP (i.e., bounded by a high degree polynomial in the condition number).

- T
- Regardless of these approaches, this problem is interesting in itself as it may tell us something about the complexity of other quantum methods for other problems.

Quantum state verification (QSV) in the QLSP



- Goal: Decide, with high probability, whether a given quantum state ρ is close or far from the solution of the QLSP. ("Close" means within trace distance 1/8. "Far" means beyond trace distance 1/2.)

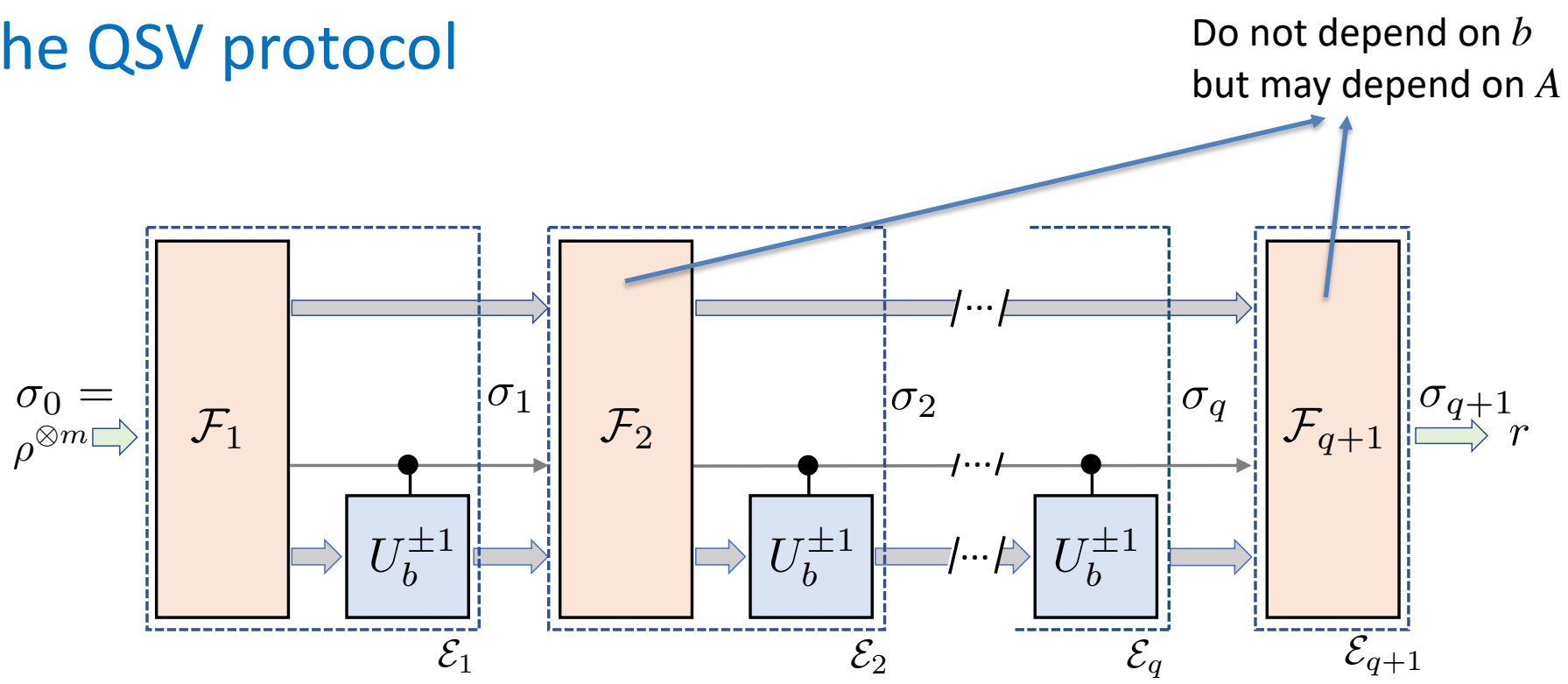
- Build a quantum protocol $\mathcal{E}$ that outputs a bit *r* as follows

$$\Pr(r=1)\begin{cases}\geq 2/3 & \text{if} \quad D_{\rho,x}\leq 1/8,\\ \leq 1/3 & \text{if} \quad D_{\rho,x}>1/2.\end{cases}$$

where

$$D_{\rho,x}=\frac{1}{2}\mathrm{Tr}|\rho-|x\rangle\langle x||$$

The QSV protocol



The protocol $\mathcal{E}$:

- A sequence of rules (quantum operations) that depend on the unknown initial state preparation unitary U_b.

- The maximum number of uses of this unitary is q. However, the protocol may stop and return the bit r before, where the number of uses of U_b is random.

QSV in the QLSP

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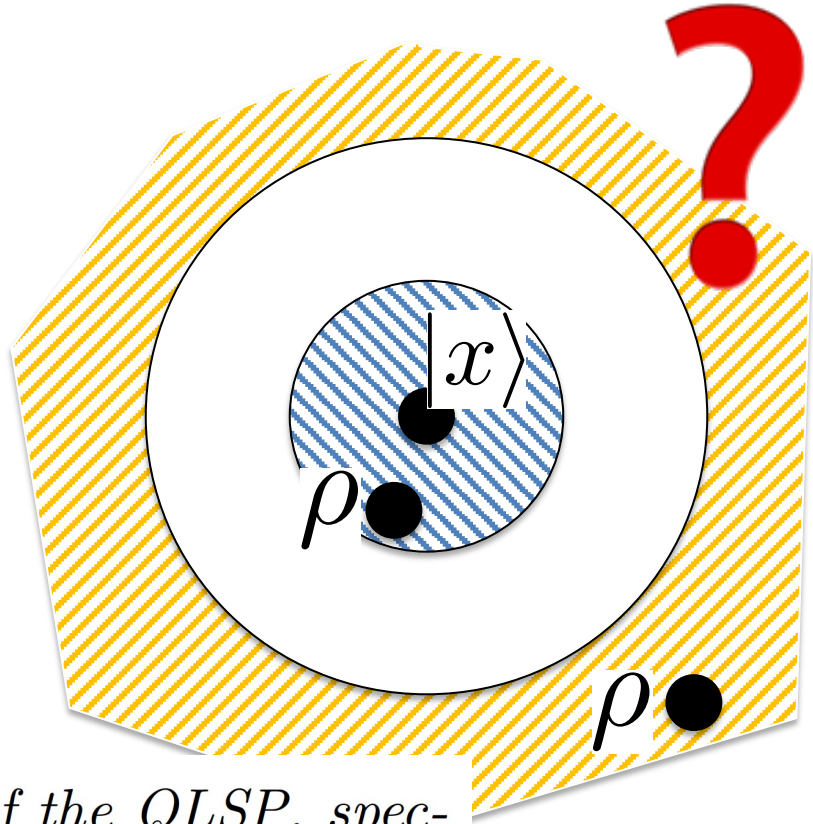

- Main theorem:

Theorem 1. *Consider any instance of the QLSP, specified by A and $\vec{b}$, and any protocol for QSV as above. Then, for all quantum states ρ that satisfy $D_{\rho,x} \leq 1/8$, the number of $cU_b^{\pm 1}$'s required to implement $\mathcal{E}$ on input $\sigma_0 = \rho^{\otimes m}$ satisfies*

$$\Pr\left(q_{A,b} > \frac{1}{13}\,\frac{\kappa}{\|A^{-1}\,|b\rangle\,\|}\right) \geq \frac{1}{6}\,. \qquad (5)$$

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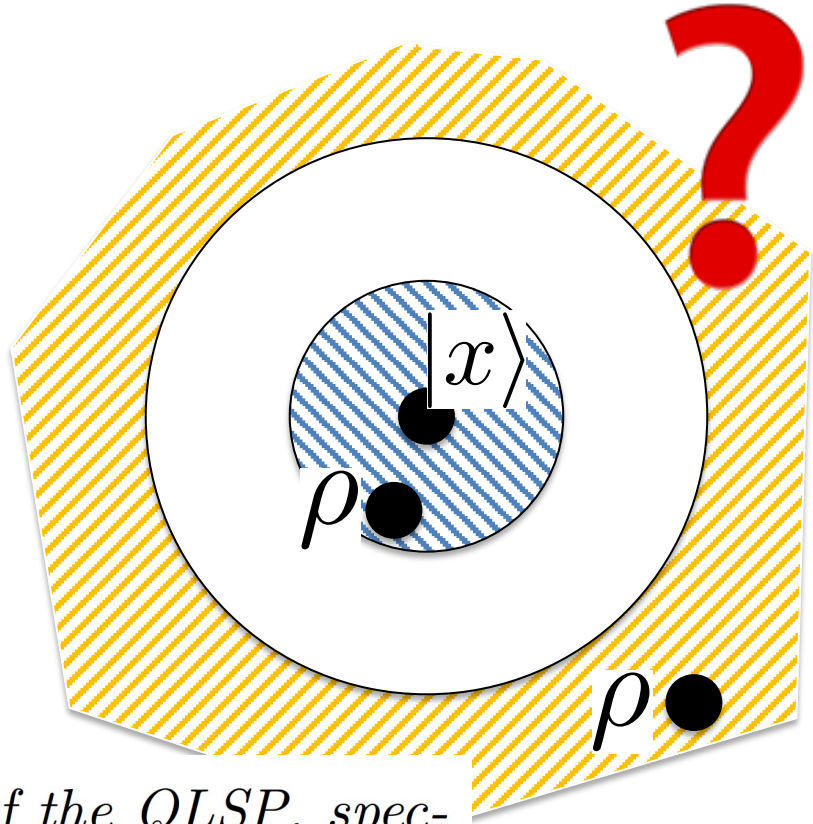
QSV in the QLSP

- Goal: Decide, with high probability, whether a given quantum state ρ is close or far from the solution of the QLSP. (Close means within trace distance 1/8. Far means beyond trace distance 1/2.)



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QSV in the QLSP

It is simple to show:

$$1 \leq \| A^{-1} |b\rangle \| \leq \kappa$$

best case

worst case

But typically, we showed: $\| A^{-1} |b\rangle \| \sim \sqrt{\kappa}$

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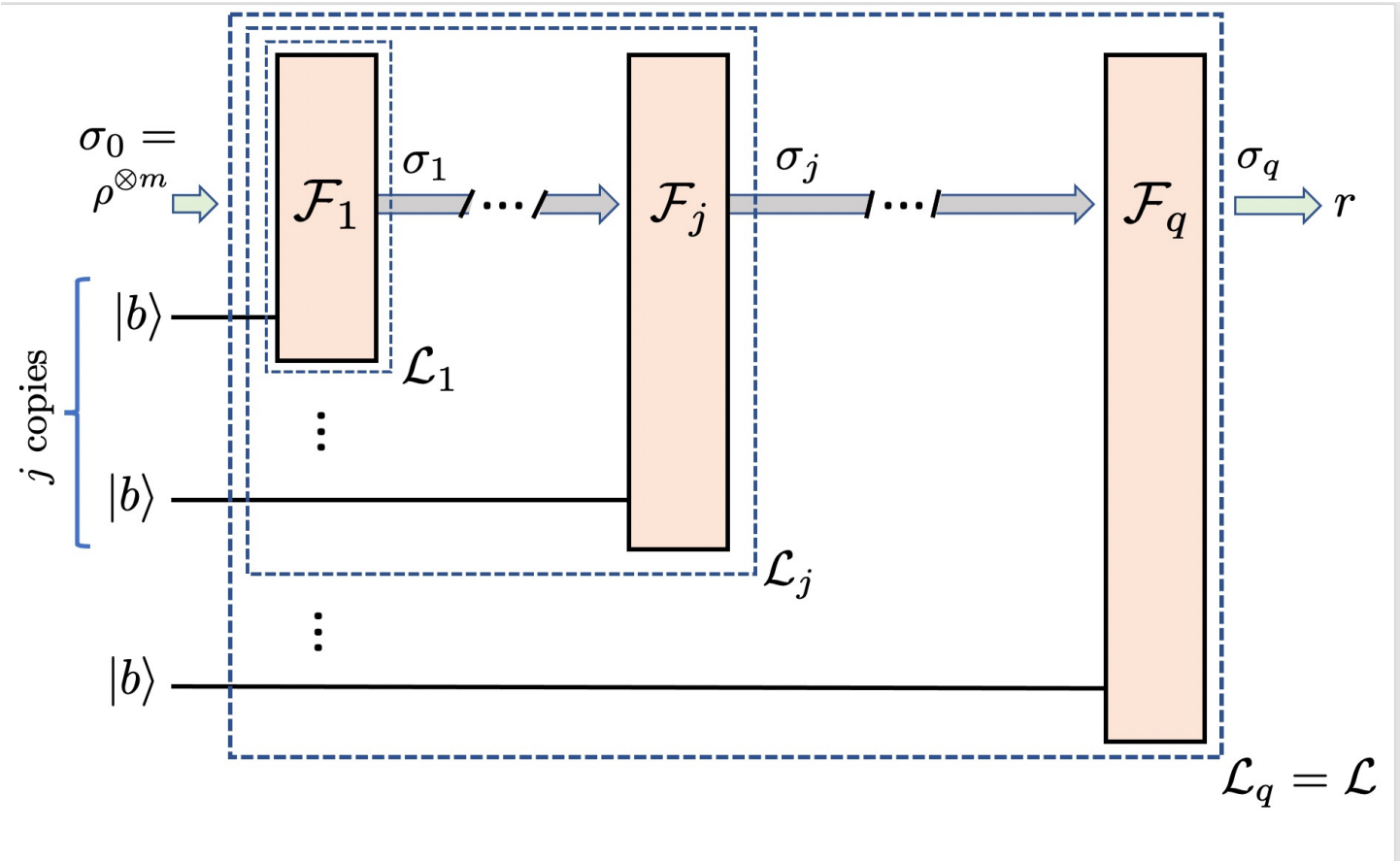
- Quantum state verification in the QLSP requires a number of resources (query complexity) that goes, at least, as the square root of the condition number, which can be very large!

- It can be shown that the best way to verify is to solve the QLSP with one of the algorithms I presented (e.g., HHL) and then use the swap test – Matching upper bound for the query complexity.

- Bad news for variational and related approaches.

QSV in the QLSP

Things are actually worse for a restricted class of verification procedures, called prepare-and-measure:



QSV in the QLSP

Things are actually worse for a restricted class of verification procedures, called prepare-and-measure:

Theorem 3. *Consider any instance of the QLSP specified by A and $\vec{b}$, and any protocol for QSV of the PM type as above. Then, for all quantum states ρ that satisfy $D_{\rho,x} \leq 1/8$, the number of copies of $|b\rangle$ required by $\mathcal{L}$ for $\sigma_0 = \rho^{\otimes m}$ satisfies*

$$\Pr\left(q_{A,b} > \frac{1}{150}\frac{\kappa^2}{\|A^{-1}|b\rangle\|^2}\right) \geq \frac{1}{6}\,. \tag{9}$$

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QSV in the QLSP

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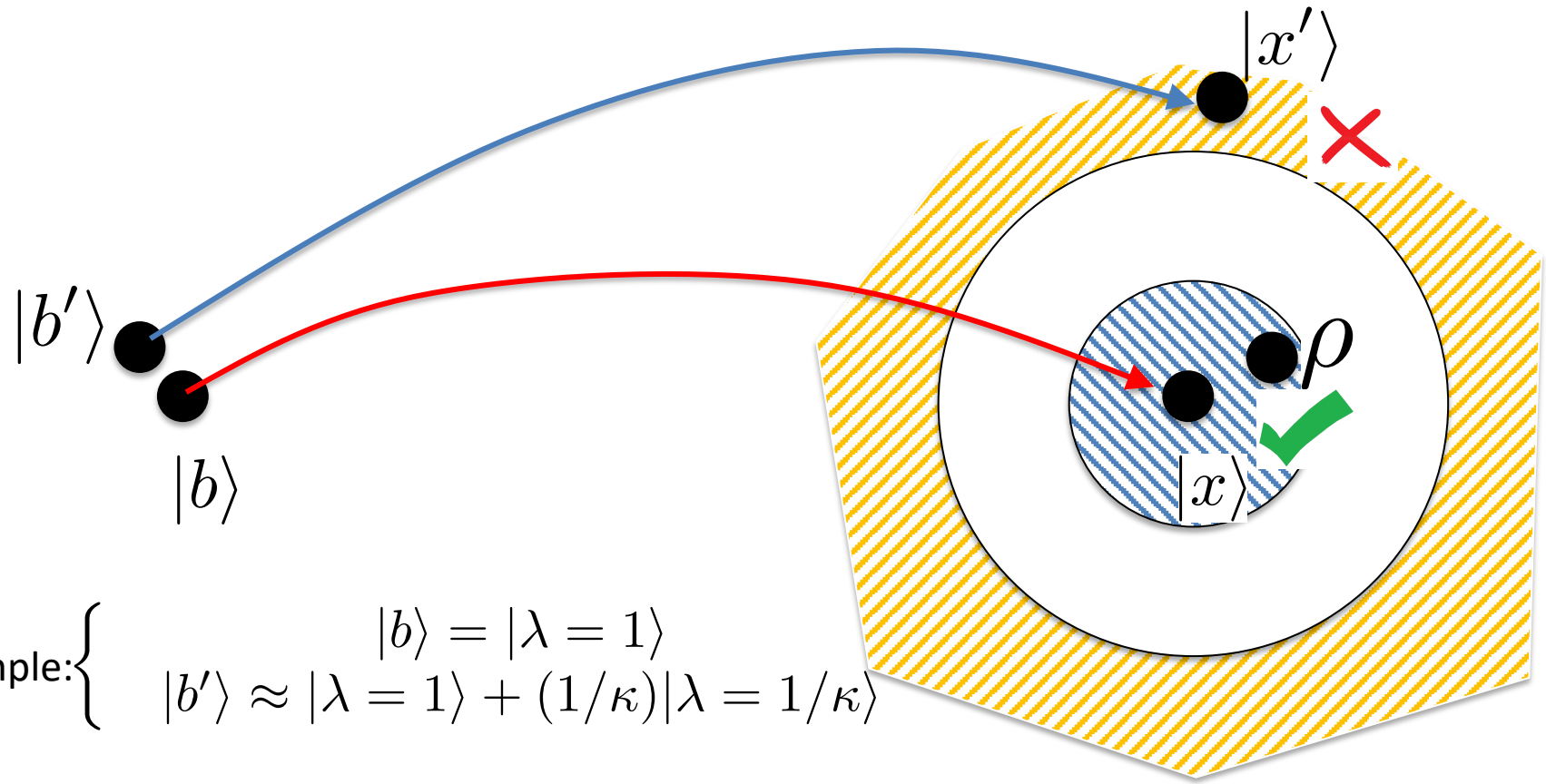
- The protocols used by proposed variational approaches can be cast as of this type. The typical complexity will be **at least** linear in κ.
- In fact, proposed variational approaches do worse due to sampling noise, with a complexity that scales with κ^4.

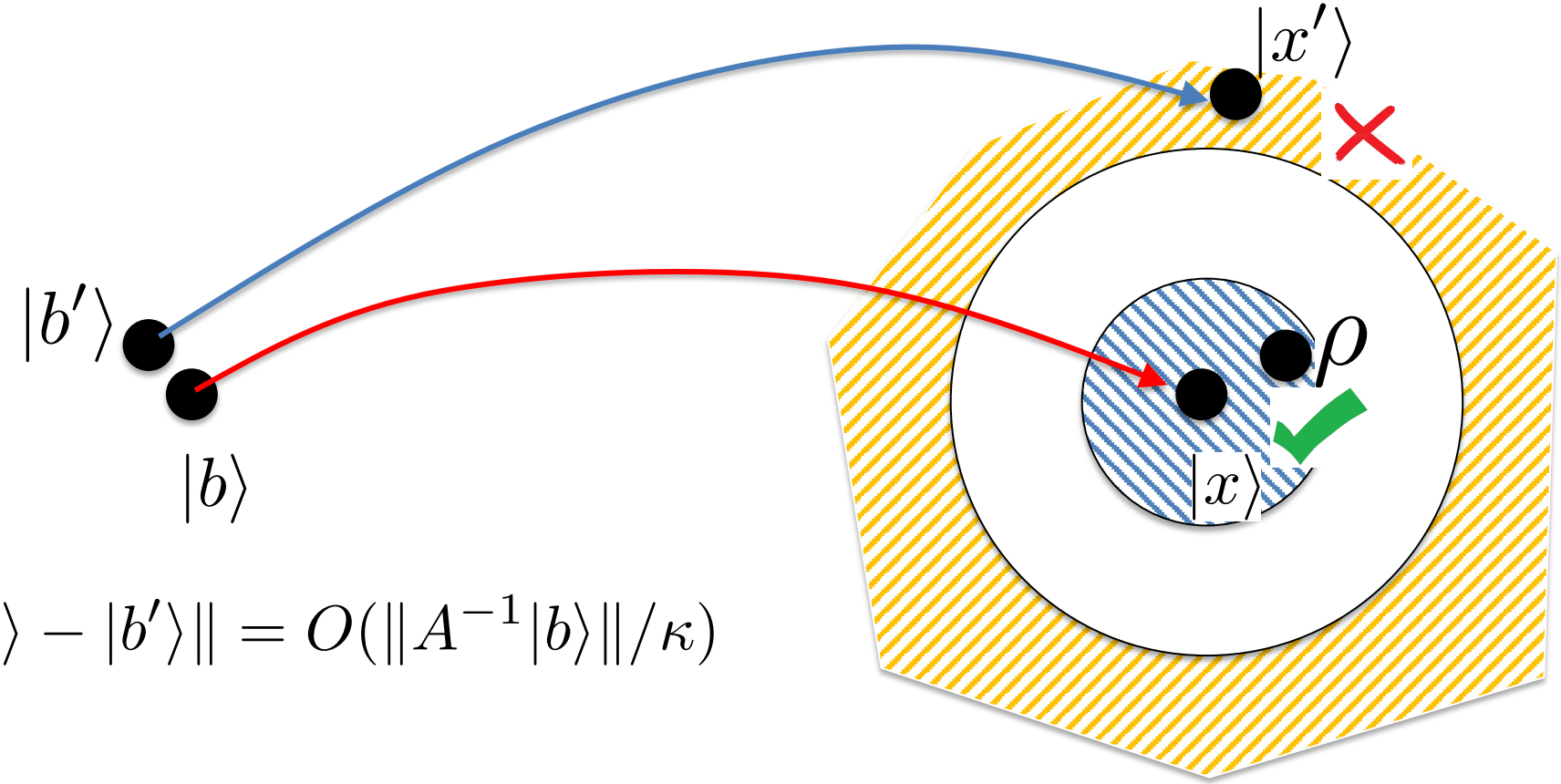
Basic idea for proof



Example: $\begin{cases} |b\rangle = |\lambda = 1\rangle \\ |b'\rangle \approx |\lambda = 1\rangle + (1/\kappa)|\lambda = 1/\kappa\rangle \end{cases}$

- A “small” perturbation in the initial state can lead to a “big” change in the solution (accept/reject): These are adversarial instances.
- One state must be accepted while the other must be rejected (whp).

Basic idea for proof



$$\||b\rangle - |b'\rangle\| = O(\|A^{-1}|b\rangle\|/\kappa)$$

- A “small” perturbation in the initial state can lead to a “big” change in the solution (accept/reject): These are adversarial instances.
- A quantum operation for QSV must resolve the difference between both instances: complexity goes with the inverse of the difference of initial states.

Basic idea for proof

- It is important to note that for each instance of the QLSP there is an adversarial one. Therefore, one cannot make the statement that QSV may be done more efficiently in typical cases, etc.

- The actual proof is more technically involved. The bit r can be output after any number of uses of the unitaries, and this number can be random. We also need to show a way to construct the adversarial instance.

- The quadratically worse bound is simply due to the fact that the trace distance between m identical copies of two states increases only with the square root of m.

- See paper for full proof

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QSV in the QLSP

The results apply to a weaker form of QSV for which some states that are close to the solution of the QLSP can also be rejected. This is what happens in variational and related optimization algorithms.

$$\Pr(r=1)\begin{cases}\geq 2/3 & \text{if} \quad C(\rho)\leq C_{\min} \\ \leq 1/3 & \text{if} \quad D_{\rho,x}>1/2\end{cases}$$

Theorem 4. *Consider any instance of the QLSP, specified by A and $\vec{b}$, and any protocol for QSV as above. Then, for all quantum states ρ that satisfy $C(\rho)\leq C_{\min}$, the number of $cU_b^{\pm 1}$'s required to implement $\mathcal{E}$ on input $\sigma_0=\rho^{\otimes m}$ satisfies*

$$\Pr\left(q_{A,b}>\frac{1}{13}\,\frac{\kappa}{\|A^{-1}\,|b\rangle\,\|}\right)\geq\frac{1}{6}\,. \qquad (11)$$

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Conclusions

- Quantum computing is promising. Several quantum algorithms for problems in linear algebra with significant speedups exist

- I presented quantum algorithms to solve the quantum linear systems problem. The techniques can be generalized to apply other operators (other than the inverse of a matrix) to quantum states.

- The advantages of the LCU algorithm are that the complexity dependence on precision is only polylogarithmic, exponentially improving previous algorithms for this problem. Further improvements are known.

- The advantages of the adiabatic algorithm are that it doesn't require many ancillary qubits and the problem reduces to a simple Hamiltonian simulation problem

- It would be important to understand the applicability of the QLSP to scientific problems beyond the ones I mentioned.

Conclusions

- I also showed that the problem of quantum state verification in the QLSP is costly. In fact, the complexity of recent alternatives (variational algorithms) is significantly higher than that of the HHL or LCU algorithms

- And it appears that one fast way of doing QSV is by using the HHL or LCU algorithms

- Last, it'd be interesting to study related problems to the QLSP. In that case, known lower bounds for the QLSP, including our results on QSV, may not apply

Thank you.