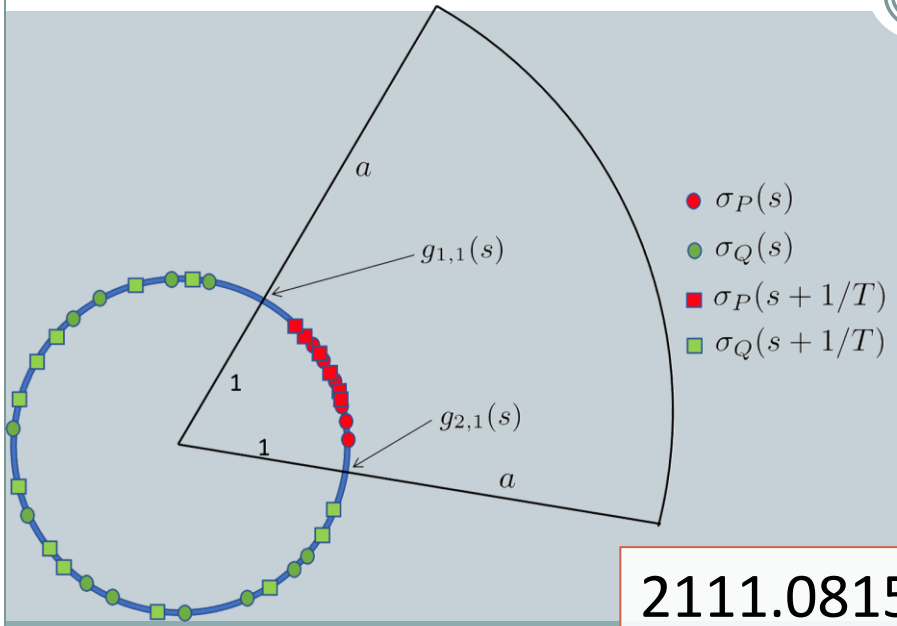
Optimal scaling quantum linear systems solver via discrete adiabatic theorem



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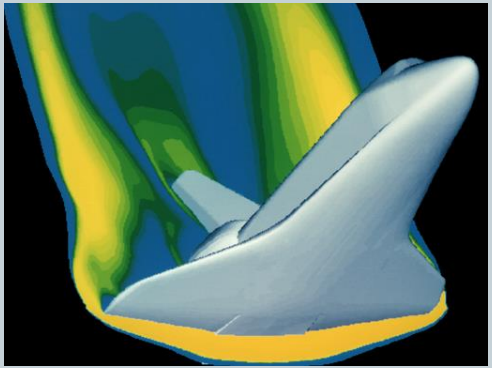
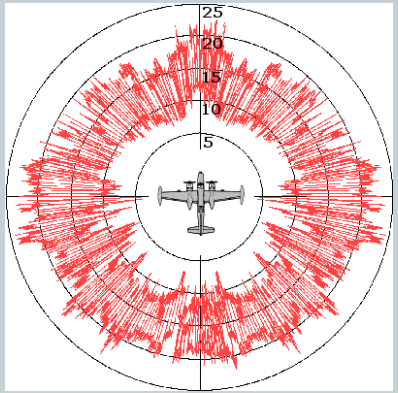
Why do we care?

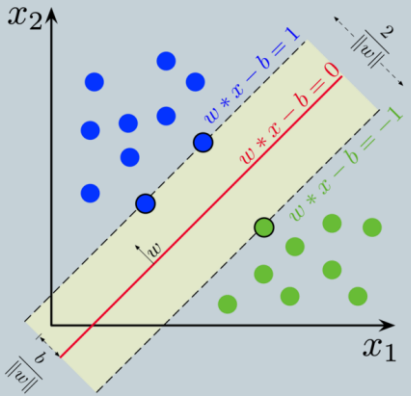
- Many problems can be posed as systems of linear equations.



Partial differential equations



EM scattering cross-section



Machine learning

- Many problems can be solved by adiabatic algorithms.
  - Ground states
  - Discrete optimisation

Quantum linear systems problem

- Need to solve

$$A\vec{x} = \vec{b}$$

- Initially prepare state

$$|b\rangle = \sum_{j=1}^{N} b_j |j\rangle$$

- Apply operation A^{-1}

$$|x\rangle = A^{-1}|b\rangle$$

- Obtain global properties from sampling $|x\rangle$ (not explicit listing).
- Exponential speedup in N.

A.W. Harrow, A. Hassidim, S. Lloyd, Physical Review Letters **103**, 150502 (2008).

Complexity scaling

- Two parameters:
  1. κ – condition number (ratio of maximum & minimum singular values)
  2. ϵ – allowable error in solution

Year	Reference	Primary innovation	Complexity
2008	Harrow, Hassidim, Lloyd	Phase estimation	$O(\kappa^2/\epsilon)$
2012	Ambainis (1010.4458)	Variable-time amplitude amplification	$O(\kappa(\log(\kappa)/\epsilon)^3)$
2017	Childs, Kothari, Somma (SIAM 46 1920)	Fourier/Chebyshev fitting using LCU	$O(\kappa\,\mathrm{polylog}(\kappa/\epsilon))$
2018	Subasi, Somma, Orsucci (PRL 122 060504)	Adiabatic randomisation method	$O((\kappa\log\kappa)/\epsilon)$
2019	An, Lin (1909.05500)	Time-optimal adiabatic method	$O(\kappa\,\mathrm{polylog}(\kappa/\epsilon))$
2019	Lin, Tong (Quantum 4, 361)	Adiabatic plus eigenstate filtering	$O(\kappa\log(\kappa/\epsilon))$
2021	This work (2111.08152)	Discrete adiabatic theorem	$O(\kappa\log(1/\epsilon))$

Continuous adiabatic algorithm

- For continuous adiabatic algorithm, simulate time-dependent Hamiltonian

$$i\frac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$$

- For short time, the time-evolution operator is given by Dyson series

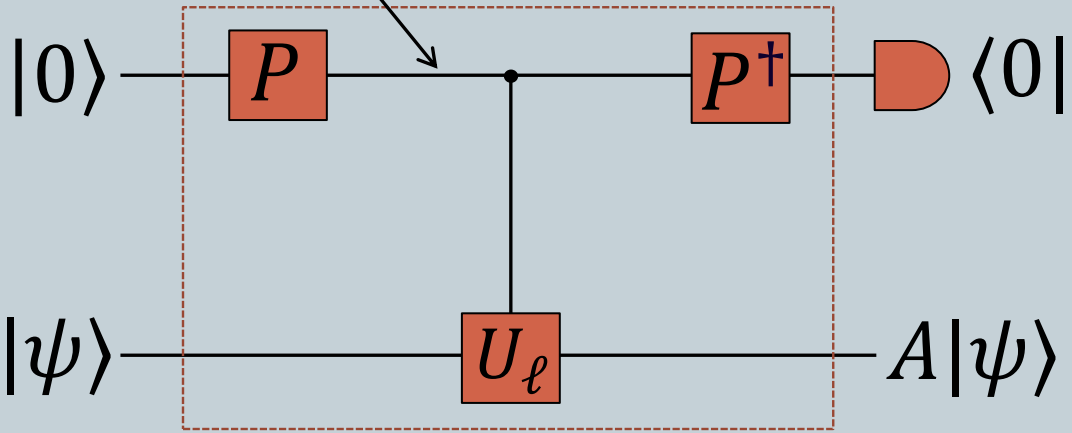
$$U(t,0) \approx \sum_{k=0}^{K}(-1)^k \int_0^t dt_1 \int_{t_1}^t dt_2 \cdots \int_{t_{k-1}}^t dt_k H(t_k)\cdots H(t_2)H(t_1)$$

- Gives $\log(\kappa/\epsilon)$ overhead for adiabatic solution of QLSP.

M. Kieferová, A. Scherer, and D. W. Berry, PRA **99**, 042314 (2019); 1805.00582.
G. H. Low and N. Wiebe, arXiv:1805.00675 (2018).

Linear combinations of unitaries

$$\sum_\ell \sqrt{w_\ell}|\ell\rangle \qquad A = \sum_\ell w_\ell U_\ell$$



Cost is typically

$$\lambda = \sum_\ell |w_\ell|$$

A. M. Childs, N. Wiebe, Quantum Information and Computation **12**, 901 (2012).

D. W. Berry, A. M. Childs, R. Cleve, R. Kothari, R. D. Somma, STOC (2014).

Block encoding

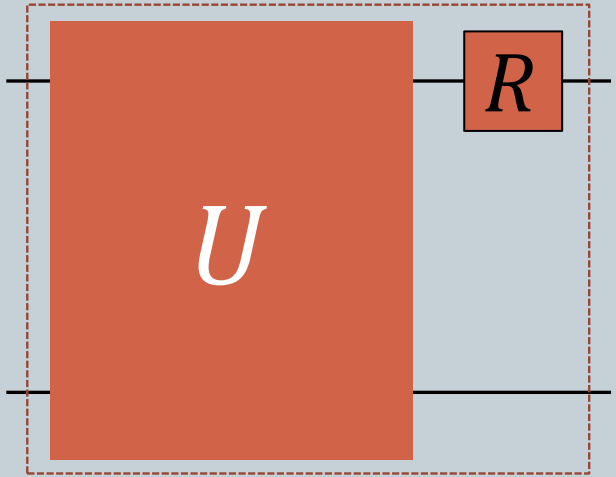
$$A = \lambda \langle 0|U|0\rangle$$

G. H. Low, I. L. Chuang, Quantum **3**, 163 (2019).

Qubitisation

- Construct quantum walk using reflection:

$$W = \equiv e^{i \arcsin A/\lambda}$$



- Eigenvalues are related to those of original matrix.

G. H. Low, I. L. Chuang, Quantum **3**, 163 (2019).

Adiabatic approach to QLSP

- Easiest for A positive-definite and Hermitian.
- Initial and final Hamiltonians with $Q_b = I_N - |b\rangle\langle b|$

$$H_0 = \begin{pmatrix} 0 & Q_b \\ Q_b & 0 \end{pmatrix} \qquad H_1 = \begin{pmatrix} 0 & AQ_b \\ Q_b A & 0 \end{pmatrix}$$

- Final eigenstate is

$$\begin{pmatrix} A^{-1}b \\ 0 \end{pmatrix}$$

- For $H(s) = \big(1 - f(s)\big)H_0 + f(s)H_1$ gap is

$$\Delta_0(s) = 1 - f(s) + f(s)/\kappa$$

- Schedule is chosen as

$$\dot{f}(s) = d_p \Delta_0^p(s), \qquad d_p = \int_0^1 \Delta_0^{-p}(u)\, du$$

- Solution is

$$f(s) = \frac{\kappa}{\kappa - 1}\left[1 - \big(1 + s(\kappa^{p-1} - 1)\big)^{\frac{1}{1-p}}\right]$$

D. An, L. Lin, arXiv:1909.05500 (2019).

Non-symmetric case

- An & Lin expand matrix for general Hermitian case

$$H_0 = \begin{pmatrix} 0 & (\sigma_z \otimes I)Q_{+b} \\ Q_{+b}(\sigma_z \otimes I) & 0 \end{pmatrix} \qquad H_1 = \begin{pmatrix} 0 & (\sigma_z \otimes A)Q_{+b} \\ Q_{+b}(\sigma_z \otimes A) & 0 \end{pmatrix}$$

- Standard (HHL) method for non-Hermitian A is to replace A with

$$\mathbf{A} = \begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix}$$

- To simplify, we use

$$A(f) = \begin{pmatrix} (1-f)I & fA \\ fA^\dagger & (1-f)I \end{pmatrix} \qquad H(s) = \begin{pmatrix} 0 & A(f)Q_b \\ Q_b A(f) & 0 \end{pmatrix}$$

- Gap is changed to

$$\Delta_0(s) = \sqrt{\big(1-f(s)\big)^2 + (f(s)/\kappa)^2} \geq (1-f(s)+f(s)/\kappa)/\sqrt{2}$$

Adiabatic walk

- Theorem for discrete sequence of operators (with integers n, T)

$$W_T(n/T), \qquad 0 \leq n \leq T-1$$

- Overall operation is sequence

$$U_T(s) = W_T(s-1/T)W_T(s-2/T)\ldots W_T(1/T)W_T(0) = \prod_{n=0}^{sT-1} W_T(n/T)$$

- We call the ideal adiabatic evolution $U_T^A(s)$.
- Aim to show error in adiabatic evolution decreases with T as

$$\left\| U_T(s) - U_T^A(s) \right\| \leq \frac{\theta}{T}$$

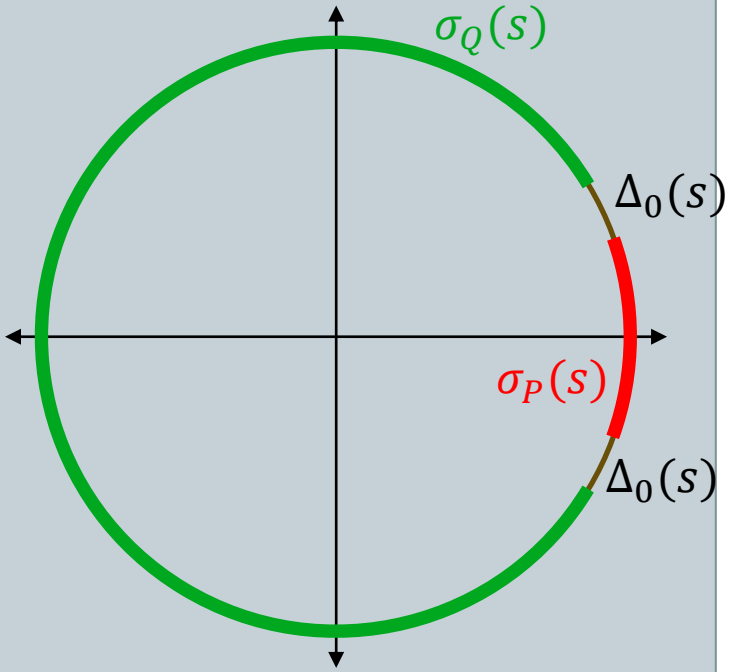
A. Dranov, J. Kellendonk, R. Seiler, Journal of Mathematical Physics **39**, 1340 (1998).

Norm of differences

- For T steps one would want difference of operators to satisfy
$$W_T(s+1/T) - W_T(s) = O(T^{-1})$$
- Need to define constant
$$\|W_T(s+1/T) - W_T(s)\| \le \frac{c_1(s)}{T}$$
- Need to define second difference:
$$DW_T(s) = W_T(s+1/T) - W_T(s), \qquad D^{(2)}W_T(s) = DW_T(s+1/T) - DW_T(s)$$
- Require bounds on multistep differences:
$$\left\|D^{(2)}W_T(s)\right\| \le \frac{c_2(s)}{T^2}$$
- Need to consider maximum over neighbouring steps:
$$\hat{c}_k(s) = \max(c_k(s-1/T), c_k(s), c_k(s+1/T))$$

Multistep gap

- Eigenvalues are on circle in complex plane.
- Gaps are needed on both sides, $\Delta_0(s)$.



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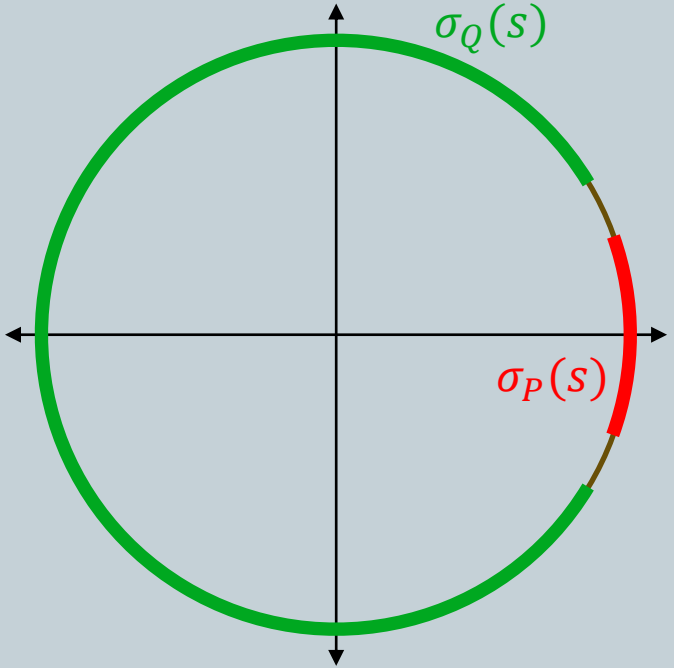
- Regions must not cross over between steps.



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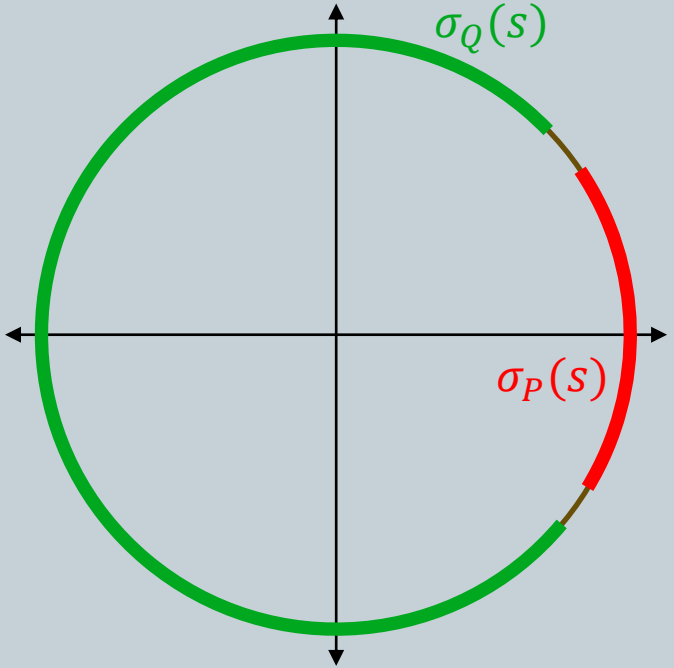
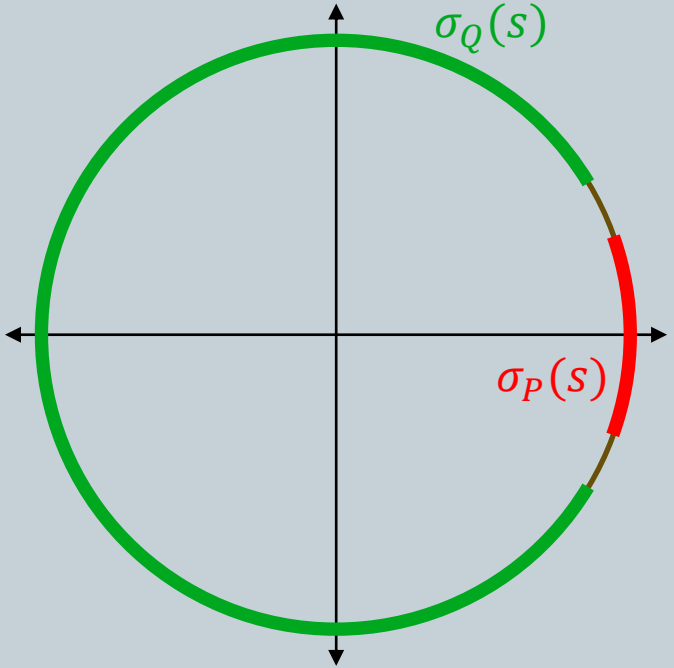


Multistep gap

- Eigenvalues are on circle in complex plane.
- Gaps are needed on both sides, $\Delta_0(s)$.
- Regions must not cross over between steps.
- Consider unified regions between three successive steps.



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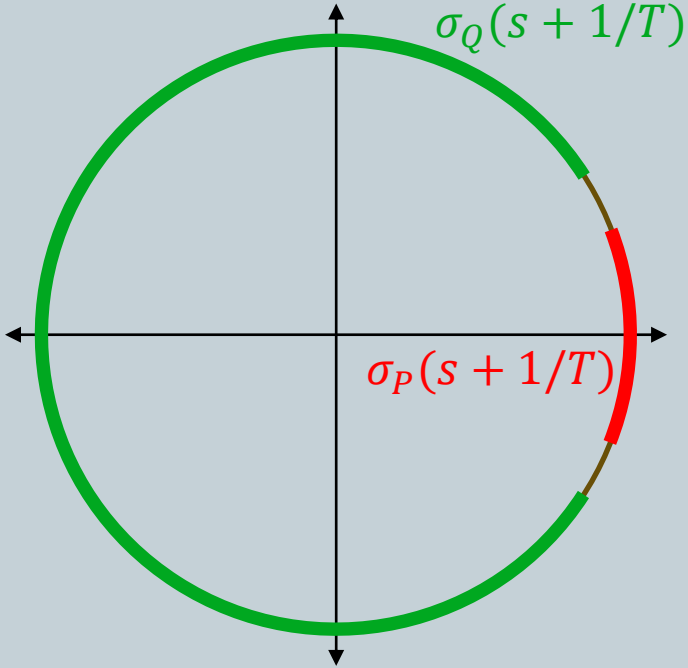

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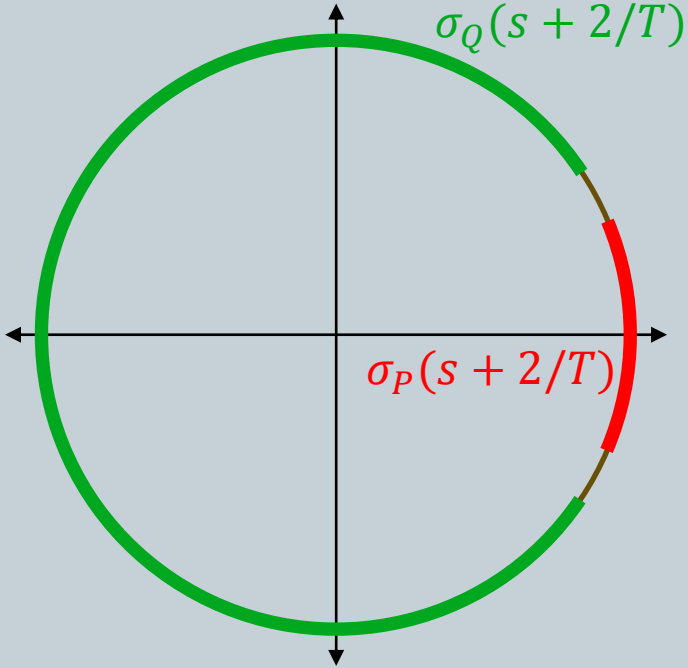
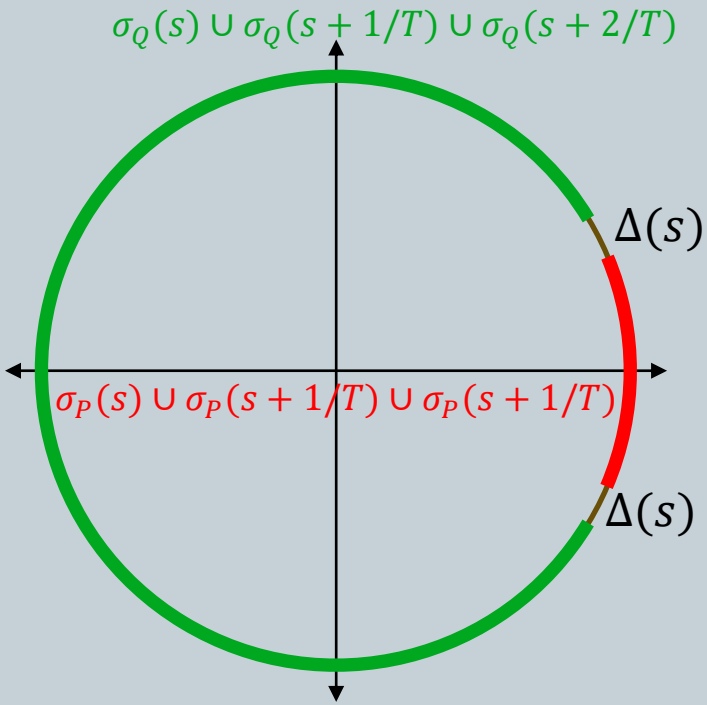


Multistep gap

- Eigenvalues are on circle in complex plane.
- Gaps are needed on both sides, $\Delta_0(s)$.
- Regions must not cross over between steps.
- Consider unified regions between three successive steps.
- We call gap between unified regions $\Delta(s)$.
- To simplify expressions need minimum over neighbouring steps too:

$$\breve{\Delta}(s) = \min(\Delta(s - 1/T), \Delta(s), \Delta(s + 1/T))$$



Discrete adiabatic theorem

The error in the adiabatic evolution is bounded as

$$\left\|U_T(s) - U_T^A(s)\right\| \leq \frac{12\hat{c}_1(0)}{T\breve{\Delta}(0)^2} + \frac{12\hat{c}_1(s)}{T\breve{\Delta}(s)^2} + \frac{6\hat{c}_1(s)}{T\breve{\Delta}(s)}$$
$$+305\sum_{n=1}^{sT-1}\frac{\hat{c}_1(n/T)^2}{T^2\breve{\Delta}(n/T)^3} + 44\sum_{n=0}^{sT-1}\frac{\hat{c}_1(n/T)^2}{T^2\breve{\Delta}(n/T)^2} + 32\sum_{n=1}^{sT-1}\frac{\hat{c}_2(n/T)}{T^2\breve{\Delta}(n/T)^2}$$

- $\hat{c}_1$ – analogous to first derivative in continuous adiabatic theorem
- $\hat{c}_2$ – analogous to second derivative in continuous adiabatic theorem

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- $\hat{c}_1$ – analogous to first derivative in continuous adiabatic theorem
- $\hat{c}_2$ – analogous to second derivative in continuous adiabatic theorem

$$\frac{\left\|H^{(1)}(0)\right\|}{T\Delta(0)^2} + \frac{\left\|H^{(1)}(s)\right\|}{T\Delta(s)^2} + \frac{1}{T}\int_0^s \left(\frac{\left\|H^{(1)}(s')\right\|^2}{\Delta(s')^3} + \frac{\left\|H^{(2)}(s')\right\|}{\Delta(s')^2}\right) ds'$$

Method to prove theorem

- "Wave operator" describes difference from ideal adiabatic evolution:

$$\Omega_T(s) = U_T^{A\dagger}(s)U_T(s)$$

- Error can be considered entirely in terms of wave operator:

$$\left\|U_T(s) - U_T^A(s)\right\| = \|\Omega_T(s) - I\|$$

- The "ripple operator" describes the change in the wave operator:

$$\Theta_T(s) = \Omega_T(s + 1/T)\Omega_T^\dagger(s)$$

- The "kernel function" describes how close this is to the identity:

$$K_T(s) = T(I - \Theta_T(s))$$

- Write wave operator in terms of these as "Volterra equation"

$$\Omega_T(n/T) = I - \frac{1}{T}\sum_{m=0}^{n-1} K_T(m/T)\Omega_T(m/T)$$

A. Dranov, J. Kellendonk, R. Seiler, Journal of Mathematical Physics **39**, 1340 (1998).

Diagonal vs off-diagonal terms

- Resolve identity as $I = P_0 + Q_0$ with initial projections $P_0 = P_T(0)$, $Q_0 = Q_T(0)$.
- Introduce to Volterra equation so

$$\|\Omega_T(s) - I\| = \frac{1}{T}\left\|\sum_{m=0}^{n-1}(P_0 + Q_0)K_T(m/T)(P_0 + Q_0)\Omega_T(m/T)\right\|$$

Diagonal vs off-diagonal terms

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$$\leq \frac{1}{T}\left\|\sum_{m=0}^{n-1}P_0K_T(m/T)P_0\Omega_T(m/T)\right\| + \frac{1}{T}\left\|\sum_{m=0}^{n-1}Q_0K_T(m/T)Q_0\Omega_T(m/T)\right\| \quad \text{“diagonal”}$$

$$+\frac{1}{T}\left\|\sum_{m=0}^{n-1}P_0K_T(m/T)Q_0\Omega_T(m/T)\right\| + \frac{1}{T}\left\|\sum_{m=0}^{n-1}Q_0K_T(m/T)P_0\Omega_T(m/T)\right\|$$

“off-diagonal”

Summation by parts formula

- Off-diagonal term can be rewritten as, with $V_T(s) = W_T^A(s)W_T^\dagger(s)$,

$$\sum_{n=1}^{sT} Q_0 U_T^{A\dagger}\left(\frac{n}{T}\right)\left(I - V_T^\dagger\left(\frac{n-1}{T}\right)\right)U_T^A\left(\frac{n}{T}\right)P_0\Omega_T\left(\frac{n-1}{T}\right)$$

- Summation by parts formula gives

$$\sum_{n=1}^{l} Q_0\, U_T^{A\dagger}\left(\frac{n}{T}\right)X\left(\frac{n}{T}\right)U_T^A\left(\frac{n}{T}\right)P_0 Y\left(\frac{n}{T}\right) = B - \frac{1}{T}S$$

- B is "boundary term"
- S is "sum term" – it still involves a sum, but is easier to bound.
- Requires operator that can only be described by contour integral:

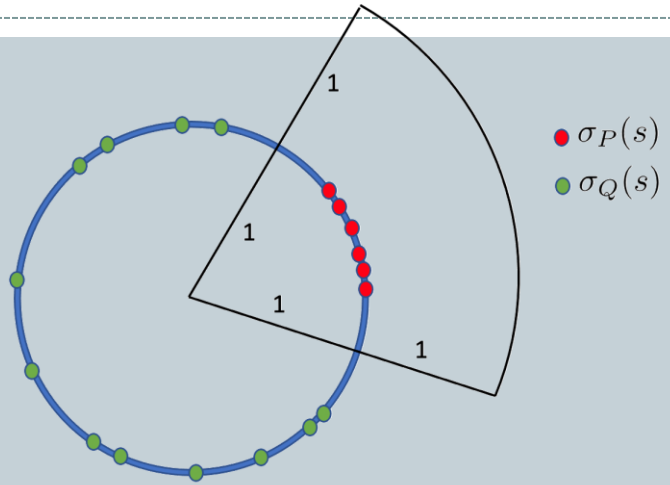
$$\tilde{X}(s) = -\frac{1}{2\pi i}\oint_{\Gamma_T(s)} R_T(s,z)X(s)R_T(s,z)dz\,, \qquad R_T(s,z) = (W_T(s) - zI)^{-1}$$

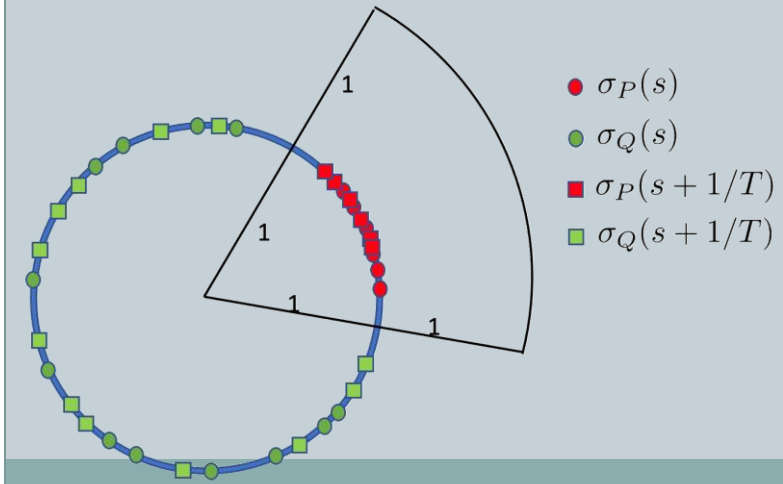
Contour integrals for bounds

- Projector can be given by contour integral:

$$P_T(s) = \frac{1}{2\pi i} \oint_{\Gamma_T(s)} R_T(s,z)dz$$

$$R_T(s,z) = (W_T(s) - zI)^{-1}$$





- Bound on difference of projectors needs contour threaded between eigenvalues for multiple steps.

$$\|DP_T(s)\| \leq \frac{2c_1(s)}{T\Delta_1(s)}$$

Theorem for $p = 1.5$

- For A positive-definite & Hermitian, bound all terms from theorem as follows:

$$\frac{\hat{c}_1(0)}{T\breve{\Delta}(0)^2} = \frac{4\sqrt{\kappa}}{T} + O\left(\frac{\kappa}{T^2}\right) \qquad \frac{\hat{c}_1(1)}{T\breve{\Delta}(1)^2} = \frac{4\kappa}{T} + O\left(\frac{\kappa}{T^2}\right) \qquad \frac{\hat{c}_1(1)}{T\breve{\Delta}(1)} = \frac{4}{T} + O\left(\frac{1}{T^2}\right)$$

$$\sum_{n=1}^{T-1} \frac{\hat{c}_1(n/T)^2}{T^2\breve{\Delta}(n/T)^3} = \frac{16\kappa}{T} + O\left(\frac{\kappa^{3/2}}{T^2}\right) \qquad \sum_{n=0}^{T-1} \frac{\hat{c}_1(n/T)^2}{T^3\breve{\Delta}(n/T)^3} \leq \frac{16}{T} + O\left(\frac{\kappa}{T^2}\right) \qquad \sum_{n=1}^{T-1} \frac{\hat{c}_2(n/T)}{T^2\breve{\Delta}(n/T)^3} \leq \frac{22\kappa}{T} + O\left(\frac{\kappa^{3/2}}{T^2}\right)$$

- Overall inequality becomes

$$\left\|U_T(s) - U_T^A(s)\right\| \leq 5632\frac{\kappa}{T} + O\left(\frac{\sqrt{\kappa}}{T}\right)$$

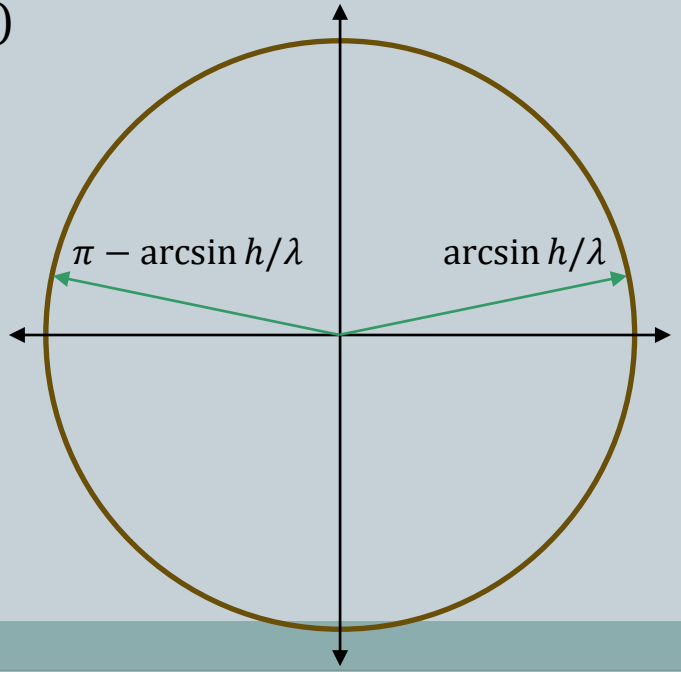
- For general A, gap has factor of $1/\sqrt{2}$ – replace $\breve{\Delta}$ with $\breve{\Delta}/\sqrt{2}$.
- Updated inequality is

$$\left\|U_T(s) - U_T^A(s)\right\| \leq 15307\frac{\kappa}{T} + O\left(\frac{\sqrt{\kappa}}{T}\right)$$

Multiple eigenvalues problem

- The discrete adiabatic theorem is for target eigenspace being in one region.
- For quantum walk zero eigenvalue of Hamiltonian maps to ± 1 for walk operator; eigenstates ($|k\rangle$ is eigenstate on system)

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle|k\rangle \pm i|0k^{\perp}\rangle)$$



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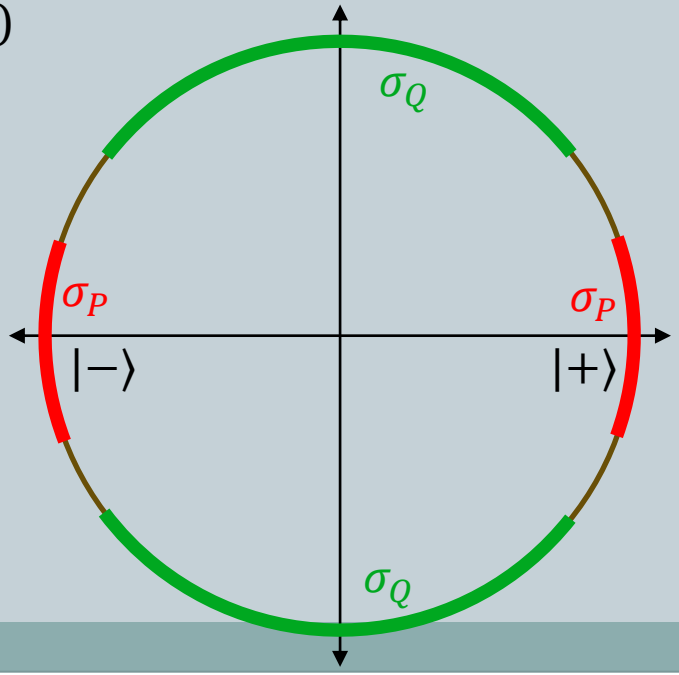
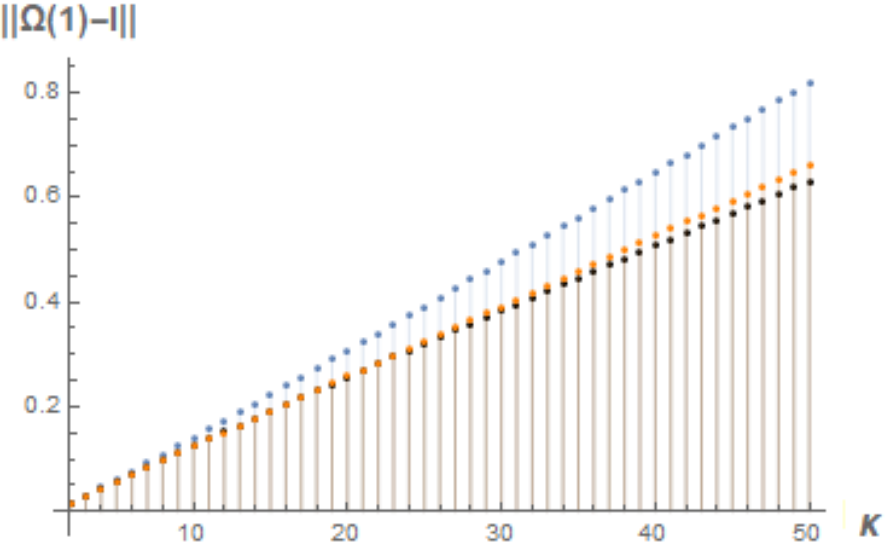
$$|0\rangle|k\rangle = \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$$

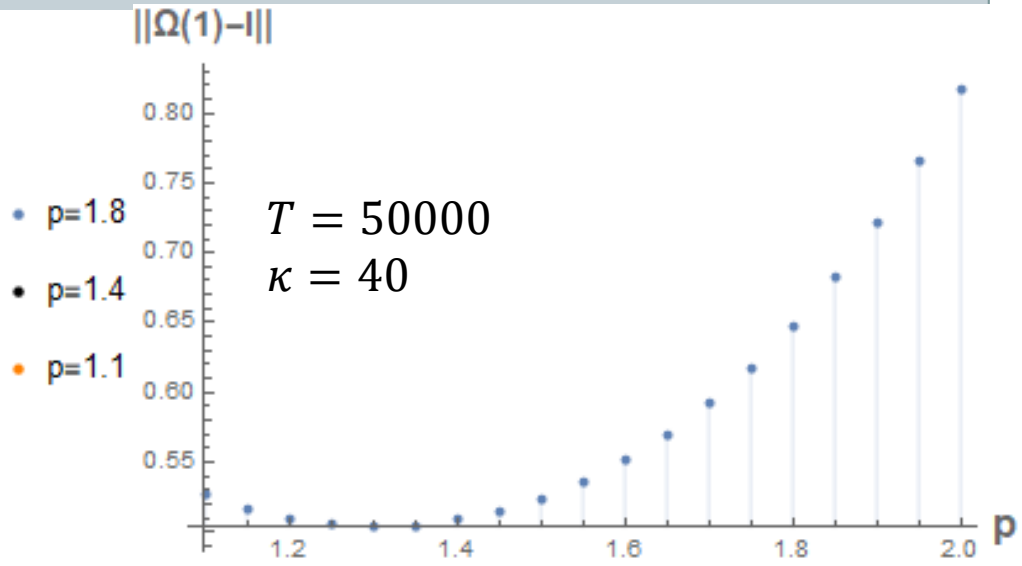
- We show phase between $|+\rangle$ and $|-\rangle$ is preserved.
- We show orthogonal degenerate eigenstates do not cross. $\begin{pmatrix} A(f)^{-1}\boldsymbol{b} \\ 0 \end{pmatrix}$ vs $\begin{pmatrix} 0 \\ \boldsymbol{b} \end{pmatrix}$



Numerical testing for constant factor

- Theorems for QLSP use many simplifications with loose inequalities.
- Numerically test with the complete discrete adiabatic theorem.
- $\|\Omega(1) - I\| \approx 1/2$, and $\kappa/T = 40/50000 = 1/1250$, so $\|\Omega(1) - I\| \geq 625\kappa/T$.
- About 9 times better than theorem.





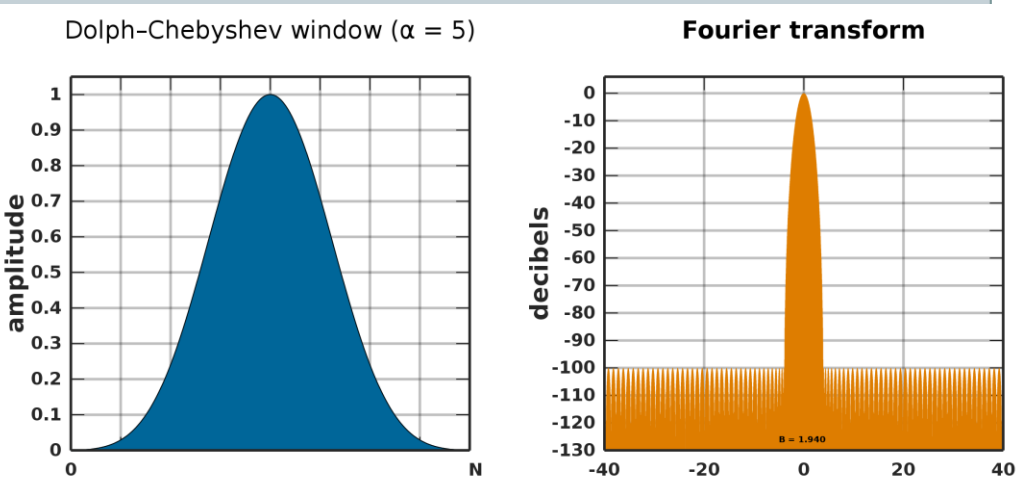
Filtering solution

- To obtain solution with precision ϵ need to filter the eigenstate.
- Lin & Tong use quantum signal processing – drawback is computing rotation angles.
- We instead apply linear combination of unitaries $\sum_j w_j W_T^j$.
- LCU maps superposition of eigenstates as

$$\sum_k \psi_k |k\rangle \mapsto \sum_k \tilde{w}(\phi_k)\psi_k |k\rangle ,$$

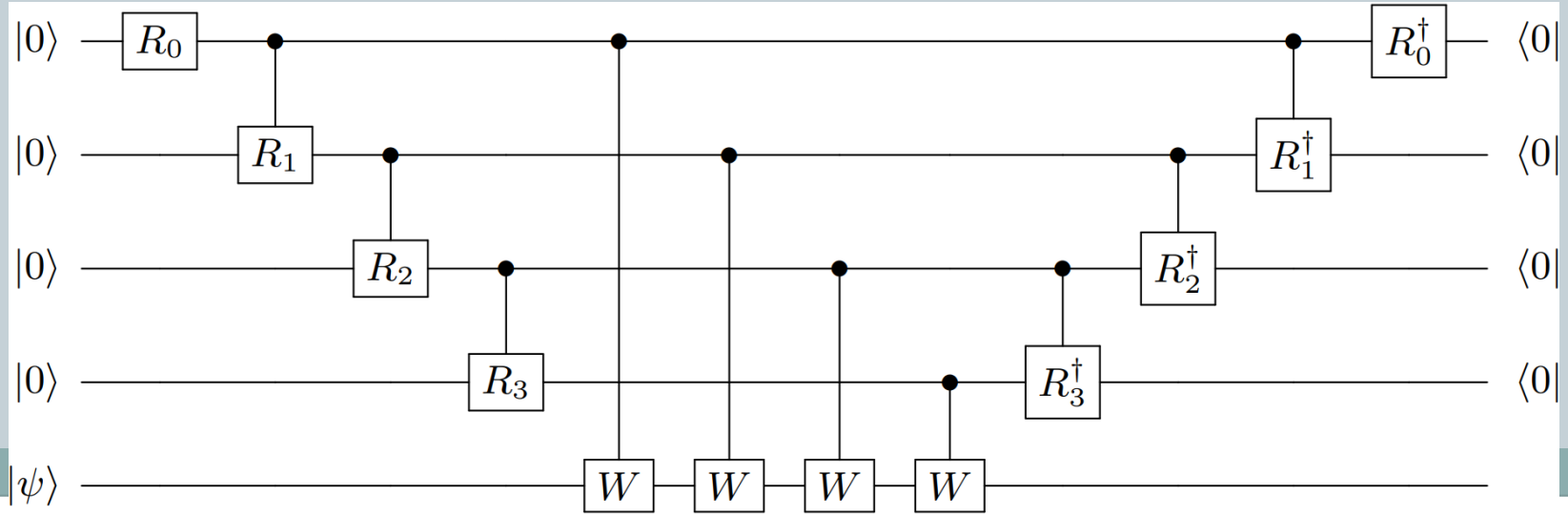
$$\tilde{w}(\phi) = \frac{1}{\sum_j w_j} \sum_j w_j e^{ij\phi}$$

- Error goes like $\tilde{w}(\phi)$ for incorrect phases – minimised for Dolph-Chebyshev window.



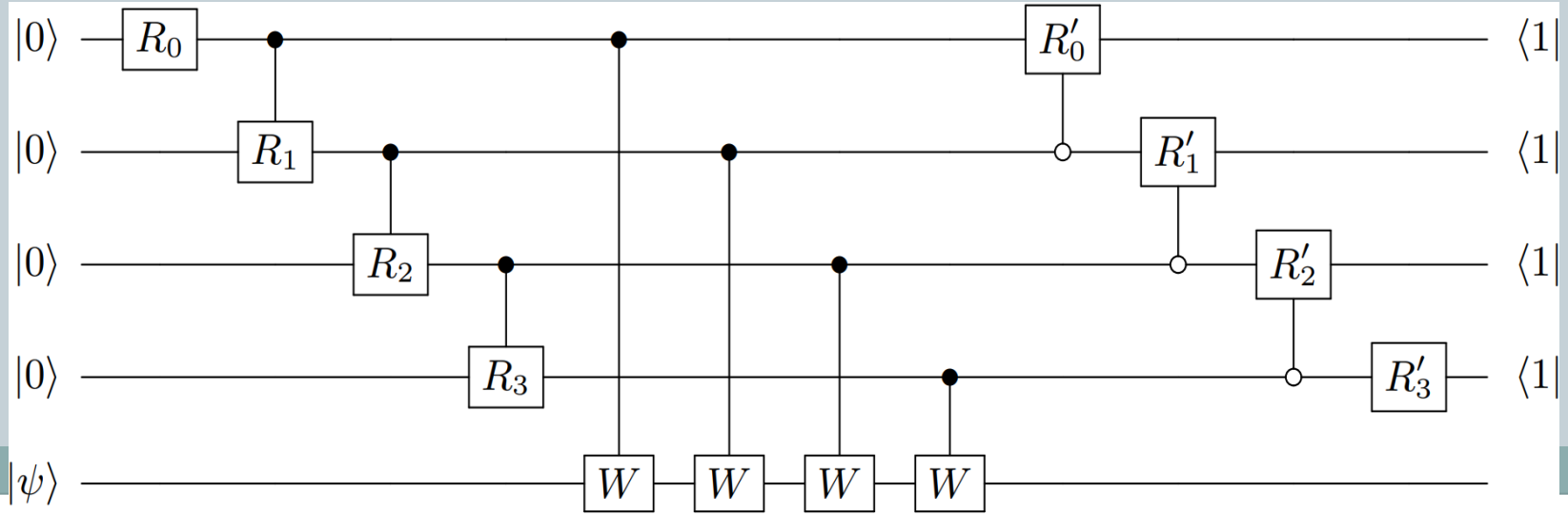
LCU with two qubits

- Normally LCU would require a large number of qubits for control.
- A single ancilla qubit is given as major advantage of quantum signal processing.
- We can do LCU using just two ancilla qubits.
- First consider control state in unary:



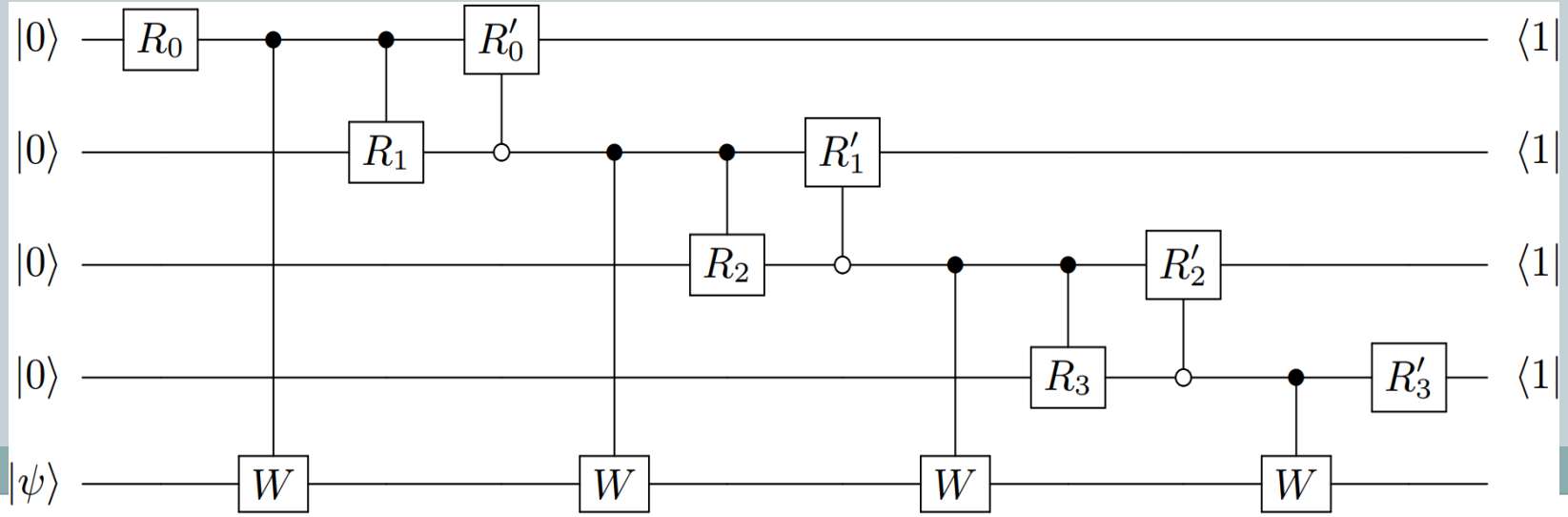
LCU with two qubits

- Normally LCU would require a large number of qubits for control.
- A single ancilla qubit is given as major advantage of quantum signal processing.
- We can do LCU using just two ancilla qubits.
- Switch sequence of controlled operations for inverse preparation:



LCU with two qubits

- Normally LCU would require a large number of qubits for control.
- A single ancilla qubit is given as major advantage of quantum signal processing.
- We can do LCU using just two ancilla qubits.
- Shift order of operations so we use two qubits at a time:



Putting it all together

- We can use these results for solving the QLSP with complexity

$$O(\kappa \log(1/\epsilon))$$

  in terms of calls to a block encoding to A, as well as preparation of $|b\rangle$.
- The procedure is:
  1. Construct a quantum walk step from the block encoding of A.
  2. Use the discrete adiabatic theorem to solve for $|A^{-1}b\rangle$ with fixed precision $1/2$. Complexity is $O(\kappa)$.
  3. Filter solution using LCU; complexity is $\kappa \log(2/\epsilon)$ steps of walk.
  4. In case of failure, repeat discrete adiabatic procedure and filtering. Average of two attempts needed.

Lower bound

- Kothari and Harrow have proven lower bound for sparse matrices (unpublished)

$$\Omega\left(\sqrt{d}\kappa \log(1/\epsilon)\right)$$

- Our complexity for general block-encoded matrices is

$$\Omega(\kappa \log(1/\epsilon))$$

- For sparse matrices, this would need to be multiplied by complexity of block-encoding sparse matrices, typically d.
- Low has demonstrated $\sqrt{d}$ scaling for Hamiltonian simulation up to logarithmic factors (STOC 2019).
- Similar approach here would make scaling no longer optimal in κ and ϵ.

Conclusions

- Fastest possible quantum algorithm for the quantum linear systems problem in terms of κ and ϵ (we don't consider sparsity d).
- Lower bound of Kothari and Harrow is $\Omega\left(\sqrt{d}\kappa \log(1/\epsilon)\right)$.
- Our discrete adiabatic algorithm with qubitisation gives speedup for all adiabatic algorithms too.
- Method for LCU with two ancilla qubits can be used generally.

Future work:

- There could be scope for improving constant factors.
- How to achieve optimal scaling in d at the same time is open problem.

P. C. S. Costa, D. An, Y. R. Sanders, Y. Su, R. Babbush, D. W. Berry, 2111.08152 (2021).