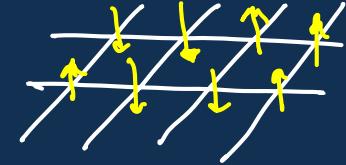


Intro to Quantum Gibbs Sampling: Algorithmic Ingredients.

Sandy Irani
UC Irvine.

Classical Gibbs Distribution



Ex:

Classical local Hamiltonian

Ising

$$-\sum_{\langle i,j \rangle} z_i \cdot z_j$$

Eigenstates : $S_n = \{0,1\}^n$

Goal is to sample from

$$P(x) = \frac{e^{-\beta E_x}}{Z}, \quad Z = \sum_x e^{-\beta E_x}$$

Discrete Time Markov Chain

Random walk on S_n

$$P(X_t=j | X_{t-1}=i) = P_{ij}$$

$X_t \in S_n$ location at time t.

P: stochastic matrix.

Classical Metropolis Algorithm

Set of jump operators A^a

A^a selected with probability $p(a)$.

Ex: flip a randomly chosen spin.

Current slate = x .

- Pick A^a w.p. $p(a)$.
 $\beta = O(\text{poly}(n))$
- Apply A^a to $x \rightarrow y$.
- Accept move w.p. $\min\{1, \exp(-\beta(E_y - E_x))\}$
 $\gamma_f(E_x, E_y)$
- If reject, go back to x .

Classical Metropolis Algorithm

Gibbs distribution π_p is a fixed point
of Metropolis

Detailed balance :

$$e^{-\beta E_x} \gamma_p(E_x - E_y) = e^{-\beta E_y} \gamma_p(E_y - E_x)$$

If jump operators mix enough then
the fixed point is unique.

Quantum Gibbs Sampling

Quantum Hamiltonian H

Eigenstates $\{|q_j\rangle\}_j$ Eigenvalues $\{E_j\}_j$

Prepare distribution: $|q_i\rangle$ w.p. $e^{-\beta E_j}/Z$.

Mixed State:

$$\rho_\beta = \sum e^{-\beta E_j} |q_j\rangle \langle q_j| = \frac{\exp(-\beta H)}{\text{Tr}[\exp(-\beta H)]}$$

Quantum Gibbs Sampling

Challenges:

- (1) Given eigenstate $|4j\rangle$ cannot calculate E_j exactly
- (2) Rejection procedure requires backing up after a quantum measurement.

Classical Continuous-time Markov Chains

State $X(t)$ is a function of $t \in \mathbb{R}^{>0}$

Markov:

$$\Pr(X(t+s) = j \mid X(s) = i) \\ = \Pr(X(t+s) = j \mid X(s) = i, \text{ events before } t-s)$$

Time-Homogeneous

$$\Pr(X(t+s) = j \mid X(s) = i) = P_{ij}(t)$$

independent
of
start time s .

Classical Continuous-time Markov Chains

One way to specify
cont-time M.c. $P_{ij}(t)$ for all t .

Instead use generator matrix Q :

$$Q \triangleq \lim_{\Delta t \rightarrow 0} \frac{P(\Delta t) - I}{\Delta t}$$

Properties of Q :

- $P_{ij} \geq 0$ if $i \neq j$.
- $P_{ii} \leq 0$
- Rows sum to 0.

Classical Continuous-time Markov Chains

$$\frac{dP}{dt} = P \cdot Q$$

$$\frac{d\pi}{dt} = \pi Q$$

π : distribution over states.

$$\Rightarrow P(t) = e^{Qt} = \sum_{n=0}^{\infty} \frac{1}{n!} Q^n t^n$$

π_0 is a fixed point if

$$\pi_0 = \pi_0 P(t) \quad \forall t$$



$$\pi_0 Q = 0.$$

From
Lecture Notes by
Miranda
Holmes-Cerfon
(UBC)

Classical Continuous-time Markov Chains

$$Q = \begin{bmatrix} & & \\ & \geq 0 & \\ & & \end{bmatrix}$$

Classical Continuous - time Markov Chains

$$Q = \begin{bmatrix} q_{i1} & q_{i2} & \dots & \dots & q_{id} \end{bmatrix}$$

$q_{ii} = - \sum_{j \neq i} q_{ij}$

For any π

$$\sum_i \frac{d\pi_i}{dt} = 0 = \pi Q \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}$$

Generator for Classical Continuous Metropolis:

Jump operators A^a non-negative matrices (not nec. stoch.)

$\sum_a p(a) A^a$ is symmetric

$$Q_{ij}^{\pm} = \sum_a p(a) \left[\underbrace{\gamma_p(E_j - E_i)}_{\text{accept}} A_{ij}^a - \delta_{ij} \underbrace{\sum_{k \neq i} \gamma_p(E_k - E_i) A_{ki}^a}_{\text{reject.}} \right]$$

$$\pi_p \cdot Q_{ij}^{\pm} = 0$$

Evolution of Closed Quantum Systems.

Hamiltonian H

Schrödinger's Equation

$$\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle$$

$$|\psi(t)\rangle = e^{-iHt} |\psi(0)\rangle$$

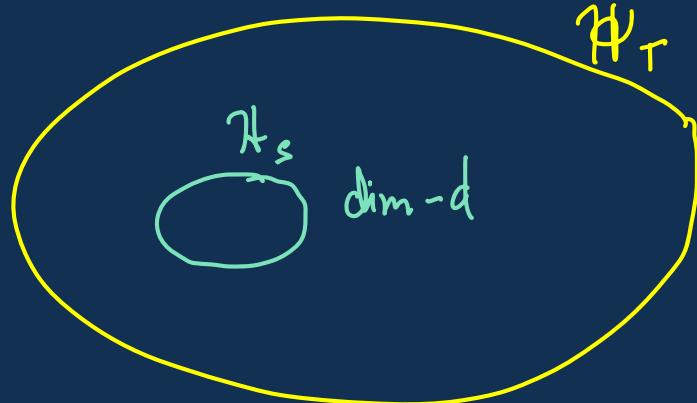
Simulation in QC

[Abrams + Lloyd '97]

Generalize : Classical \rightarrow Quantum
Quantum Closed \rightarrow Quantum Open } Lindbladian.

Closed Quantum Systems

Open



$$\dim \mathcal{H}_T = D.$$

Pure state $|\psi_T\rangle$

D -dim vector $\langle\psi_T|\psi_T\rangle=1$

↓ trace out $T-S$

Ensemble of states

$$\{ |\psi_j\rangle, p_j \} \quad |\psi_j\rangle \in \mathcal{H}_S.$$

$$P_S = \sum_j p_j |\psi_j\rangle \langle \psi_j|$$

{ density : positive operator
matrix $\text{Trce} = 1.$

A Bit About Mixed States (density matrices)

$$\rho = \sum p_i |\psi_i\rangle\langle\psi_i|$$

Unitary evolution $\rho \xrightarrow{U} U \rho U^*$

Schrödinger's Equation $\frac{d|\psi\rangle}{dt} = -iH|\psi\rangle$

$$\frac{d\rho}{dt} = -i(H\rho - \rho H) = -i[H, \rho]$$

$$[A, B] \triangleq AB - BA$$

Fock-Liouville

$$\rho \rightarrow |\rho\rangle \quad d^2 \times 1.$$

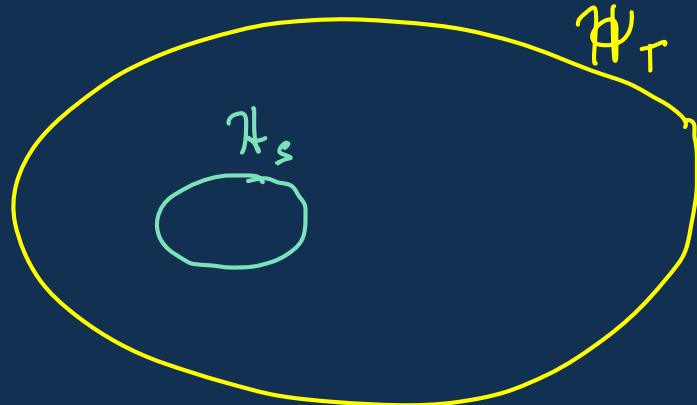
$$\text{Tr} [\phi^\dagger \rho] = \langle \phi | \rho \rangle$$

Linear op $\frac{1}{2}$ on ρ

$$\hat{\rho} |\rho\rangle$$

$$d^2 \times \overrightarrow{d^2}$$

Open Quantum Systems



Is there a linear map λ

$$\frac{d\rho}{dt} = \lambda\rho$$

$$V(t) = e^{iHt} \text{ for all } t ? \text{ (Not Always)}$$

Ref: A Short Intro to the Lindblad Master Equation, D. Manzano.

ρ_T evolves according to H_T .

$$\left| \psi(0) \right\rangle \xrightarrow{e^{-iH_T t}} \left| \psi(t) \right\rangle$$

\downarrow trace out $T-S$

$$\rho_0 \xrightarrow{V(t)} \rho_T$$

completely positive
trace-preserving map.
(CPTP)

What is the most general form for linear map \mathcal{L}

$$\frac{d}{dt} \rho = \mathcal{L} \rho$$



such that $V(t) = e^{2t}$ is CPTP?

If V is a linear map $B(H) \rightarrow B(H)$ Bounded lin ops
on H .

(1) V is completely positive iff $V(\rho) = \sum_i L_i \rho L_i^*$

(2) V is CPTP iff also $\sum_i L_i L_i^* = I$

Start with $V(t)$ is C.P. basis for ops.

$$\mathcal{L} = \lim_{\Delta t \rightarrow 0} \frac{V(\Delta t) - I}{\Delta t} \quad \frac{1}{\Delta t} I = K_1, \dots, K_d$$

$$Tr(K_i^+ K_j) = 0 \quad i \neq j.$$

$$\Rightarrow Tr(K_j) = 0 \quad j \leq z.$$

$$V(\Delta t) \rho = c(\Delta t)_{ij} K_i \rho K_j^+$$

$$\mathcal{L} \rho = \sum_{i,j=2}^{d^2} g_{ij} K_i \rho K_j^+ + \underbrace{\sum_{i=2}^{d^2} g_{i,1} K_i \rho}_{G \rho} + \underbrace{\sum_{j=2}^{d^2} g_{1,j} \rho K_j^+}_{\rho G^+} + g_{1,1} I$$

$$\begin{aligned}
 \mathcal{L}\rho &= \sum_{i,j=2}^{d^2} g_{ij} K_i \rho K_j^\dagger + \underbrace{\sum_{i=2}^{d^2} g_{i,1} K_i \rho}_{G\rho} + \underbrace{\sum_{j=2}^{d^2} g_{1,j} \rho K_j^\dagger}_{\rho G^\dagger} + g_{1,1} I \\
 &= \underbrace{\sum_{i,j=2}^{d^2} g_{ij} K_i \rho K_j^\dagger}_{\text{Trace} = 0} + F\rho + \rho F - iH\rho + i\rho H \\
 &\quad - i[H, \rho].
 \end{aligned}$$

$G = F - iH$
 $\begin{matrix} \overline{F} \\ \downarrow \end{matrix}$ anti-herm. $\begin{matrix} \overline{H} \\ \downarrow \end{matrix}$ herm.

Apply trace-preserving condition

$$D = \text{Tr} \left[\frac{d\rho}{dt} \right] = \text{Tr} [\mathcal{L}\rho] \quad F = -\frac{1}{2} \sum_{i,j=2}^{d^2} g_{ij} K_i K_j^\dagger$$

Lindbladian Master Equation

$$\begin{aligned}\{A, B\} &= AB + BA \\ [A, B] &= AB - BA\end{aligned}$$

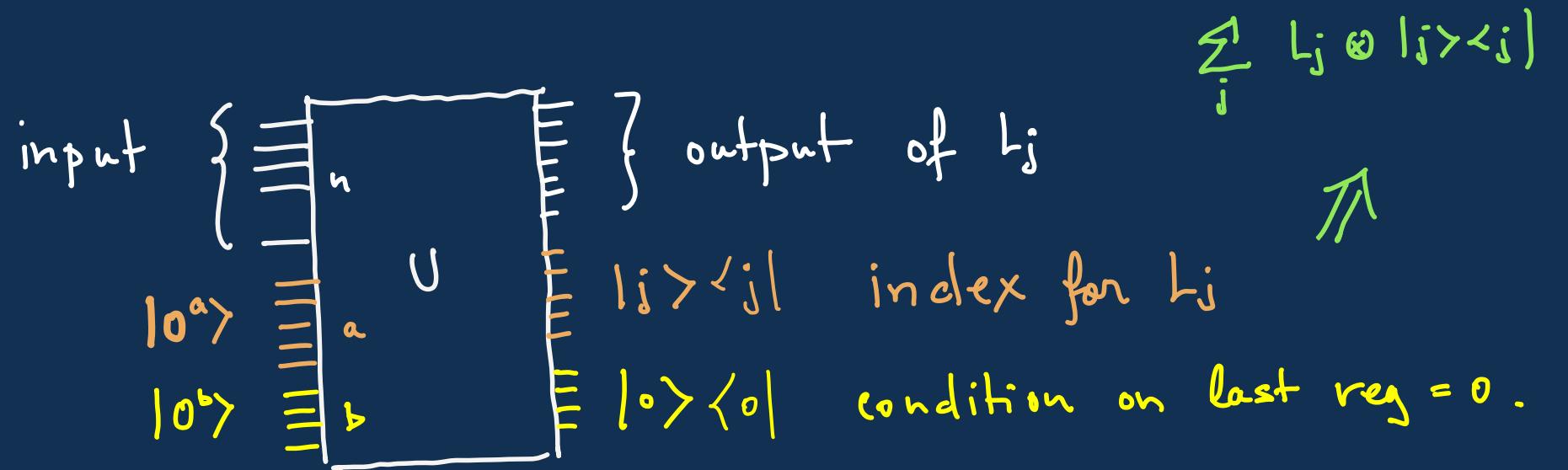
$$\dot{\rho} = \underbrace{\sum_k L_k \rho L_k^+}_{\text{"Accept"}} - \underbrace{\frac{1}{2} \{ L_k L_k^+, \rho \}}_{\text{"Reject"} \text{ to preserve trace.}} - i [H, \rho]$$

$$\text{w.l.o.g } \text{Tr}[L_k] = 0$$

Goal : Simulate e^{iHt}

How to specify $\{L_k\}_k$?

Block Encoding

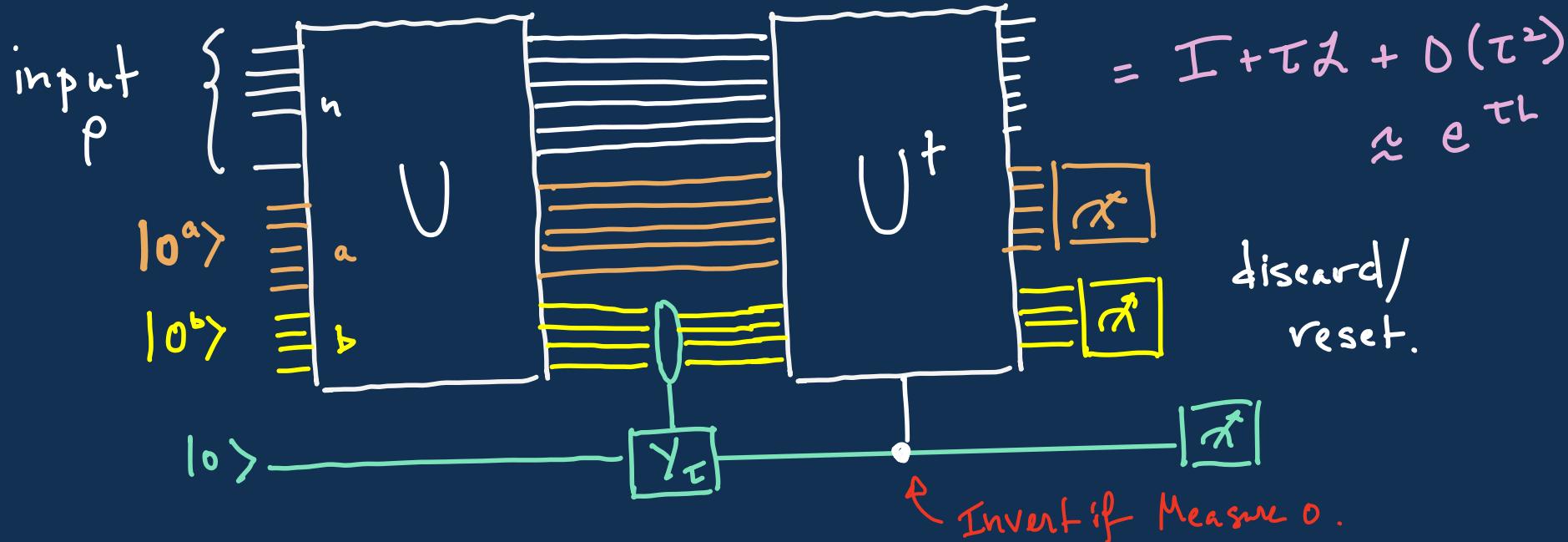


Given a block - encoding of $\{L_j\}$ can simulate $e^{t\hat{\mathcal{L}}}$

$$\mathcal{L}[\rho] = \sum_j L_j \rho L_j^\dagger - \frac{1}{2} L_j L_j^\dagger \rho - \frac{1}{2} \rho L_j L_j^\dagger$$

[Cleve-Wang '17, Li-Wang '22, CGKB '23]

Weak-Measurement Lindblad Implementation



$$Y_\tau = |0^b\rangle\langle 0^b| \otimes \begin{bmatrix} \sqrt{1-\tau} & -\sqrt{\tau} \\ \sqrt{\tau} & \sqrt{1-\tau} \end{bmatrix} + (I - |0^b\rangle\langle 0^b|) \otimes I.$$

Weak-Measurement Lindblad Implementation

Mixing time for 1: T_{mix}

steps for weak-meas. implementation:

$$T_{\text{mix}} / \tau$$

Total error: $\frac{T_{\text{mix}}}{\tau} \cdot \tau^2 = T_{\text{mix}} \tau$

Neglect $\tau = O(1/T_{\text{mix}})$ # steps $\sim (T_{\text{mix}})^2$

Quantum Phase Estimation

$$V |\Phi\rangle = e^{i\varphi 2\pi} |\Phi\rangle$$

Input: $|0^r\rangle |\Phi\rangle$ $2^r = R \sim \text{poly}(n)$.

$$\downarrow H^{\otimes n} \otimes I$$

$$\frac{1}{R} \sum_t |t\rangle |\Phi\rangle \quad t \in \{0, \dots, R-1\}$$

$$V = e^{iH/k}$$

$$k \geq \frac{\|H\|}{2\pi}$$

$$\downarrow |t\rangle \langle t| \otimes V^t$$

$$\frac{1}{\sqrt{R}} \sum_t e^{i\varphi 2\pi t} |t\rangle |\Phi\rangle$$

$$\downarrow QFT^+$$

$$|\tilde{\varphi} \cdot R\rangle |\Phi\rangle$$

$$H |\psi_j\rangle = E_j |\psi_j\rangle$$

$$V |\psi_j\rangle = e^{i\varphi_j 2\pi} |\psi_j\rangle$$

$$E_j = \varphi_j \cdot 2\pi \cdot k.$$

Quantum Phase Estimation

$$V |\Phi\rangle = e^{i\varphi 2\pi} |\Phi\rangle$$

Input: $|0^r\rangle |\Phi\rangle \quad 2^r = R$

$$\downarrow H^{\otimes n} \otimes I$$

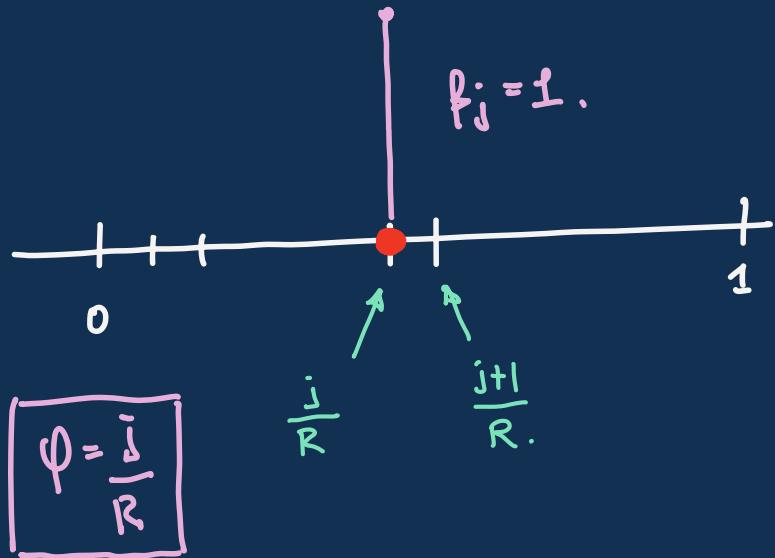
$$\frac{1}{\sqrt{R}} \sum_t |t\rangle |\Phi\rangle \quad t \in \{0, \dots, R-1\}$$

$$\downarrow |t\rangle \langle t| \otimes V^t$$

$$\frac{1}{\sqrt{R}} \sum_t e^{i\varphi 2\pi t} |t\rangle |\Phi\rangle$$

$$\downarrow QFT^+$$

$$|\tilde{\varphi} \cdot R\rangle |\Phi\rangle = \sum_j \beta_j |j\rangle |\Phi\rangle$$



Quantum Phase Estimation

$$V |\Phi\rangle = e^{i\varphi 2\pi} |\Phi\rangle$$

Input: $|0^r\rangle |\Phi\rangle$ $2^r = R$

$$\downarrow H^{\otimes n} \otimes I$$

$$\frac{1}{R} \sum_t |t\rangle |\Phi\rangle \quad t \in \{0, \dots, R-1\}$$

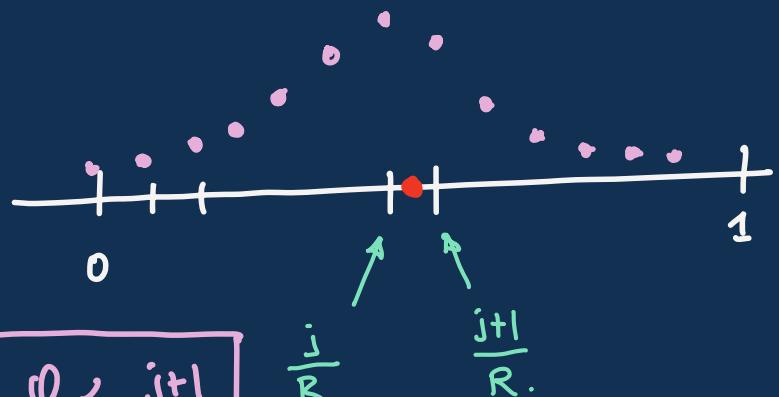
$$\downarrow |t\rangle \langle t| \otimes V^t$$

$$\frac{1}{\sqrt{R}} \sum_t e^{i\varphi 2\pi t} |t\rangle |\Phi\rangle$$

$$\downarrow QFT^+$$

$$|\tilde{\varphi} \cdot R\rangle |\Phi\rangle = \sum_j p_j |j\rangle |\Phi\rangle$$

$$\boxed{\frac{j}{R} \leq \varphi < \frac{j+1}{R}}$$



-
- ① Precision $R \sim \text{poly}$
 - ② Non-deterministic.

Quantum Phase Estimation

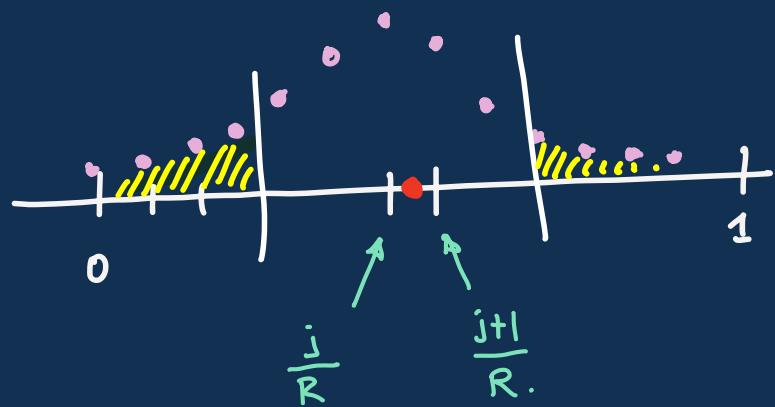
$$V |\Phi\rangle = e^{i\varphi 2\pi} |\Phi\rangle$$

Input: $|0^r\rangle |\Phi\rangle$ $2^r = R$

\Downarrow QPE.

$$|\tilde{\varphi} \cdot R\rangle |\Phi\rangle = \sum_j \beta_j |j\rangle |\Phi\rangle$$

$$\sum_{j:} |\beta_j|^2 \sim |\tilde{\varphi} \cdot R|^{-\alpha}$$

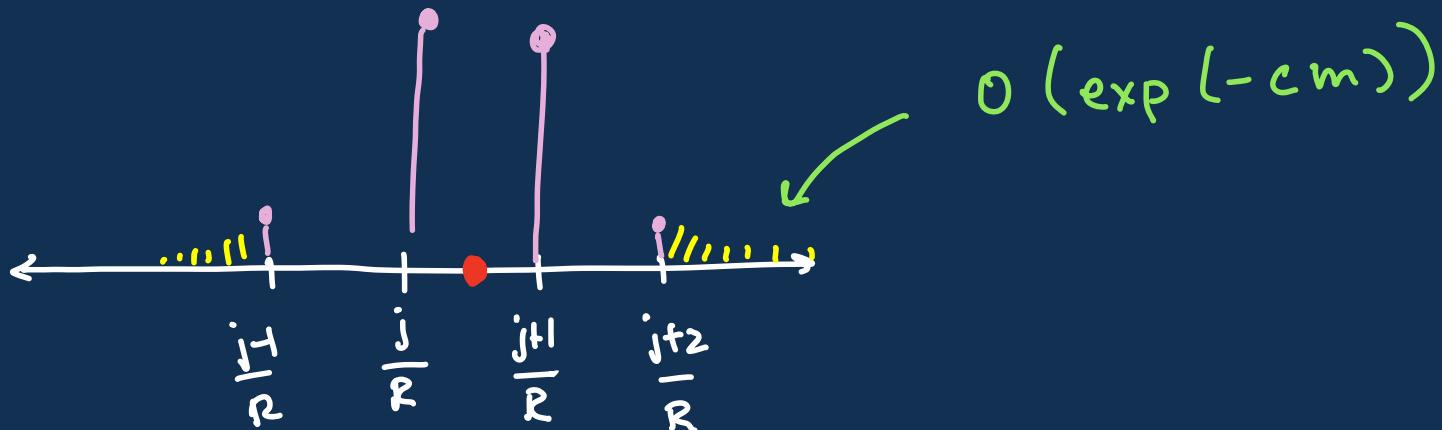


Boosted QPE : Median of multiple runs. [NC]

$$\underbrace{|0^r\rangle|0^r\rangle \dots |0^r\rangle|0^r\rangle}_{\otimes m} |\Phi\rangle \xrightarrow{\text{QPE}^{\otimes m}} |j_1\rangle \dots |j_m\rangle|0^r\rangle|\Phi\rangle$$

median

$$\longrightarrow |j_1\rangle \dots |j_m\rangle|\bar{j}\rangle|\Phi\rangle.$$



Boosting QPE by Filters

Input: $|0^r\rangle |\Phi\rangle \quad 2^r = R$

$$\downarrow H^{\otimes n} \otimes I$$

$$\frac{1}{\sqrt{R}} \sum_t |t\rangle |\Phi\rangle \quad t \in \{0, \dots, R-1\}$$

$\left. \begin{array}{c} \text{prepare} \\ \text{filter.} \end{array} \right\}$

$$\downarrow |t\rangle \langle t| \otimes V^t$$

$$\frac{1}{\sqrt{R}} \sum_t e^{i\Phi 2\pi t} |t\rangle |\Phi\rangle$$

$$\downarrow QFT^+$$

$$|\hat{\phi} \cdot R\rangle |\Phi\rangle$$

- Kaiser Filter for QPE

arXiv 2209.13581 v22

- Patel, Tan, Subasi, Sornborger
2024

CGKB: Gaussian Filter

$$|g_\sigma\rangle = \frac{1}{\sqrt{\text{Norm}}} \sum_t e^{-\frac{t^2}{4\sigma^2}} |t\rangle$$

$$QFT^+ |g_\sigma\rangle \approx |g_{w/\sigma}\rangle$$

Boosting QPE by Filters

$$|g_\sigma\rangle = \frac{1}{\sqrt{\text{Norm}}} \sum_t e^{-\frac{t^2}{4\sigma^2}} |t\rangle$$

Input: $|0^r\rangle |\Phi\rangle$ $2^r = R$



$$|g_\sigma\rangle |\Phi\rangle$$



$$|t\rangle \langle t| \otimes V^t$$

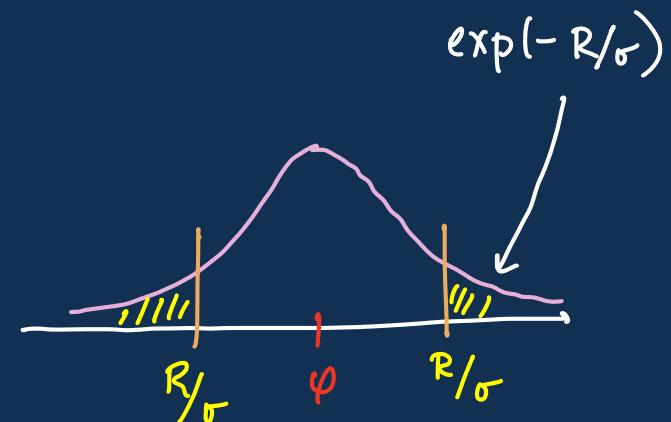
$$\frac{1}{\sqrt{\text{Norm}}} \sum_t e^{-\frac{t^2}{4\sigma^2}} e^{i\varphi 2\pi t} |t\rangle |\Phi\rangle$$

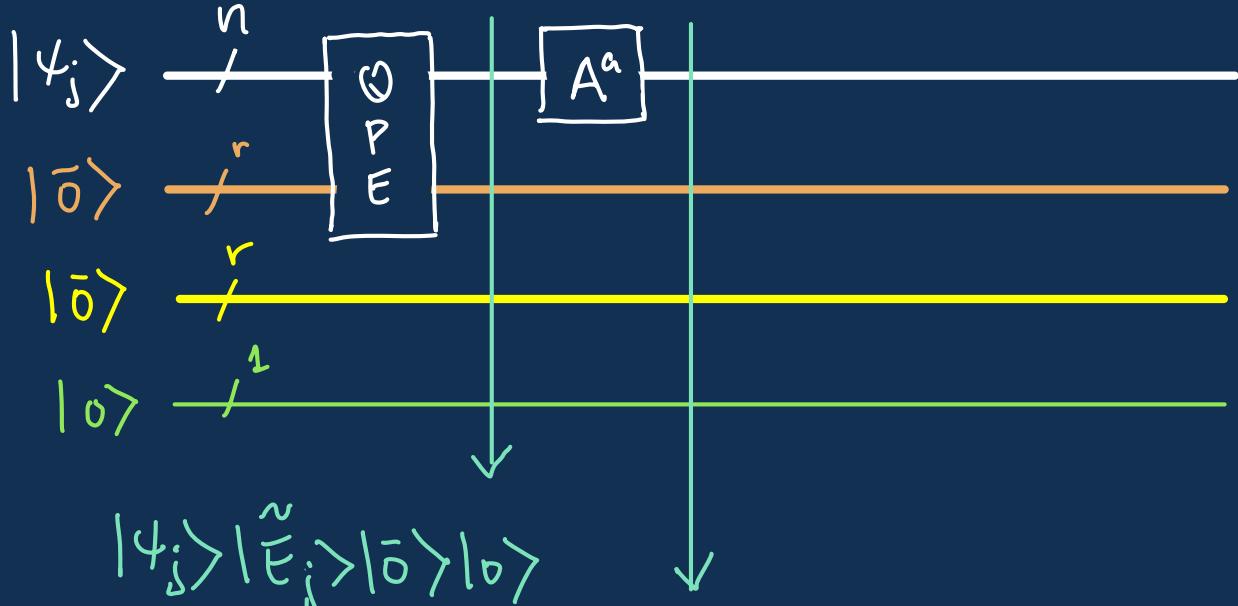


$$|\tilde{\phi} \cdot R\rangle |\Phi\rangle$$

$$|\tilde{\phi}R\rangle = |g_{R/\sigma}\rangle$$

shifted by $\varphi \cdot R$.

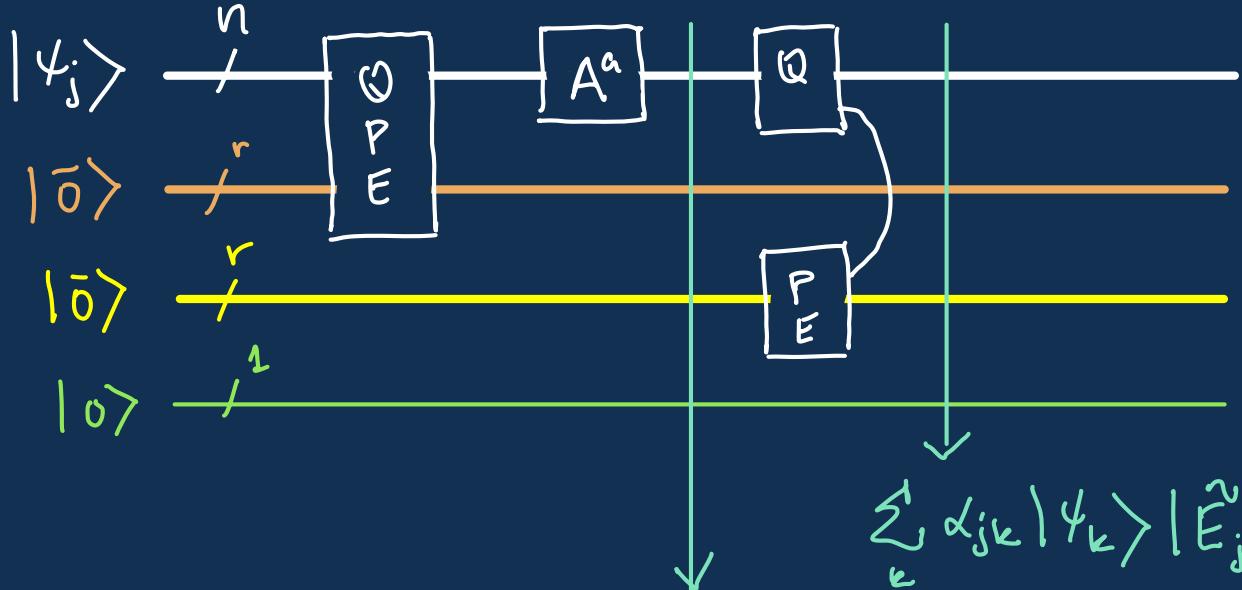




A Metropolis-like
Lindbladian

Select jump op A^a with prob. $p^{(a)}$.

$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\bar{0}\rangle |_0\rangle$$

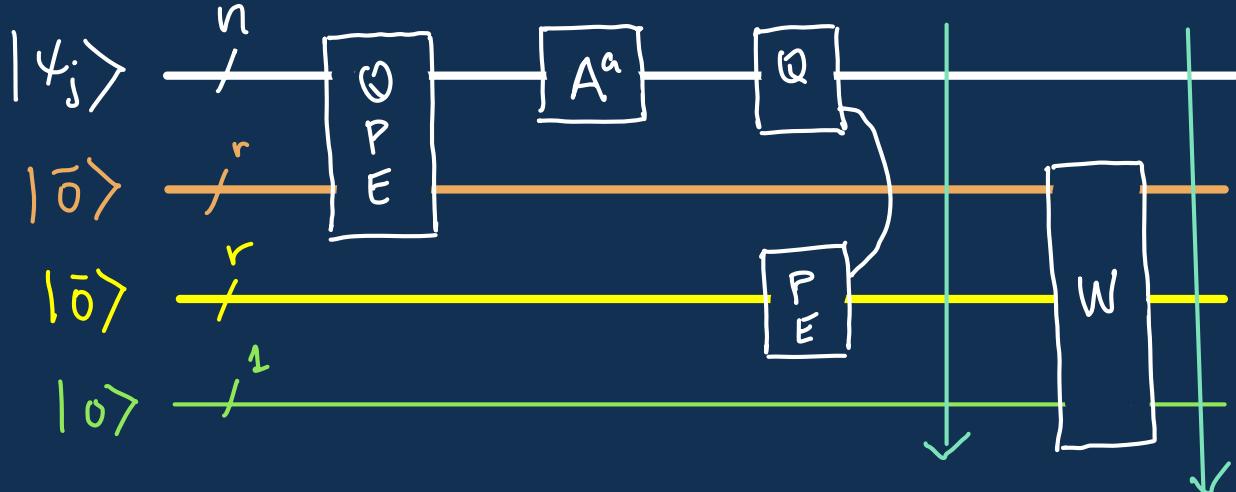


A Metropolis-like
Lindbladian

Select jump op A^a
with prob. $p^{(a)}$.

$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\tilde{E}_k\rangle |_0\rangle$$

$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_i\rangle |\tilde{E}_j\rangle |_0\rangle$$



$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\tilde{E}_k\rangle |_0\rangle$$

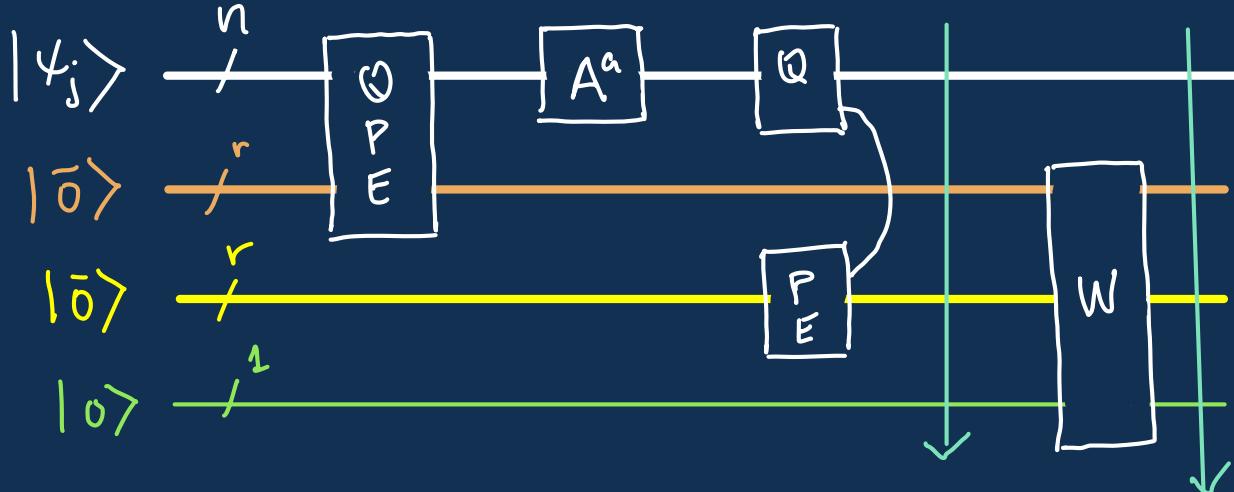
A Metropolis-like
Lindbladian

Select jump op A^a
with prob. $p^{(a)}$.

$$\gamma = \min\{1, \exp(-\beta(E_k - E_j))\}$$

$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\tilde{E}_k\rangle \otimes \frac{(\sqrt{1-\gamma}|_0\rangle + \sqrt{\gamma}|1\rangle)}{\sqrt{\gamma}}$$

Rej Acc



A Metropolis-like
Lindbladian

Select jump op A^a
with prob. $p^{(a)}$.

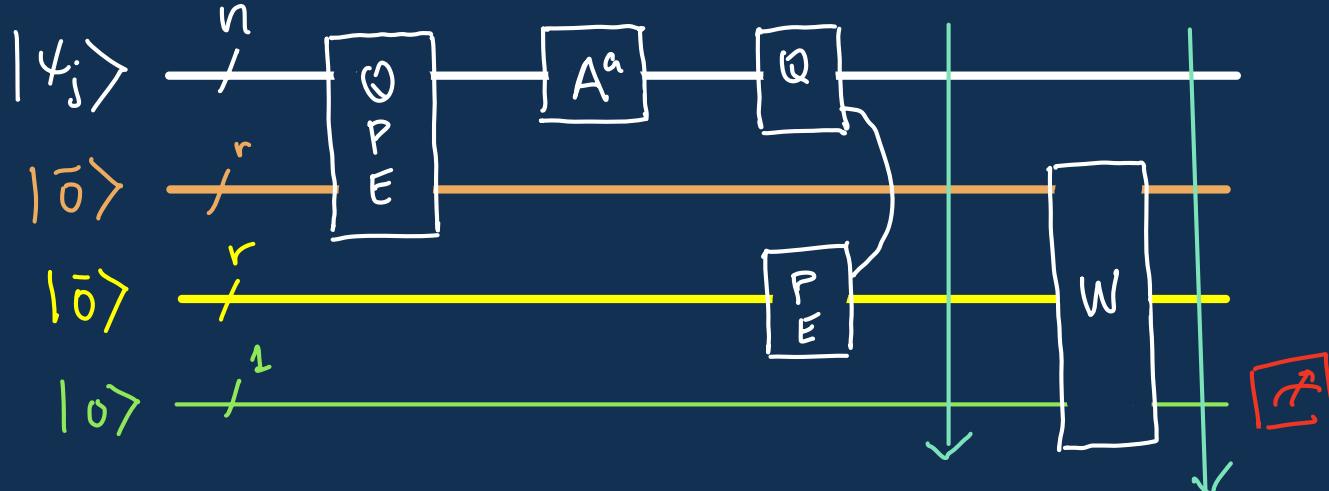
$$\gamma = \min\{1, \exp(-\beta(E_k - E_j))\}$$

$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\tilde{E}_k\rangle |_0\rangle$$

$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\tilde{E}_k\rangle \otimes \frac{(\sqrt{1-\gamma}|_0\rangle + \sqrt{\gamma}|_1\rangle)}{\sqrt{\gamma}}$$

$$W = \sum_{EE'} |EE'\rangle \langle EE'| \otimes \begin{bmatrix} \sqrt{1-\gamma_{EE'}} & -\sqrt{\gamma_{EE'}} \\ \sqrt{\gamma_{EE'}} & \sqrt{1-\gamma_{EE'}} \end{bmatrix}$$

T0VPV 2013



Meas 1: Accept.
Meas 0: Reject.

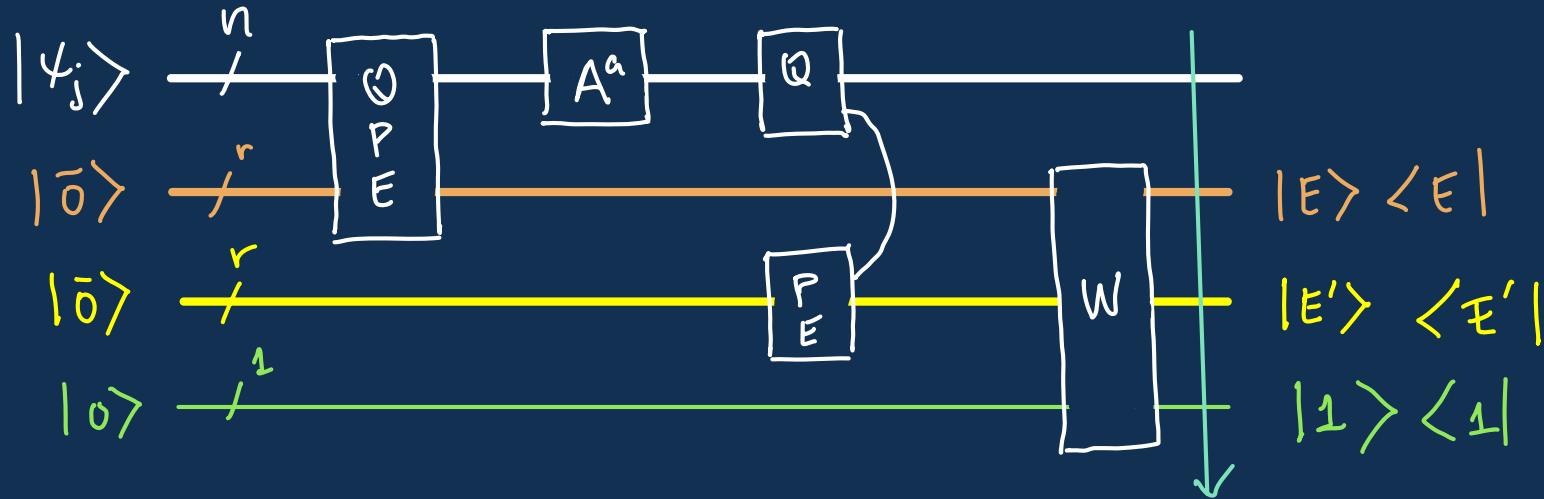
Back up via
Mariott-Watrous.

$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\tilde{E}_k\rangle |0\rangle$$

$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\tilde{E}_k\rangle \otimes \begin{cases} \sqrt{1-\gamma} |0\rangle + \sqrt{\gamma} |1\rangle & \text{Acc} \\ \sqrt{\gamma} |0\rangle - \sqrt{1-\gamma} |1\rangle & \text{Rej} \end{cases}$$

$$W = \sum_{EE'} |EE'\rangle \langle EE'| \otimes \begin{bmatrix} \sqrt{1-\gamma_{EE'}} & -\sqrt{\gamma_{EE'}} \\ \sqrt{\gamma_{EE'}} & \sqrt{1-\gamma_{EE'}} \end{bmatrix}$$

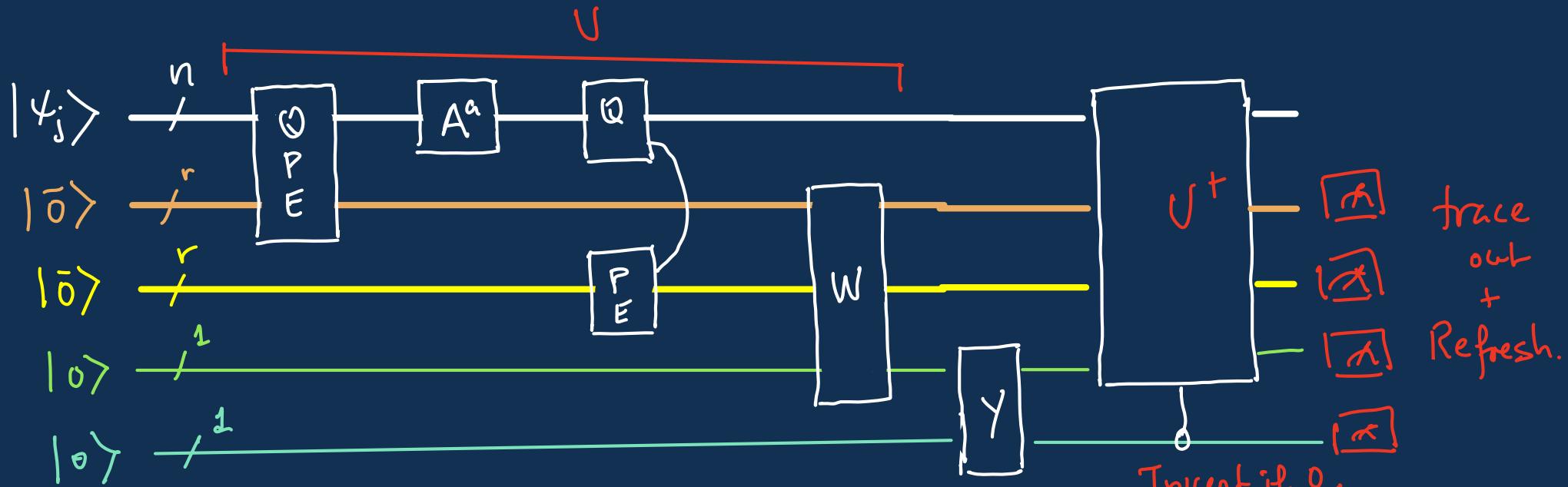
Define Lindbladian Operators $\{L_{EE'}\}_{EE'}$



$$\sum_k \alpha_{jk} |\psi_k\rangle |\tilde{E}_j\rangle |\tilde{E}_k\rangle \otimes \left(\frac{\sqrt{1-\gamma}}{\text{Rej}} |0\rangle + \frac{\sqrt{\gamma}}{\text{Acc}} |1\rangle \right)$$

Define Lindbladian Operators

$$\{L_{EE'}\}_{EE'} \Rightarrow \mathcal{L}$$



$$Y = \frac{|1\rangle\langle 1|}{A} \otimes \begin{bmatrix} \sqrt{1-\tau} & \sqrt{\tau} \\ \sqrt{\tau} & \sqrt{1-\tau} \end{bmatrix}$$

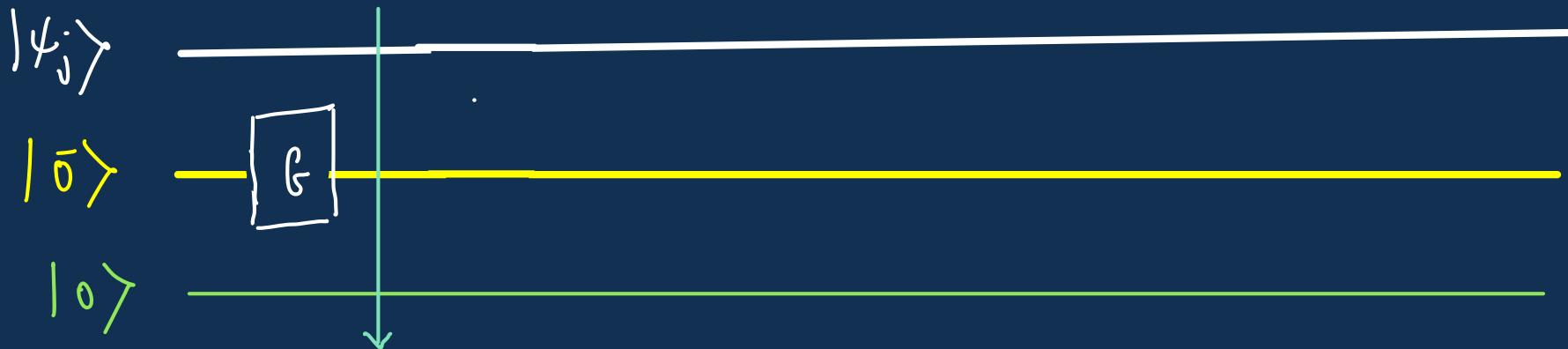
$$+ \frac{|0\rangle\langle 0|}{R} \otimes I$$

Implement $e^{i\omega t}$ via weak measurement.

Lindbladian Operators from

CGKB '23

Select A^a w.p. $P^{(a)}$.



$$|4j\rangle \otimes \underbrace{\sum_t g_t |t\rangle \otimes |0\rangle}_{\text{L}}$$

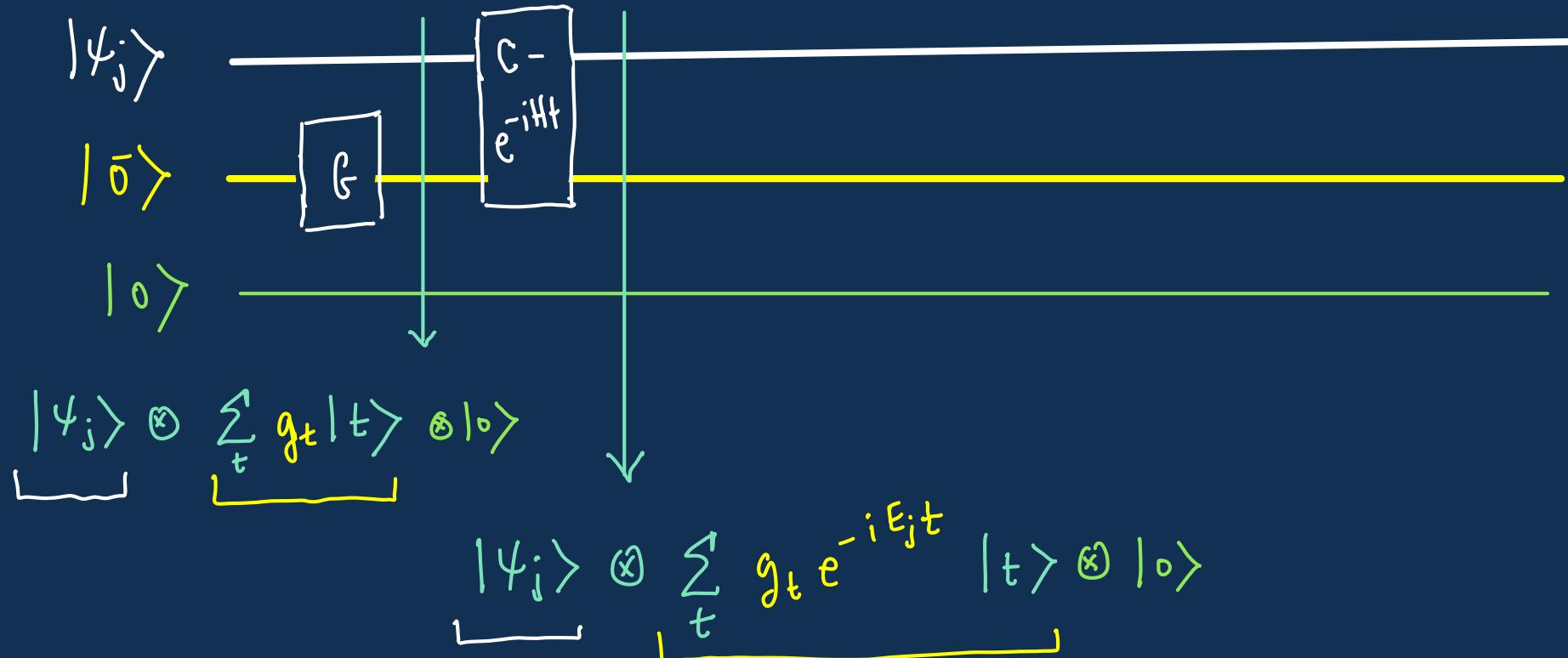
Apply controlled time-evolved jump operator

$$\left[e^{iHt} \quad A^a \quad e^{-iHt} \right] \otimes |t\rangle \langle t|$$

Lindbladian Operators from

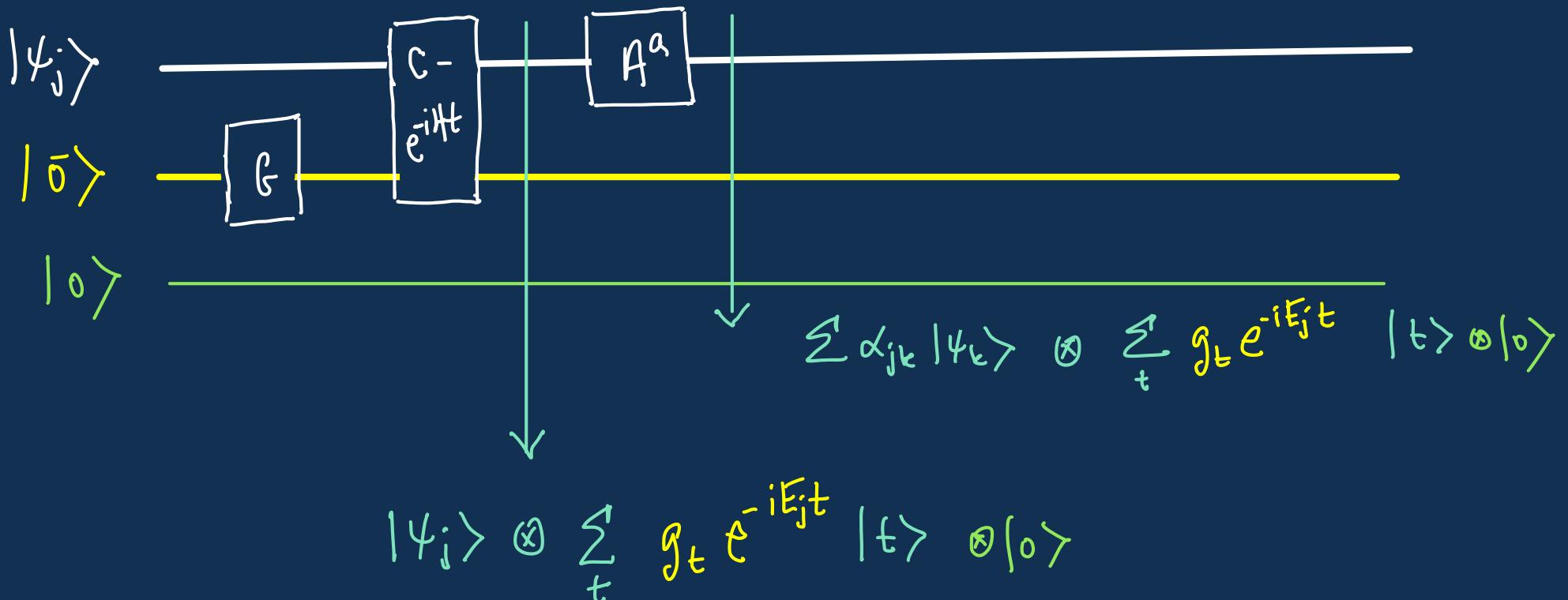
CGKB '23

Select A^α w.p. P^α .



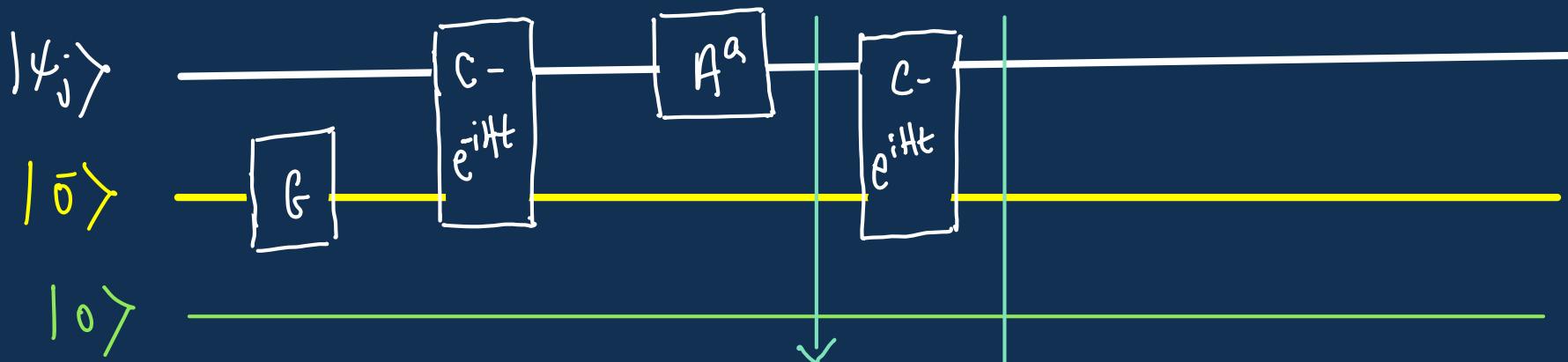
Lindbladian Operators from CGKB '23

Select A^a w.p. $P^{(a)}$.



Lindbladian Operators from CGKB '23

Select A^a w.p. $P^{(a)}$.

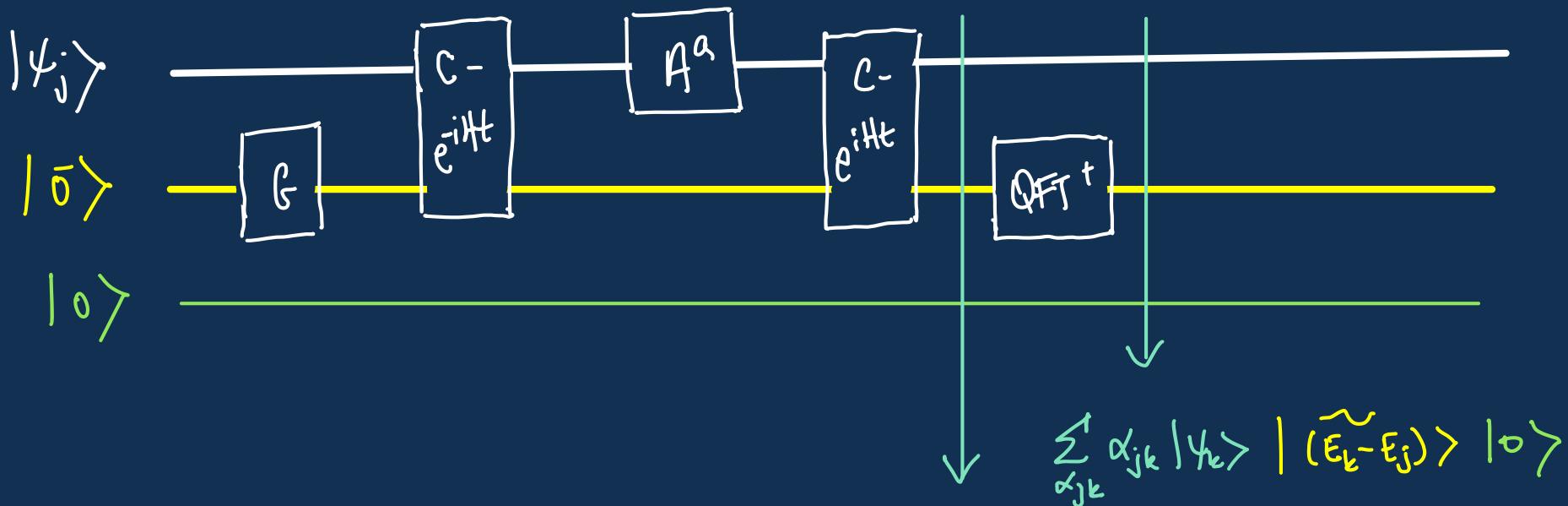


$$\sum \alpha_{jk} |4k\rangle \otimes \sum_t g_t e^{-iE_j t} |t\rangle \otimes |0\rangle$$

$$\sum \alpha_{jk} |4k\rangle \otimes \sum_t g_t e^{i(E_k - E_j)t} |t\rangle \otimes |0\rangle$$

Lindbladian Operators from CGKB '23

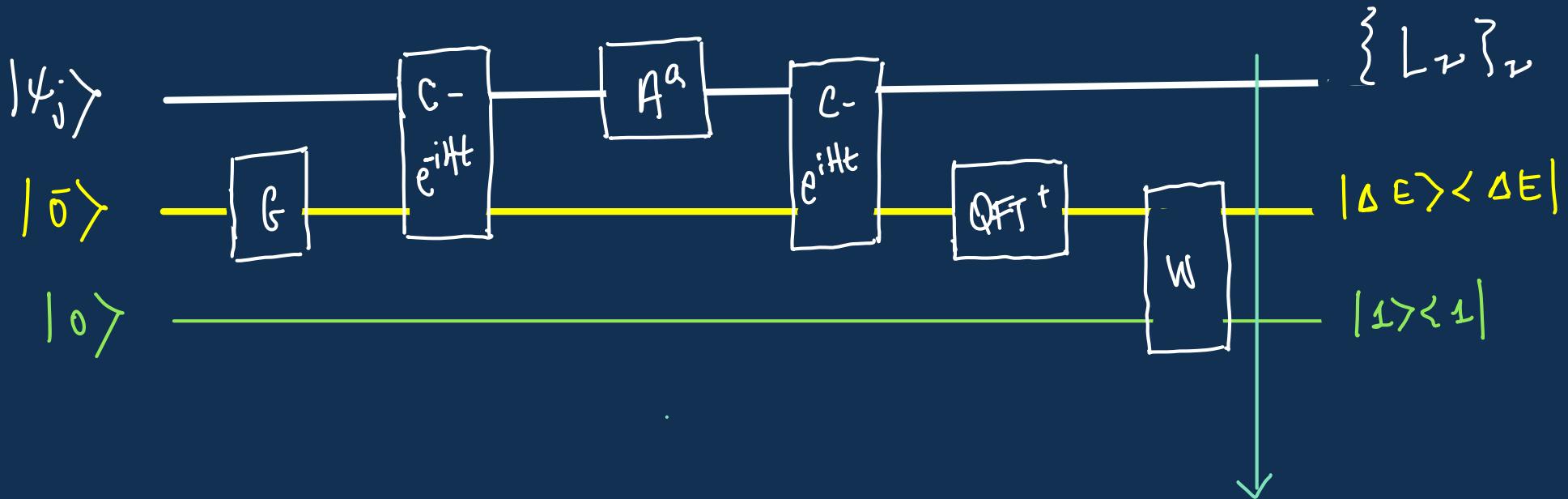
Select A^a w.p. $P^{(a)}$.



$$\sum \alpha_{jk} |4k\rangle \otimes \sum_t g_t e^{i(\epsilon_k - \epsilon_j)t} |t\rangle \otimes |0\rangle$$

Lindbladian Operators from CGKB '23

Select A^α w.p. $P^{(\alpha)}$.

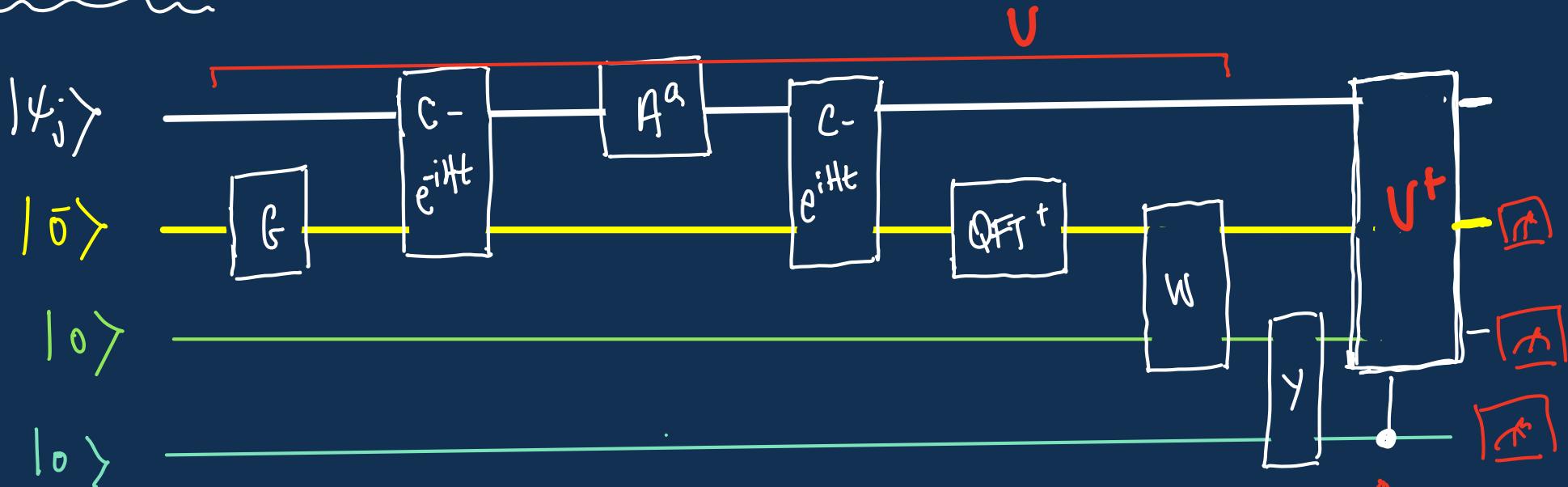


$$\sum_{jk} \alpha_{jk} |4_k> |(\tilde{E}_k - E_j)> [\sqrt{1-\gamma} |0> + \sqrt{\gamma} |1>]$$

$$\gamma = \min \{ 1, \exp(-\beta (\tilde{E}_k - E_j)) \}$$

Lindbladian Operators from CGKB '23

Select A^a w.p. $P(a)$.



One iteration of CGKB
using weak-measurement
Lindbladian implementation.

$$Y = |1\rangle\langle 1| \otimes \begin{bmatrix} \sqrt{1-\tau} & -\sqrt{\tau} \\ \sqrt{\tau} & \sqrt{1-\tau} \end{bmatrix}$$

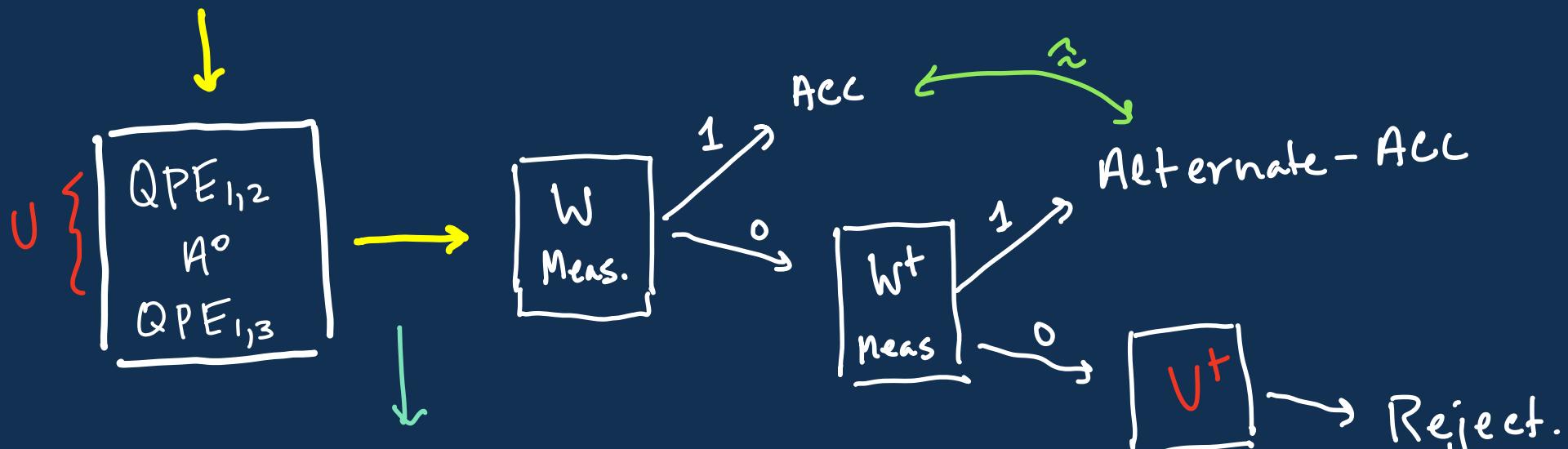
$$+ |0\rangle\langle 0| \otimes I$$

Invert
if 0.

Metropolis-Style Algorithm [Jiang, I.]

$$|4_j\rangle |0\rangle |0\rangle |0\rangle$$

$$W|EE'\rangle|0\rangle \rightarrow |EE'\rangle \left[\sqrt{1-\tau\gamma} |0\rangle + \sqrt{\tau\gamma} |1\rangle \right]$$



$$\sum_k \alpha_{jk} |4_k\rangle |0\rangle |0\rangle |0\rangle$$

$$\approx |4_j\rangle |0\rangle |0\rangle |0\rangle$$

Thank You !

