Toward Quantum Computing Phase Diagrams of Gauge Theories with Physical Thermal Pure Quantum States

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Niklas Mueller[1]

arXiv.2208.*xxxx*

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Motivation

Classical lattice gauge theory calculations can be limited by sign problems at finite chemical potential

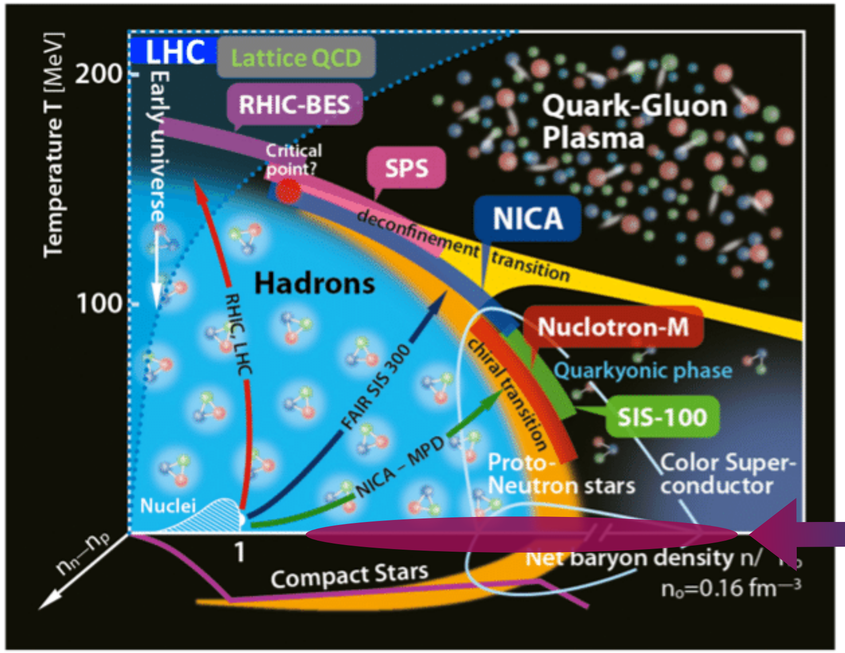
Subsequently hinders our understanding of the phase diagrams of interesting models, e.g. QCD

Extensive work has been done in the lattice QCD community in overcoming the sign problem at finite chemical potential

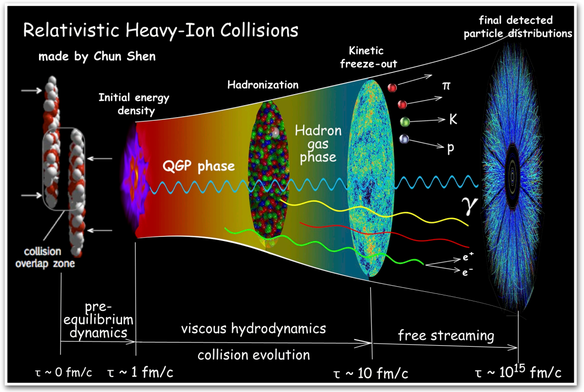
Reviews: de Forcrand, arXiv:1005.0539, Muroya, Nakamura, Nonaka, Takaishi, Prog. Theor. Phys **110** (2003)

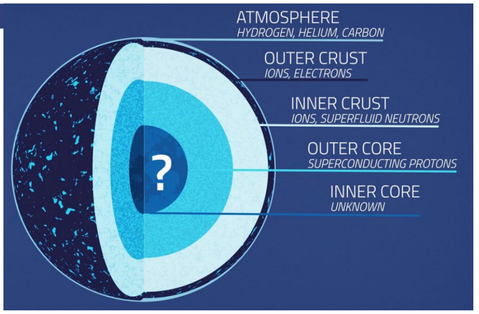
Many talks here! (Felix Ziegler, Rishabh Thakkar, Wolfgang Unger, Michael Westh Hanson, Jishnu Goswami, and more)

Existing experimental efforts are also exploring uncharted areas (and more on the way)



Sahoo, R., and Nayak, T. K., *Curr. Sci.* **121** (2021) 1403





NASA Goddard Space Flight Center / Conceptual Image Lab

There's still much to explore!

Calculating thermal values with quantum computers

Quantum computers can avoid this sign problem, but at what cost?

Finite temperature calculations are more difficult due to the mixed nature of thermal states

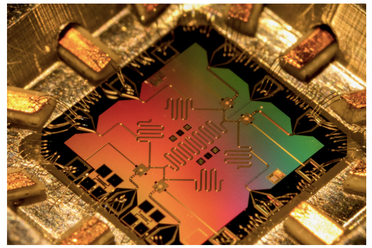


Photo: Charles Poling/LANL

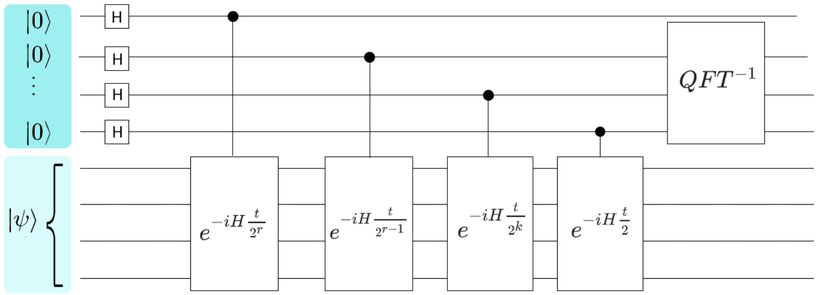
2 major categories of current methods:

Preparing the full (mixed) thermal state

- Often rely on QPE, variational methods, or ancillary registers that scale with system size or complexity

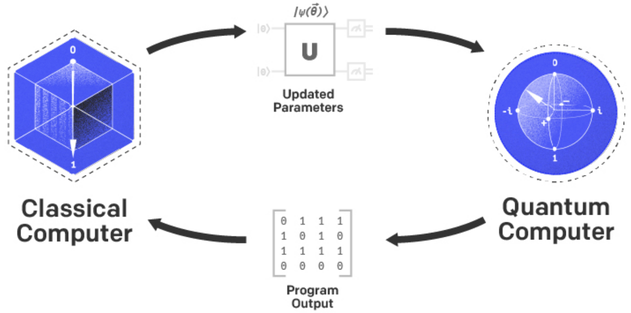
D. Poulin and P. Wocjan, Phys. Rev. Lett. **103**, 220502 (2009), A. Riera, C. Gogolin, and J. Eisert, Physical Review Letters **108** (2012), E. Bilgin and S. Boixo, Phys. Rev. Lett. **105**, 170405 (2010), G. Verdon, J. Marks, S. Nanda, S. Leichenauer, and J. Hidary, arXiv 1910.02071 (2019), J. Wu and T. H. Hsieh, Physical Review Letters **123** (2019), B. M. Terhal and D. P. DiVincenzo, Phys. Rev. A **61**, 022301 (2000), A. N. Chowdhury and R. D. Somma, Quantum Info. Comput. **17**, 41–64 (2017).

Quantum Phase Estimation Circuit Schematic



Credit: IBM

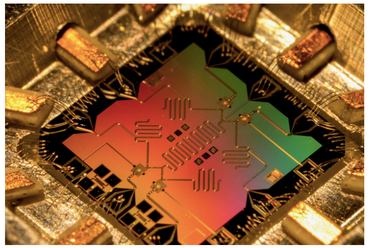
Variational Methods Workflow



Credit: IonQ

	Classical Computers	Quantum Computers
Finite Density	Sign Problem	√
Finite Temperature	√	Challenging

Calculating thermal values with quantum computers



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Sampling pure states from a thermal distribution

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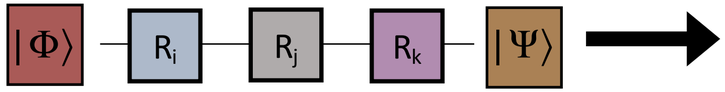
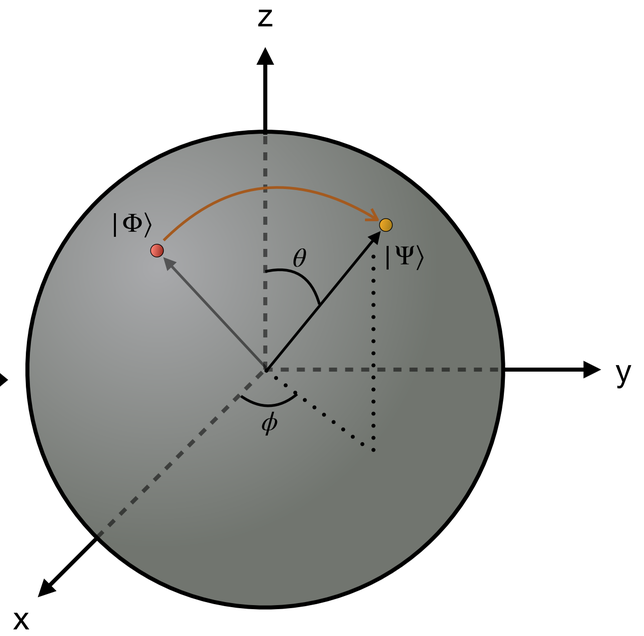
Single-qubit pure state



Circuits amount to unitary transformations



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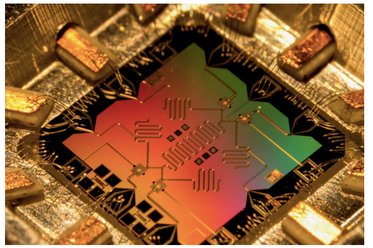

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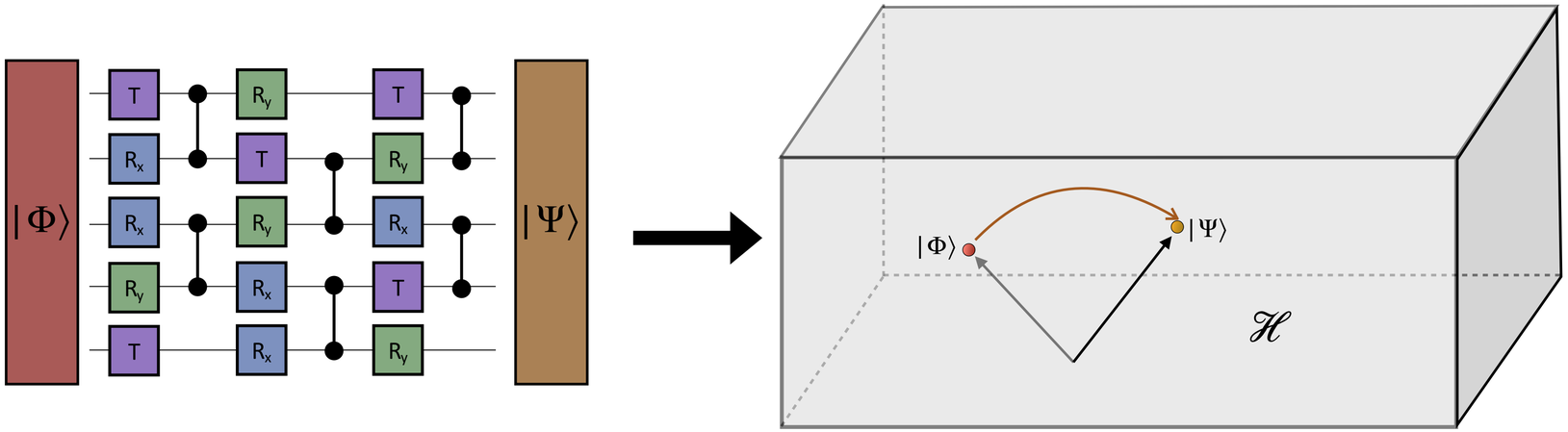

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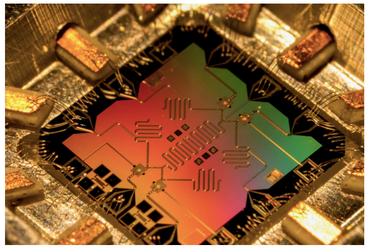

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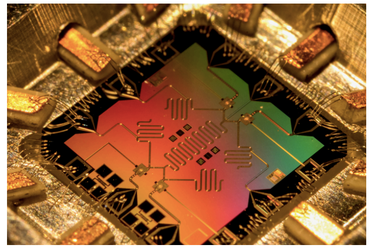
How can we avoid this required sample scaling **and** the preparation of a full thermal state?

Calculating thermal values with quantum computers



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Canonical thermal pure quantum (TPQ) states

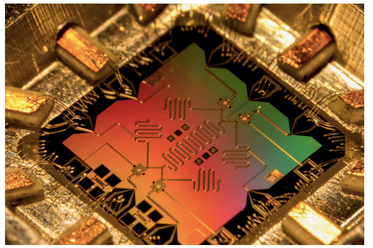
- Introduced classically in S. Sugiura and A. Shimizu, PRL **111** (2013)
- First demonstrated on quantum hardware in C.P., L.B.O., W.A.d.J., arXiv:2109.01619 (2021)

$$|\beta, N\rangle = e^{-\beta H/2}|\Psi_R\rangle$$ ← Haar-random state

Representative of true thermal states in expectation values for a large class of observables

- Average squared error using a single TPQ state is bounded by a function that becomes exponentially small with increasing system size!

Calculating thermal values with quantum computers



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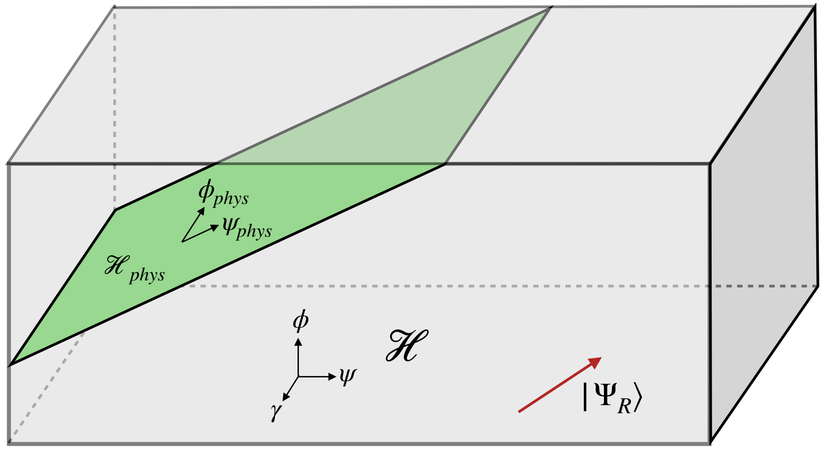
Canonical thermal pure quantum (TPQ) states

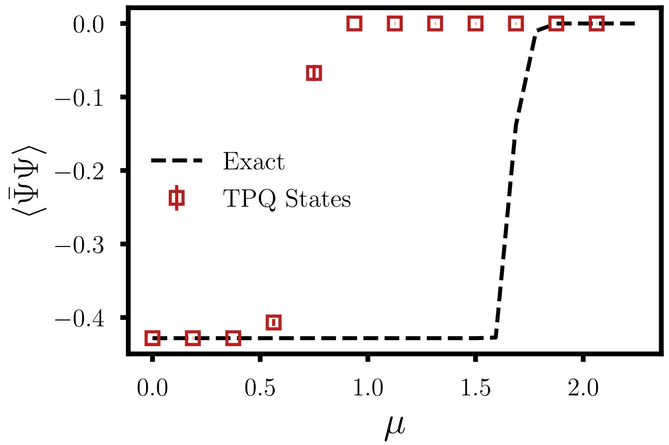
Advantages	Disadvantages
Accuracy improves with system size (inverse scaling of required samples)	Still have to perform imaginary time evolution
No QPE or variational methods required	Weakened performance at small system sizes
Flexibility in number of required ancillary qubits (as low as 0)	

What about thermal values for LGTs?

The presence of unphysical states complicates the picture…



Forming a TPQ state from a Haar-random state outside the physical subspace can lead to incorrect results!



For our application, this is especially pertinent around phase transitions

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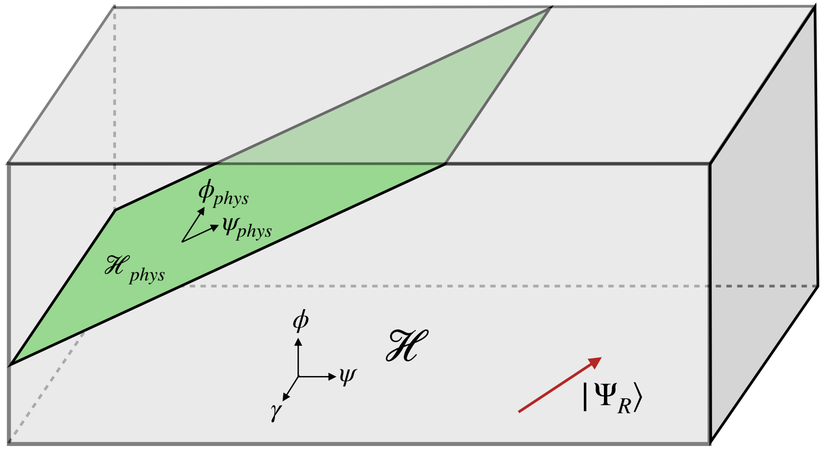

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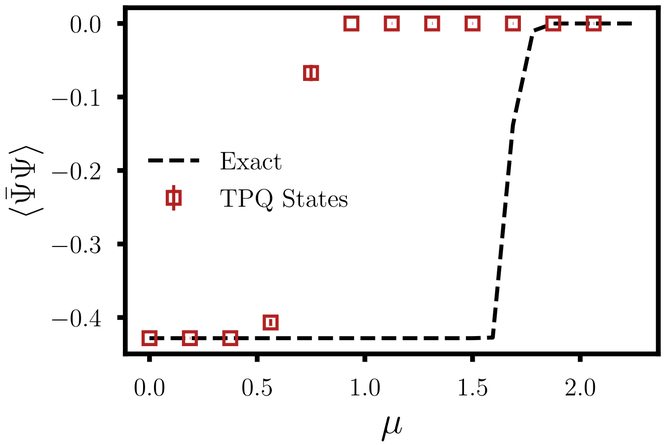
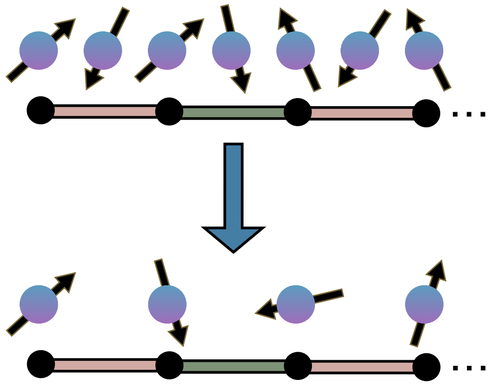


For our application, this is especially pertinent around phase transitions

Purely fermionic formulation residing in the physical subspace solves the issue…

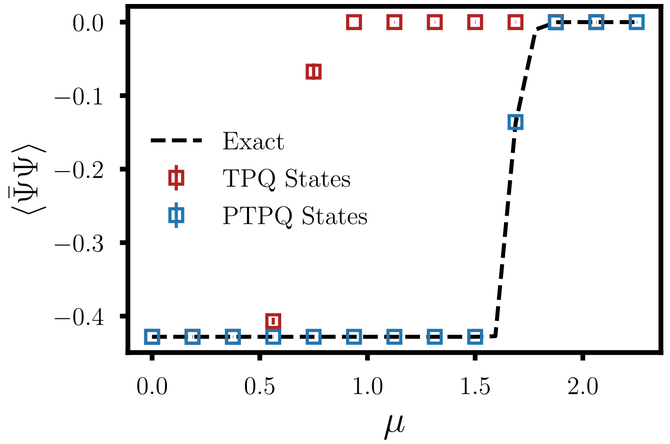


But such formulations are only possible in 1+1D with certain boundary conditions

We need a solution that works even when unphysical states exist in the Hilbert space

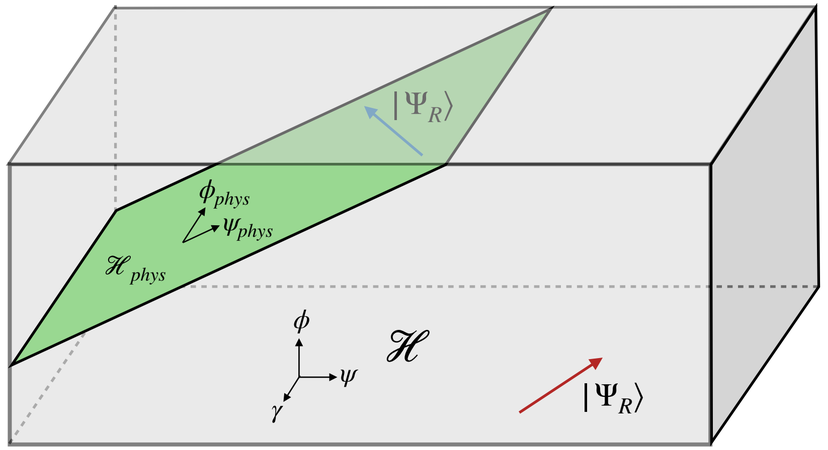
What about thermal values for LGTs?

Solution: Restrict TPQ states to the physical subspace via the enforcement of Gauss's law, forming "physical" thermal pure quantum states (PTPQ)



There are two main steps in TPQ state preparation, and thus 2 possible choices in where to enforce physicality:

1) Haar-random state preparation



Downside: would necessitate development of a random circuit structure that enforces Gauss's law

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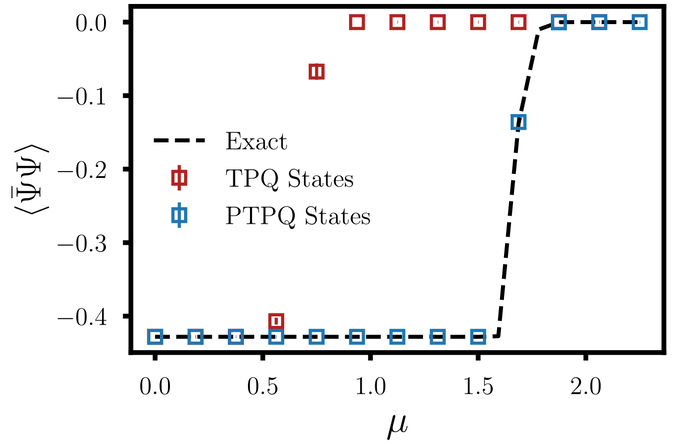


There are two main steps in TPQ state preparation, and thus 2 possible choices in where to enforce physicality:

1) Haar-random state preparation

2) Imaginary time evolution

- Can utilize existing random circuit structures with studied convergence onto Haar-random states spanning the entire Hilbert space
- Utilize a Lagrange multiplier to "guide" the TPQ state into the physical sector during imaginary time evolution

$$|\beta, N\rangle^{phys} = e^{\frac{-\beta}{2}(H+\lambda\sum_n f(G_n))}|\Psi_R\rangle$$

$f(G_n)$ chosen to penalize unphysical states

PTPQ State Preparation

Circuit Structure

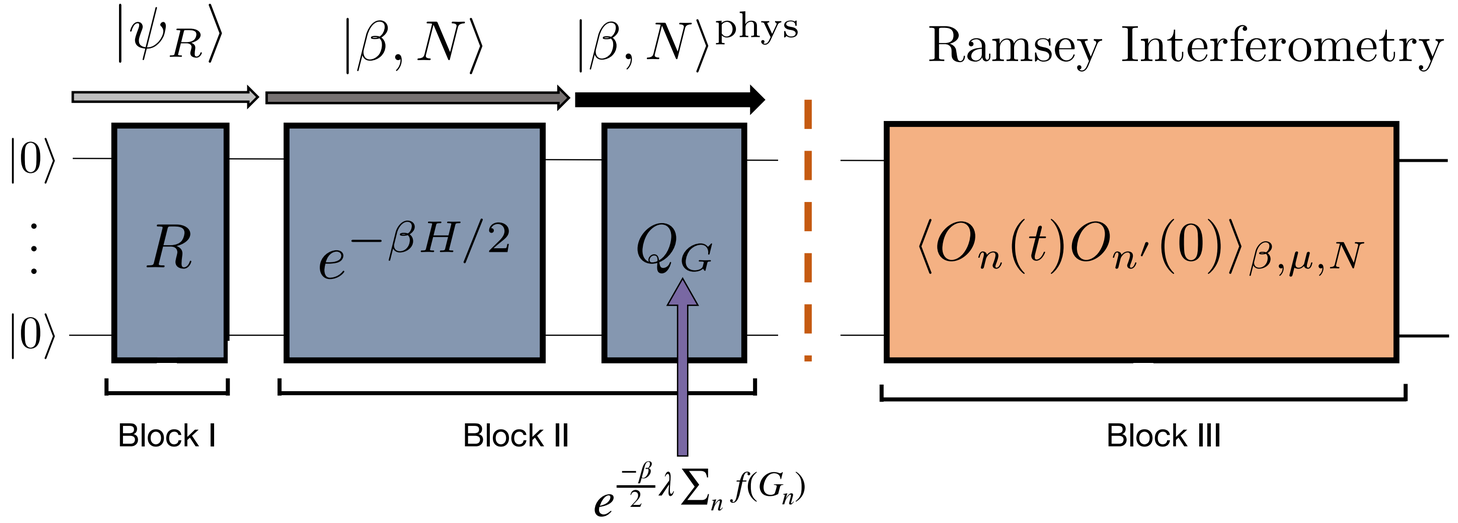
Block I. Random State Preparation

Block II. Imaginary Time Evolution

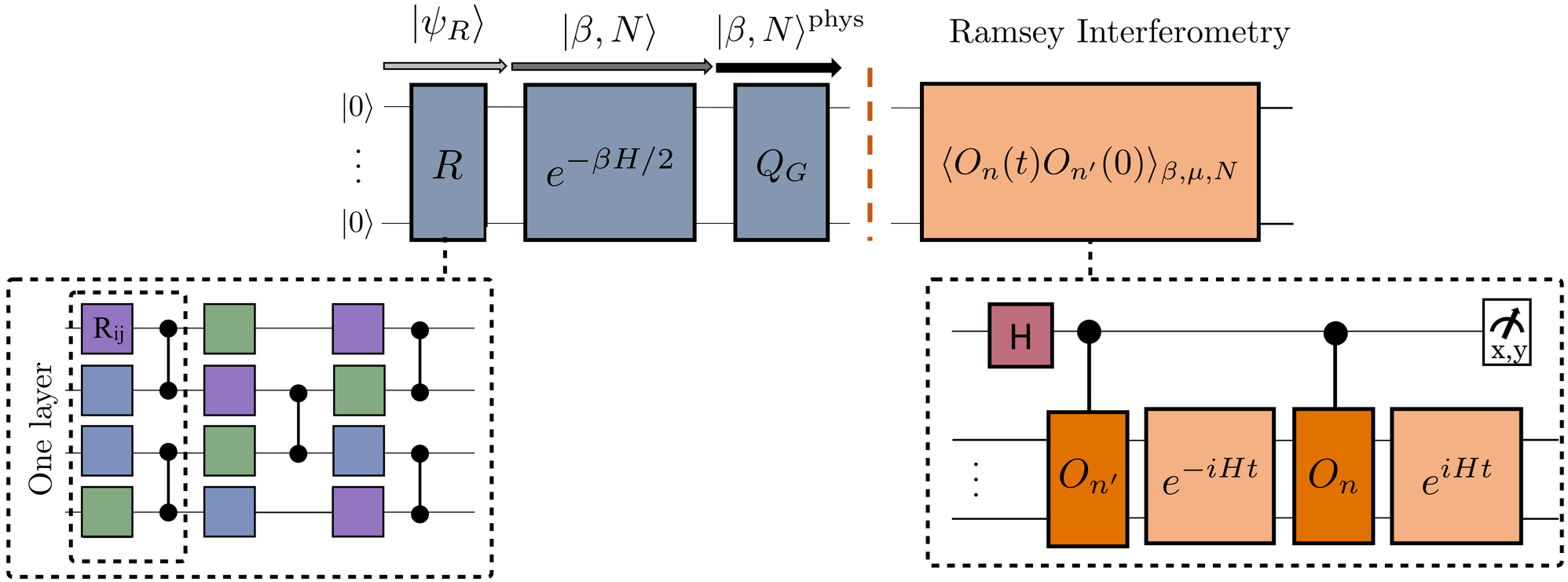
Block II.a) Standard TPQ state evolution

Block II.b) Enforcing Gauss's law

Block III. Ramsey Scheme
(if, for example, measuring non-equal time correlation functions)



PTPQ State Preparation



$$S = \{R_x(\pi/2), R_y(\pi/2), T\}$$
$$R_{ij} \in S \backslash R_{i,j-1}$$

Approximates higher t-designs as d is increased, improving approximation of Haar-random state with known scalings w.r.t. system size

Richter and Pal, PRL **126** (2021), Boixo et al., Nature Physics **14**, 595–600 (2018)

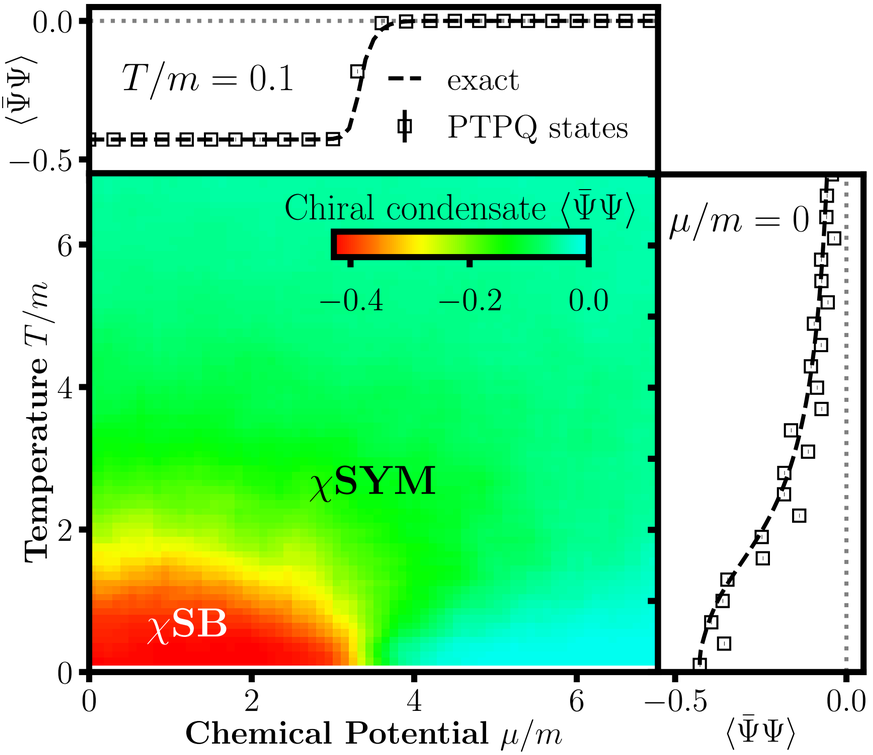
Demonstration: Finite temperature chiral phase diagram

Testbed model: $\mathbb{Z}_2^{1+1}$ coupled to massive staggered fermions

$$H = \frac{1}{2a}\sum_n (c_n^\dagger \tilde{\sigma}_n^x c_{n+1} + \mathrm{h.c.}) + \mathrm{m}\sum_\mathrm{n}(-1)^\mathrm{n} c_\mathrm{n}^\dagger c_\mathrm{n} - \epsilon\sum_\mathrm{n}\tilde{\sigma}_\mathrm{n}^\mathrm{z} - \mu\sum_{\mathrm{n=0}}^{\mathrm{N-1}} c_\mathrm{n}^\dagger c_\mathrm{n}$$

Fermionic hopping | Fermionic mass | Gauge field | Chemical potential

$$\langle\bar{\Psi}\Psi\rangle \equiv \frac{1}{N}\langle\sum_{i=0}^{N-1}(-1)^i c_i^\dagger c_i\rangle$$



$$G_n|\mathrm{phys}\rangle = |\mathrm{phys}\rangle$$

$$f(G_n) = 1 - G_n$$

Gauss's law operator $G_n = \tilde{\sigma}_n^z \tilde{\sigma}_{n-1}^z e^{i\pi Q_n}$

where $Q_n = c_n^\dagger c_n + [(-1)^n - 1]/2$

$$|\beta, N\rangle^{phys} = \exp\left(\frac{-\beta(H + \lambda\sum_n(1 - G_n))}{2}\right)|\Psi_R\rangle$$

Demonstration: Non-equal time correlation functions

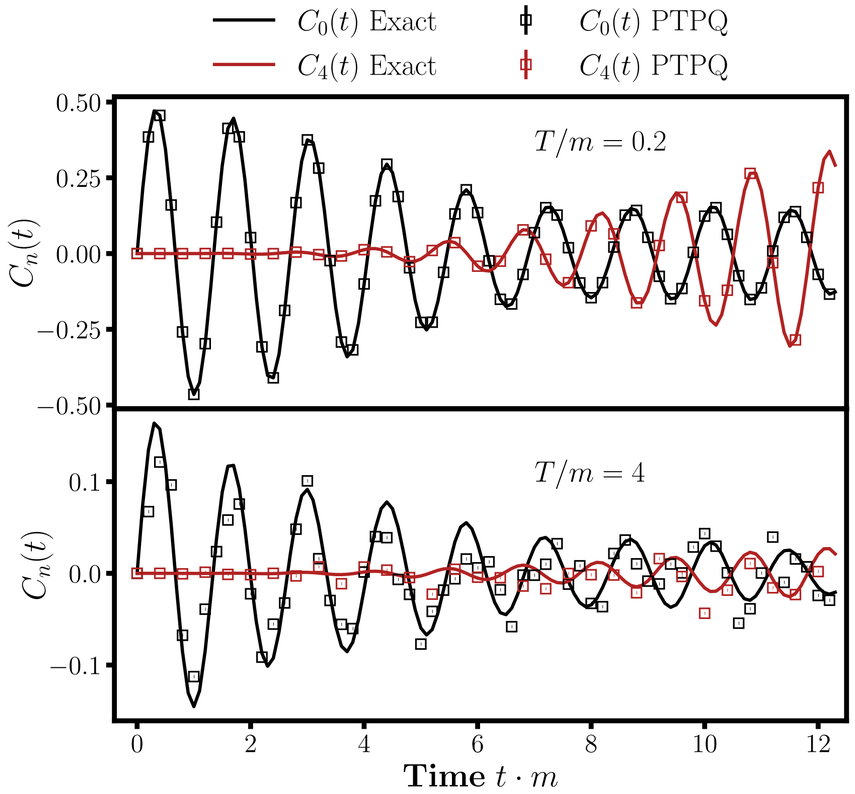
Can also be used for computing transport coefficients, e.g. electrical conductivity, bulk viscosity

$$C_n(t) = [j_n(t), j_0(t=0)]$$

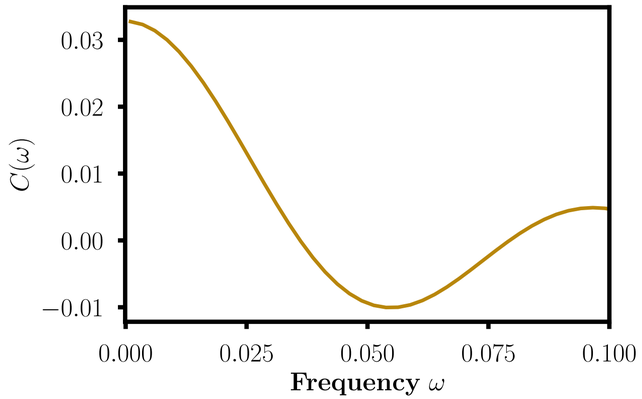
current operators

For this model, $j_n = \frac{i}{2a}(\sigma_x^+ \tilde{\sigma}_n^x \sigma_{n+1}^- - h.c.)$

$N = 6$



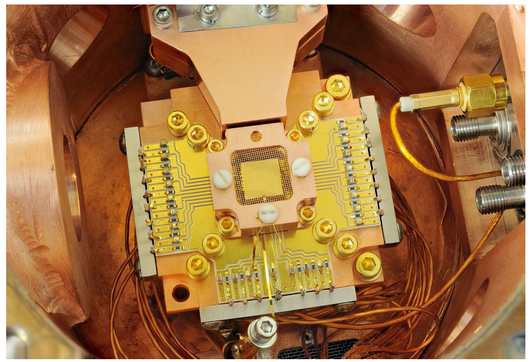
$$\sigma^{elec}_{\beta,\mu} \sim \lim_{\omega \to 0} \frac{1}{\omega} \int dt e^{i\omega t} a \sum_n \langle C_n(t) \rangle_{\beta,\mu} = \lim_{\omega \to 0} C(\omega)$$



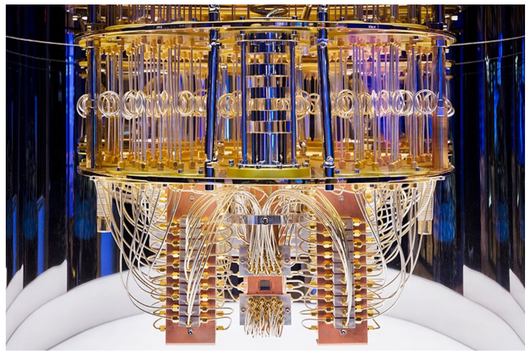
What about errors and noise?

NISQ-era device qubits are prone to a myriad of errors dependent on the device type

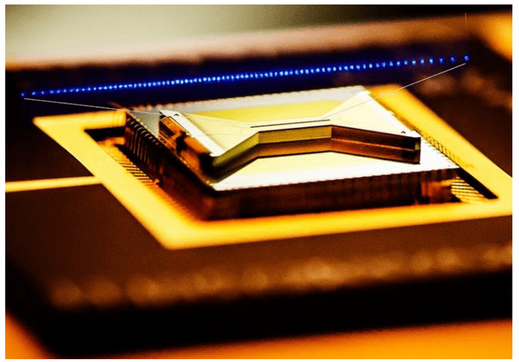
- Imperfect gates, crosstalk, decoherence, readout error, imperfect coupling resonators, …



Credit: NIST



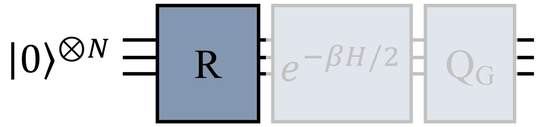
Credit: IBM

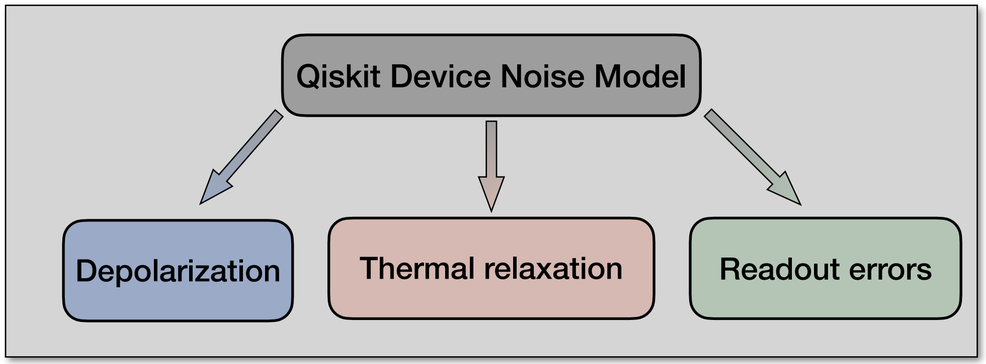


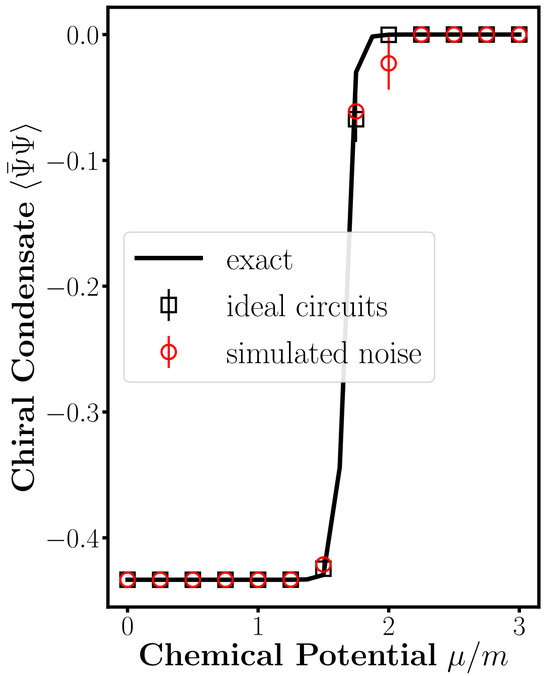
Credit: Christopher Monroe

What about errors and noise?

Want to answer the question:
How sensitive are measured thermal values to errors introduced during random state preparation?





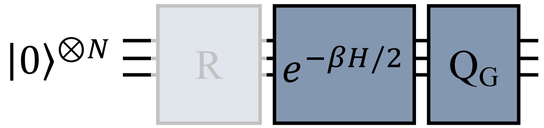


Using Qiskit's noise model for the IBM "Sydney" device

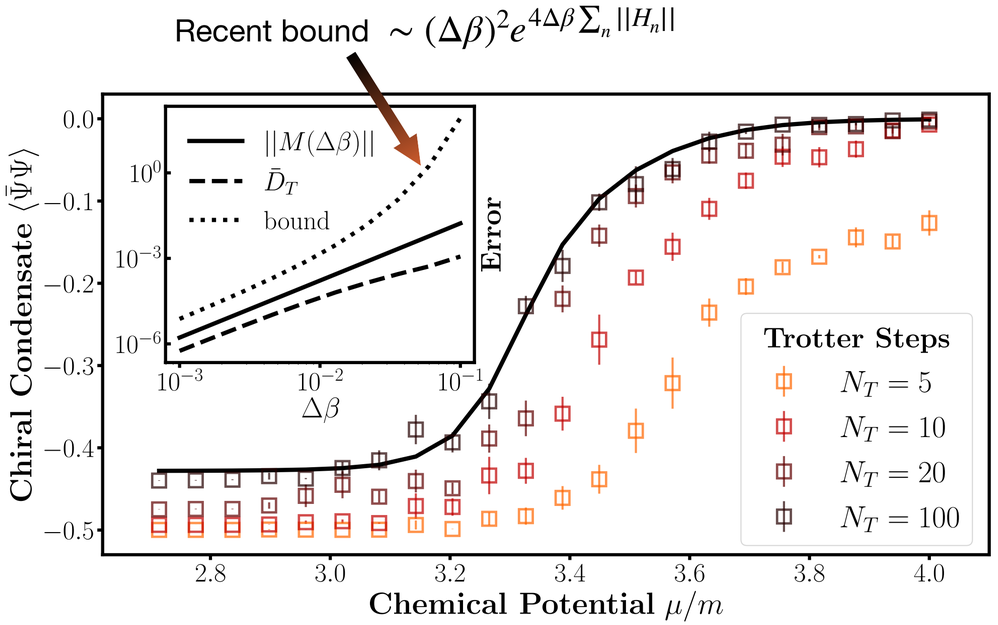
Result:
Results from PTPQ states appear to be robust to simulated device errors introduced during the random state preparation sub-circuit

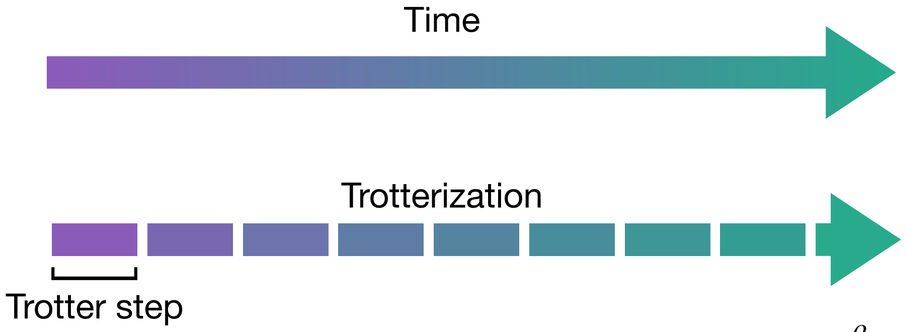
What about errors and noise?

Want to answer the question:
How sensitive are measured thermal values to Trotter errors introduced during the imaginary time evolution phase?



Childs et al., Phys. Rev. X 11, 011020 (2021).





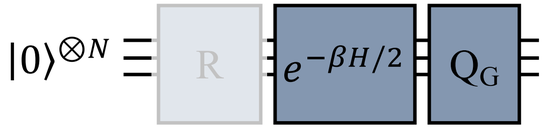
$$e^{-\beta H} \approx (\prod_n e^{-H_n \Delta\beta})^{N_T} + O(\Delta\beta) \qquad N_T = \frac{\beta}{\Delta\beta}$$

$$\prod_n e^{-H_n\Delta\beta} = e^{-\Delta\beta H}(1 + M(\Delta\beta)) \qquad D_T(\rho,\sigma) = \frac{1}{2}\mathrm{Tr}(\sqrt{(\rho-\sigma)^2}$$

- Impact on measured values follows expected behavior w.r.t. N_T
- Power law behavior observed for $||M(\Delta\beta)||$, $\approx$ scaling predicted by real-time evolution bound

What about errors and noise?

Want to answer the question:
How sensitive are measured thermal values to unitary errors introduced during the imaginary time evolution phase?

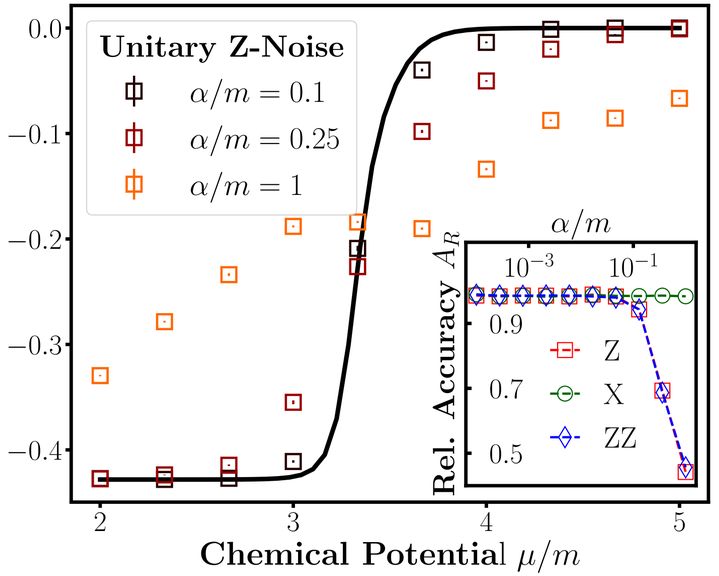


$$H = \frac{1}{2a}\sum_{n}(c_n^\dagger \tilde{\sigma}_n^x c_{n+1} + \mathrm{h.c.}) + m\sum_{n}(-1)^n c_n^\dagger c_n - \epsilon\sum_{n}\tilde{\sigma}_n^z - \mu\sum_{n=0}^{N-1} c_n^\dagger c_n + \sum_{m=0}^{2N-1} K_m^\alpha \sigma_m$$

Fermionic hopping | Fermionic mass | Gauge field | Chemical potential | Error terms

K_m^α sampled uniformly from $[-\alpha, \alpha]$

- PTPQ states show high robustness to introduced error terms that violate Gauss's law
- More sensitive to non-violating error terms, reasonably robust up to $\alpha/m \approx 0.1$



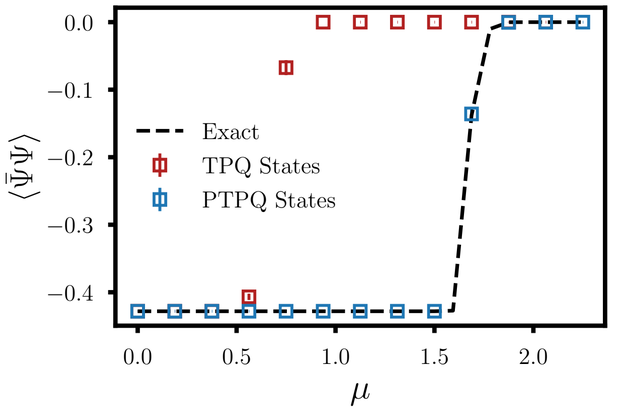
$\sigma_m \in \{\sigma_m^z, \sigma_m^x, \sigma_m^z\sigma_{m+1}^z\}$

Conclusions

Standard canonical TPQ states offer a promising route to estimating thermal expectation values on quantum computers, but cannot be used to explore LGTs

PTPQ states solve this issue, enabling finite temperature and finite μ explorations of LGTs with all of the resource requirement benefits of TPQ states

Results from a single prepared state only become more accurate with increasing system size
Flexible classical/quantum resource requirements
No dual purely fermionic model required
Robust to certain types of introduced errors



Expected utility in the NISQ era and beyond

Future Work

Exploring advantages of forming PTPQ states by enforcing Gauss's law during random state generation instead of imaginary time evolution

Thank you

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Image: RHIC/Brookhaven National Laboratory