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Examining Thermodynamics using Quantum Computers

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Southeast Quantum Computing Workshop
05/20/2022

With:

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Norbert Linke, Duke University
Chris Monroe, Duke University & IonQ

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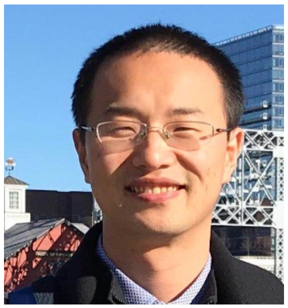

NCSU Team
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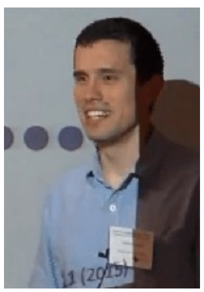
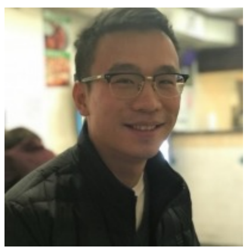
Georgetown
Jim Freericks


U Maryland Team
Daiwei Zhu
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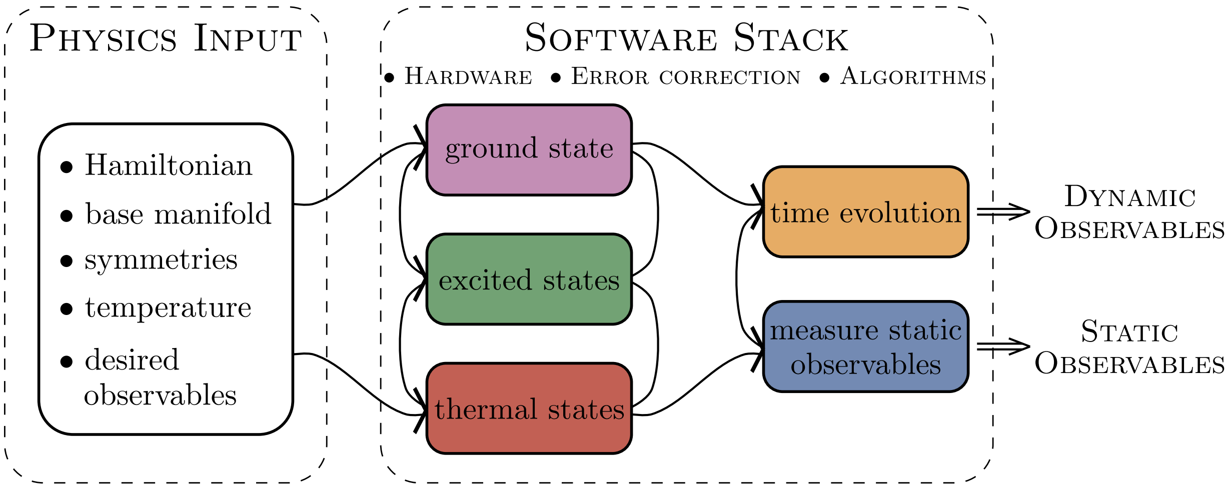
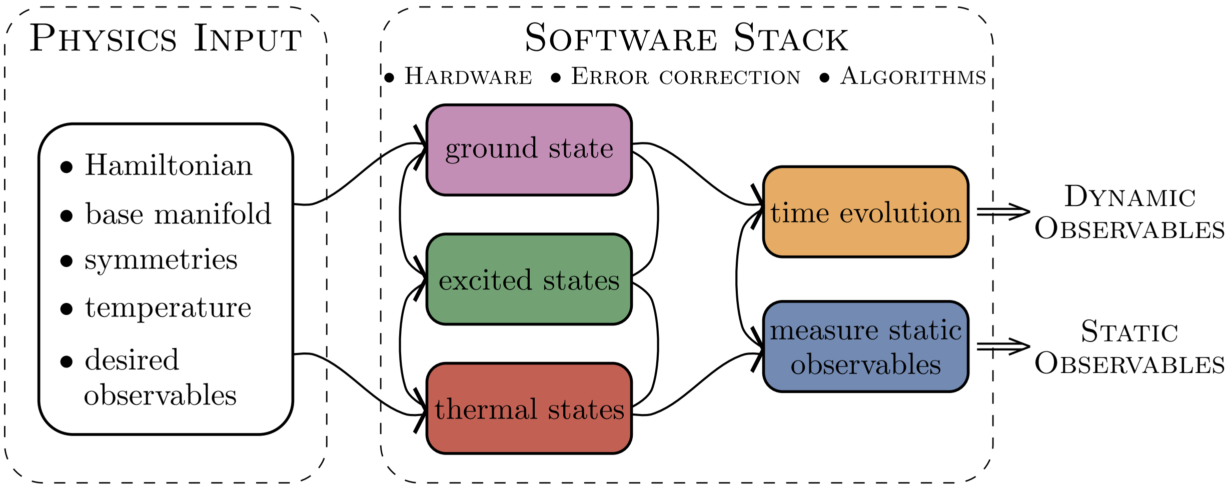
Quantum Matter meets Quantum Computing



- Measuring correlation functions
- Preparing/measuring topological states
- Modeling driven/dissipative systems
- Time evolution via Lie algebraic decomposition/compression
- Thermodynamics

Quantum Matter meets Quantum Computing



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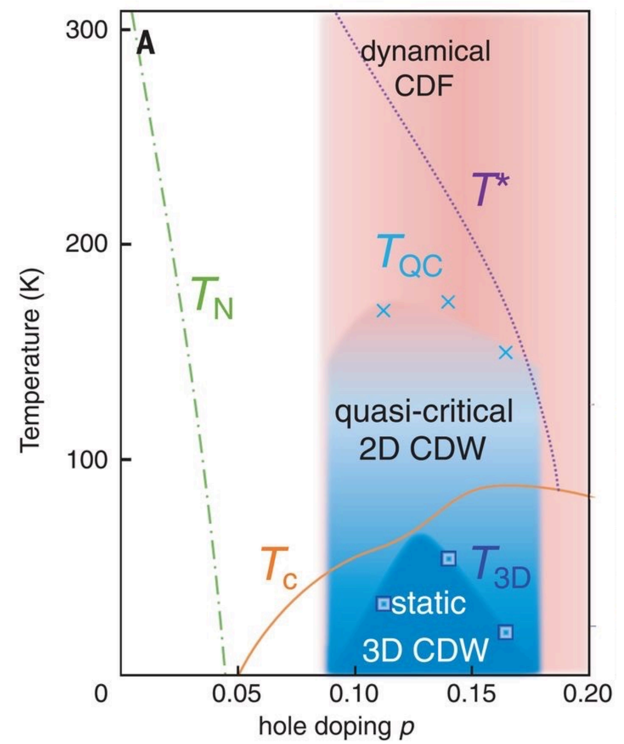
Phase diagrams and Phase transitions

“It’s not a cuprate talk unless it has a phase diagram…”

-- Overheard at APS March Meeting

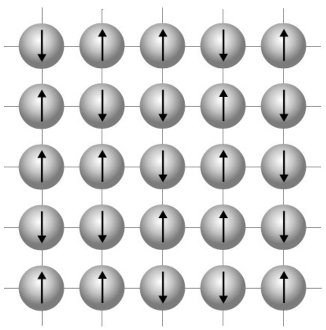
$YBa_2Cu_3O_{7-x}$

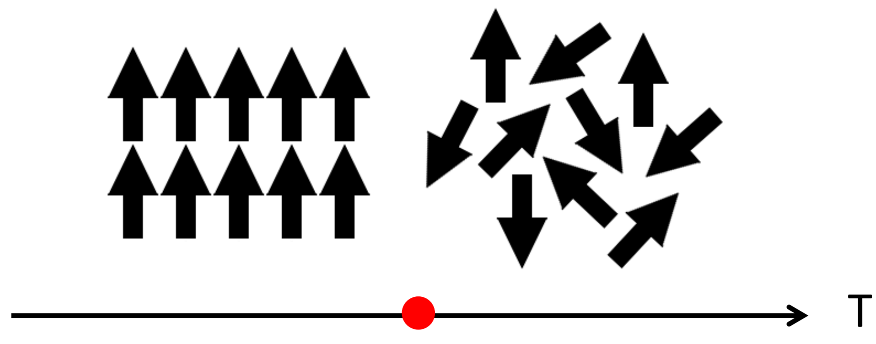


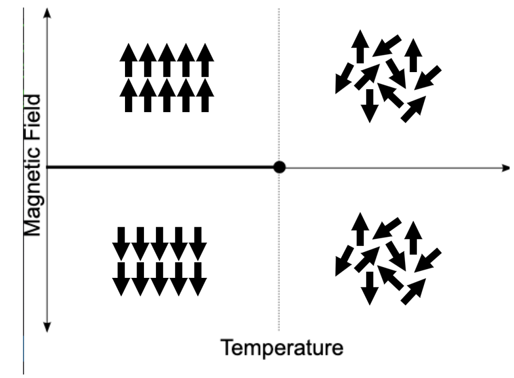
10.1126/science.aav1315

Ising Model Thermodynamics

Phase transitions:







$$\mathcal{F} = E - TS$$

$$S = -\mathrm{Tr}\,\rho \log \rho$$

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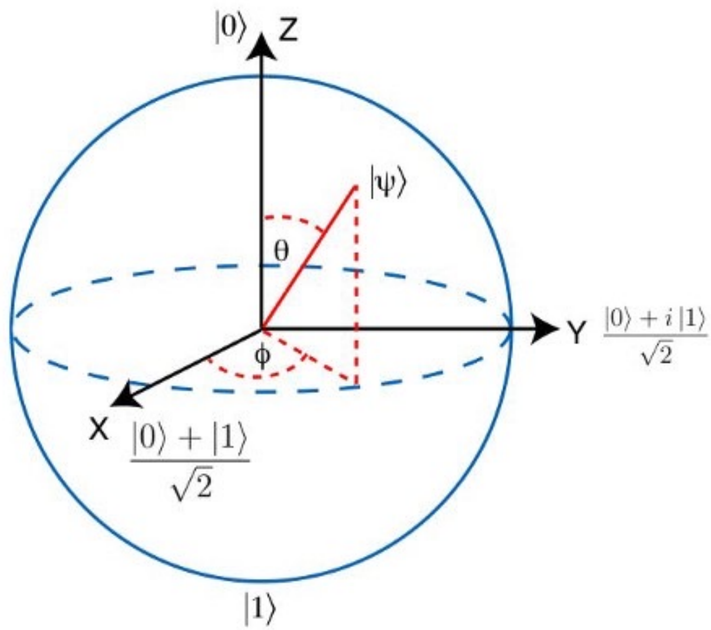
The density matrix ρ

Pure States

$$\rho = |\psi\rangle\langle\psi|$$

On the surface of the Bloch sphere

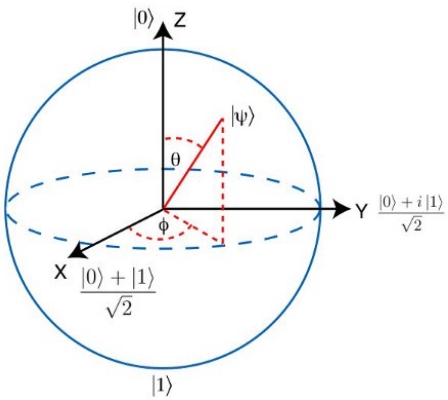


Mixed States

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

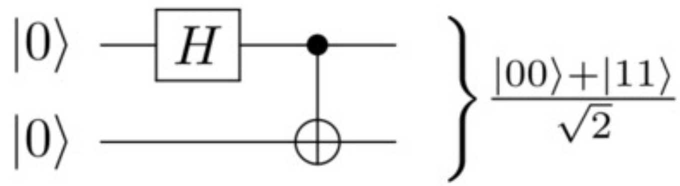
Inside the Bloch sphere

The density matrix ρ on QC

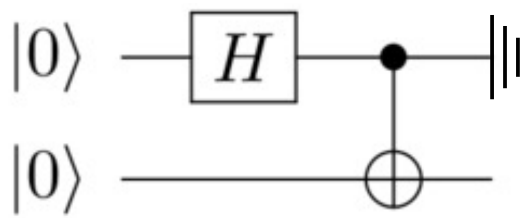


$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

Mixed states can be obtained from pure states by tracing out part of a pure state (dilation theorems).

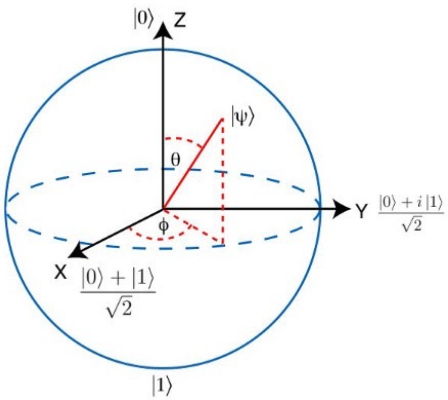


$$\rho = \frac{|00\rangle\langle 00| + |11\rangle\langle 11| + |00\rangle\langle 11| + |11\rangle\langle 00|}{2}$$



$$\rho = \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2}$$

The density matrix ρ on QC



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

$$\beta = \frac{1}{k_B T}$$

For a thermal state ρ_{th},

$$\rho = \mathcal{Z}^{-1} \sum_i e^{-\beta H} |\psi_i\rangle\langle\psi_i|$$

where $\mathcal{Z}$ is set such that $\mathrm{tr}\rho = 1$.

Big question: How do we make such a state?

The density matrix ρ on QC

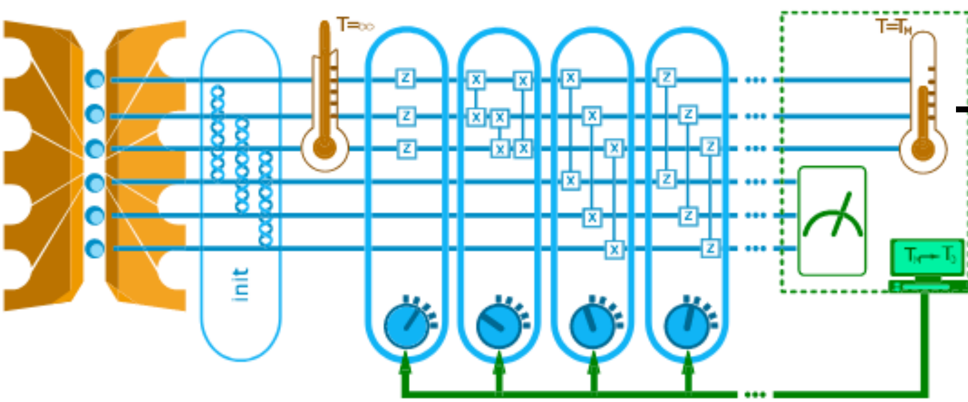
Variational Thermal Quantum Simulation via Thermofield Double States

Jingxiang Wu[1,2] and Timothy H. Hsieh[1]

Generation of thermofield double states and critical ground states with a quantum computer

D. Zhu[a,b,c], S. Johri[d], N. M. Linke[a,b], K. A. Landsman[a,b], C. Huerta Alderete[a,b,e], N. H. Nguyen[a,b], A. Y. Matsuura[d], T. H. Hsieh[f], and C. Monroe[a,b,c,g,1]

$$|TFD(\beta)\rangle = \frac{1}{\sqrt{Z(\beta)}} \sum_n e^{-\beta E_n/2} |n\rangle_A |n'\rangle_B$$



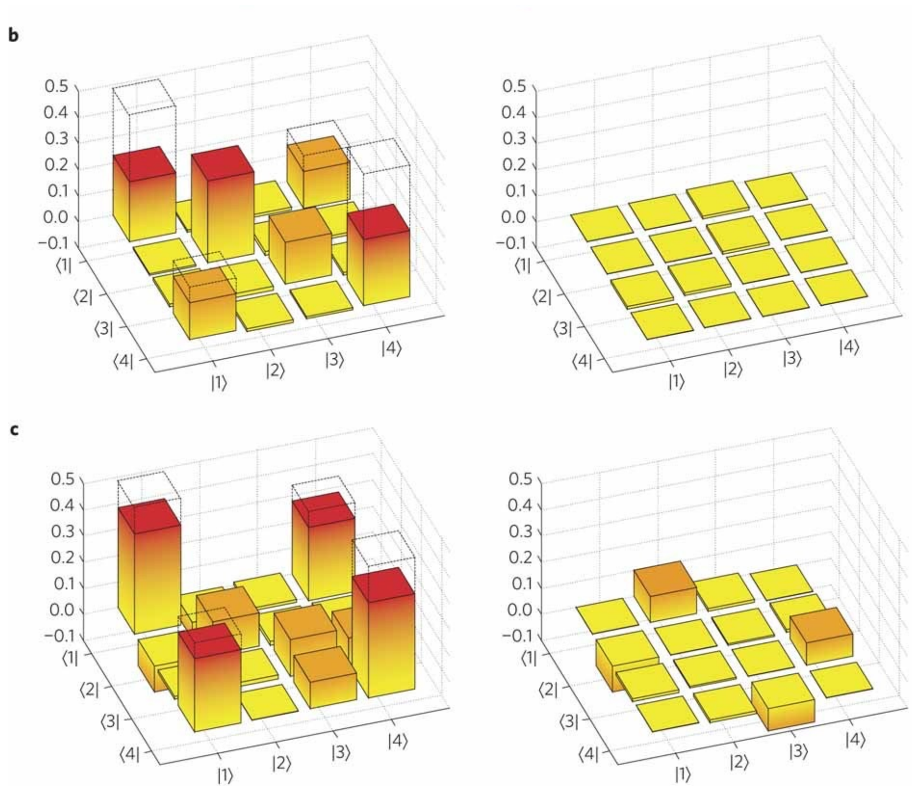
ρ →

$$\mathcal{F} = E - TS$$
$$E = \mathrm{tr}\ \rho\mathcal{H}$$
$$S = -\mathrm{tr}\ \rho \log \rho$$

PNAS October 13, 2020 117 (41) 25402-25406

The density matrix ρ on QC

Once we have one, how do we measure the density matrix ρ?



$$\sim 4^N$$

$$S = -\mathrm{tr}\ \rho \log \rho$$

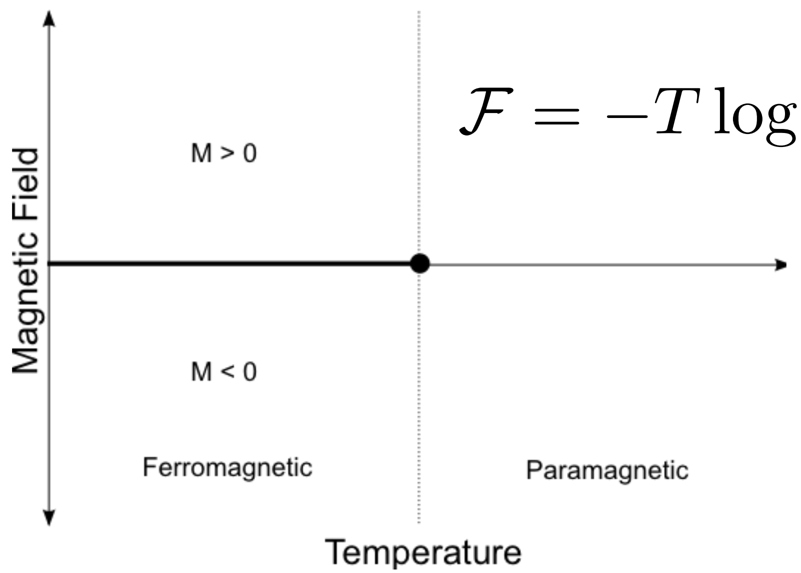
☹

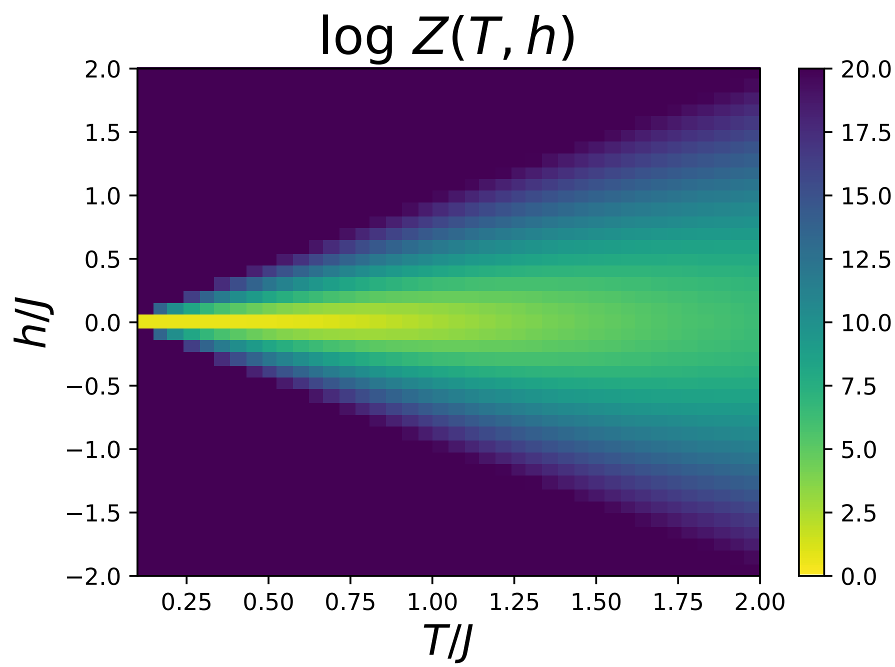
Nature Physics **volume 8**, pages 596–600 (2012)

An alternative approach: the partition function $\mathcal{Z}$

$$\hat{H} = -J \sum_i \sigma_i^z \sigma_{i+1}^z + h \sum_i \sigma_i^z \qquad \mathcal{Z}(\beta, h) = \mathrm{tr} e^{-\beta \hat{H}(h)}$$

$$\mathcal{F} = -T \log \mathcal{Z}$$

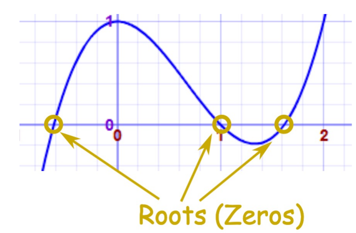




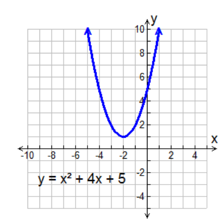
Partition Function Zeros

- Think of Z in a different way: as a function on the set of parameters of the Hamiltonian: Z(h,T)
- As long as the number of states N < ∞, Z is a “nice” function.
- Thus, it admits a polynomial expansion in h.
- Every polynomial is characterized by its zeros in its domain.
- Z is positive definite for real Hamiltonian parameters, thus the zeros must lie in the complex plane of parameters.

$$\mathcal{Z}(\beta, h) = \mathrm{tr} e^{-\beta \hat{H}(h)}$$



$$\mathcal{Z}(h) = c \prod_{h_0} (h - h_0)$$



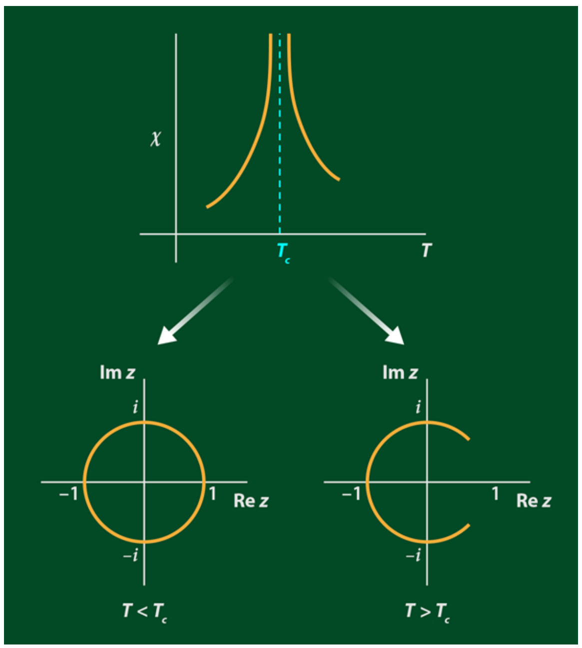
Lee, T.D. and Yang, C.N., Physical Review, ***87***, 410

Partition Function Zeros

Physics — Physics 8, 2 (2015)

Viewpoint

Imaginary Magnetic Fields in the Real World



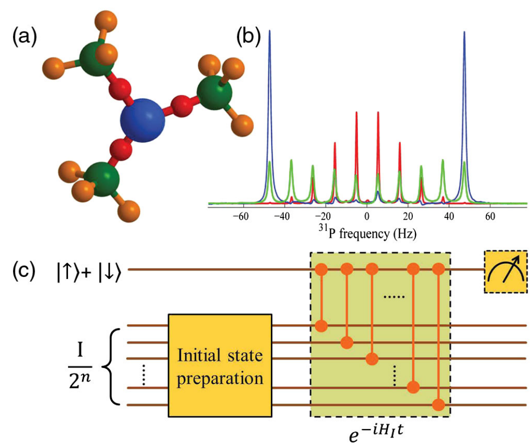
$$z = e^{2\beta z_0}$$

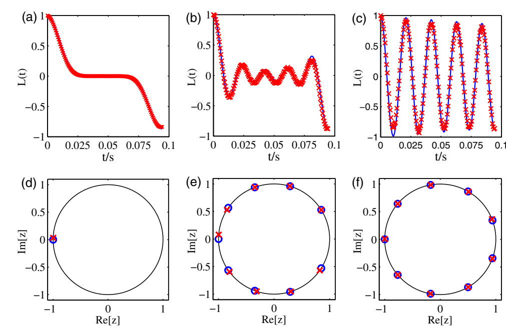
Selected for a Viewpoint in Physics
PRL 114, 010601 (2015) PHYSICAL REVIEW LETTERS week ending 9 JANUARY 2015

Experimental Observation of Lee-Yang Zeros

Xinhua Peng,[1,*] Hui Zhou,[1] Bo-Bo Wei,[2] Jiangyu Cui,[1] Jiangfeng Du,[1,†] and Ren-Bao Liu[2,‡]
[1]Hefei National Laboratory for Physical Sciences at Microscale, Department of Modern Physics, and Synergetic Innovation Center of Quantum Information & Quantum Physics, University of Science and Technology of China, Hefei 230026, China
[2]Department of Physics, Centre for Quantum Coherence, and Institute of Theoretical Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, China

(Received 11 September 2014; published 5 January 2015)





$$\mathcal{Z} = \mathrm{tr}\; e^{-\beta\sum_{i\alpha} J_\alpha \sigma_i^\alpha \sigma_{i+1}^\alpha - \beta h_r \sum_i \sigma_i^z - i\beta h_i \sum_i \sigma_i^z}$$

Thermal state ρ

Time evolution

<u>3 problems to be addressed:</u>

1. How do we produce a thermal state? *Thermofield Double States*

2. How do we accomplish the time evolution? $\rho(t) = e^{-iH_{int}t}\rho(0)e^{+iH_{int}t}$

3. How do we map this onto QC?

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Partition Function Zeros on Quantum Computers

Produce a thermal state ρ

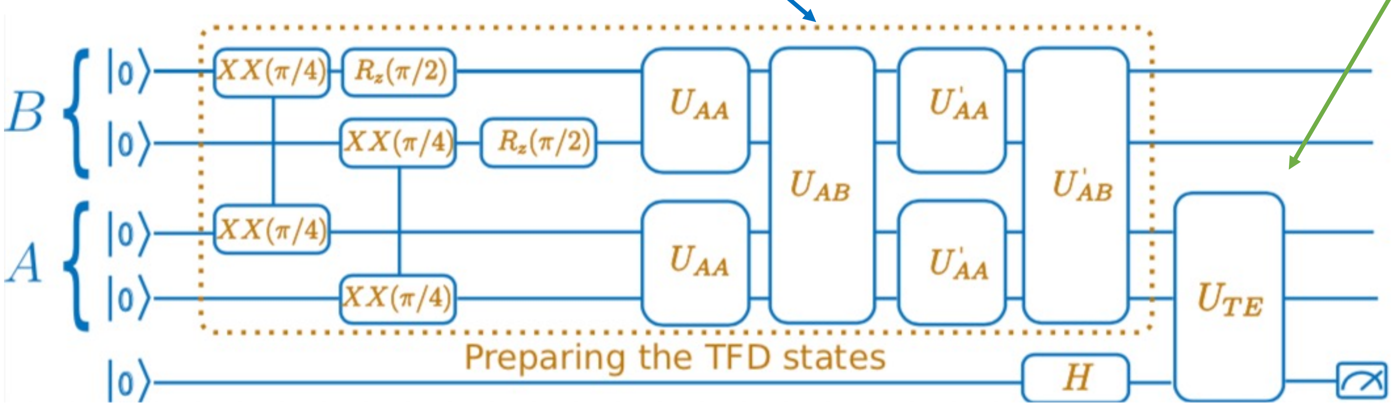
Generation of thermofield double states and critical ground states with a quantum computer

D. Zhu[a,b,c], S. Johri[d], N. M. Linke[a,b], K. A. Landsman[a,b], C. Huerta Alderete[a,b,e], N. H. Nguyen[a,b], A. Y. Matsuura[d], T. H. Hsieh[f], and C. Monroe[a,b,c,g,1]

$$|TFD(\beta)\rangle = \frac{1}{Z(\beta)} \sum_n e^{-\beta E_n/2} |n\rangle_A |n'\rangle_B$$

Time evolution
Apply imaginary *h* field

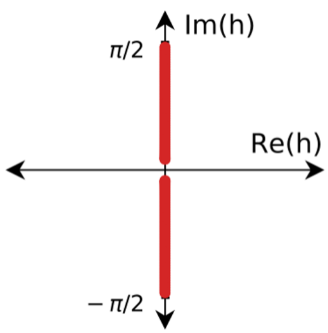
Measure ancilla coherence

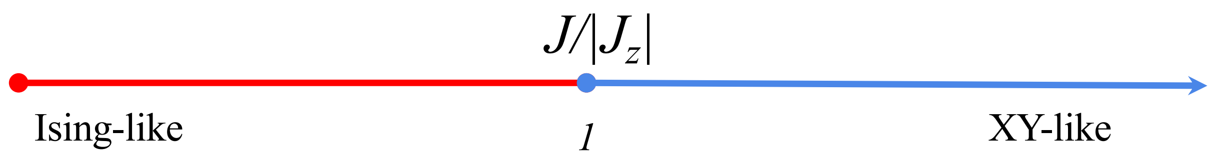


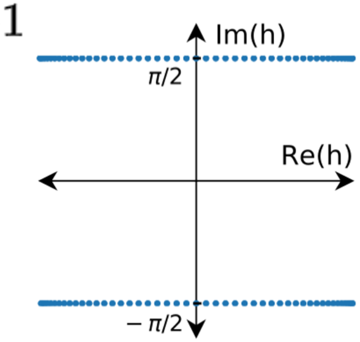
PNAS October 13, 2020 117 (41) 25402-25406

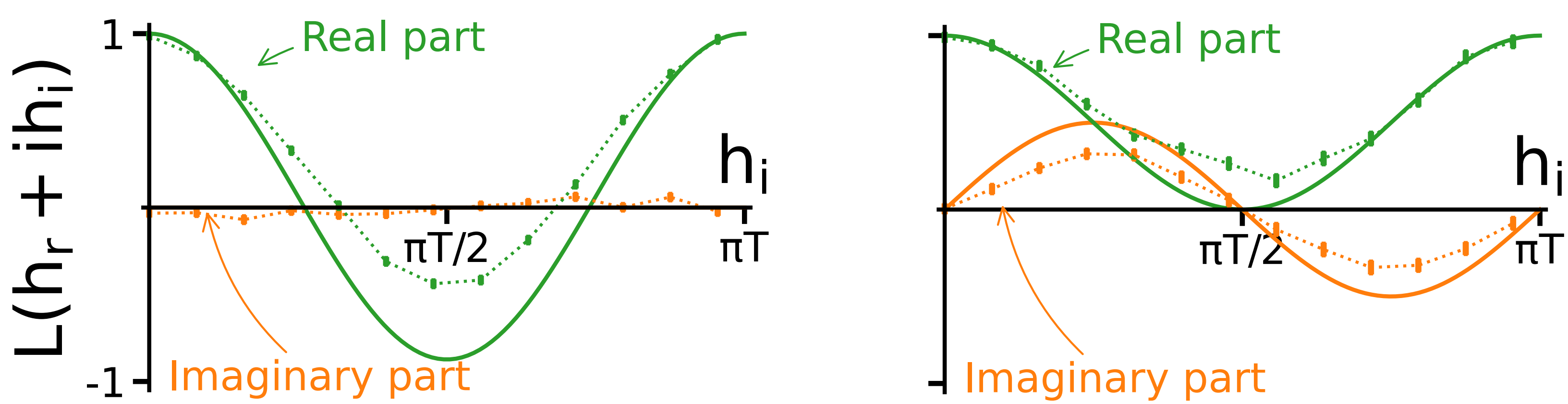
Partition Function Zeros of the XXZ model

$$H = J\sum_i(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) + J_z\sum_i \sigma_i^z\sigma_{i+1}^z$$



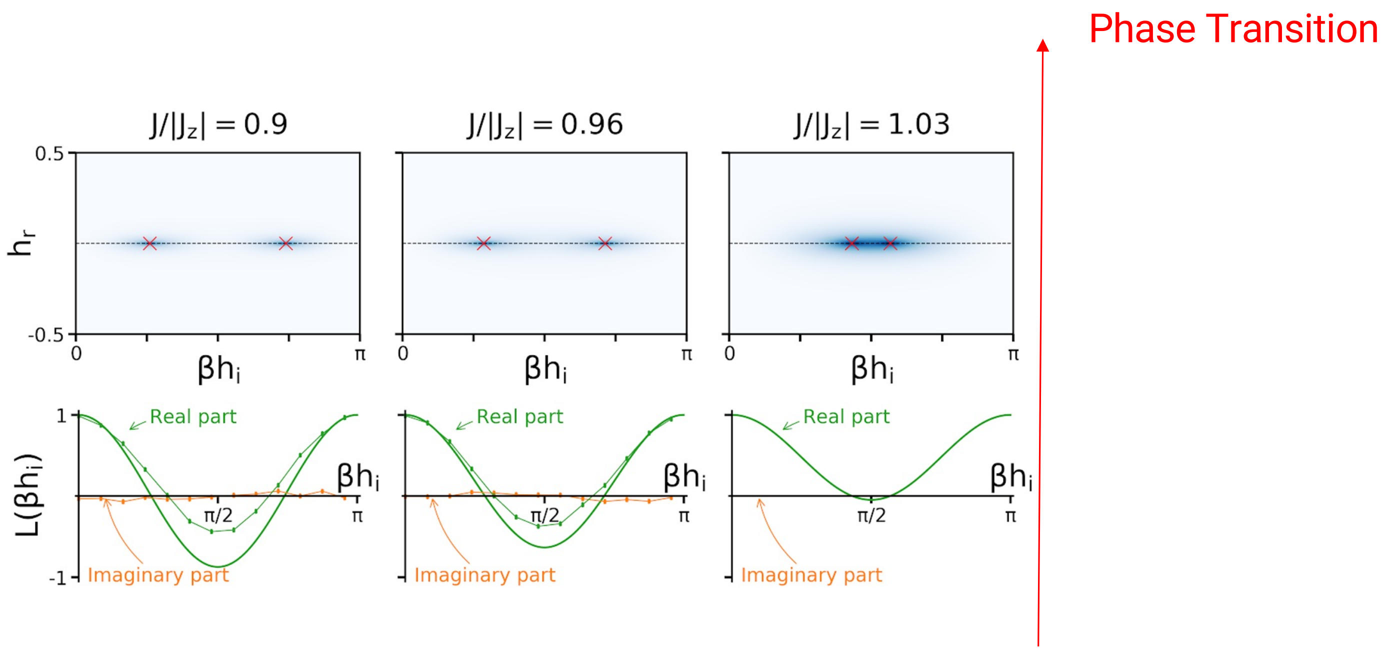






Trapped Ion Quantum Computer results from D. Zhu, C. Huerta Alderete, C. Monroe and N. Linke

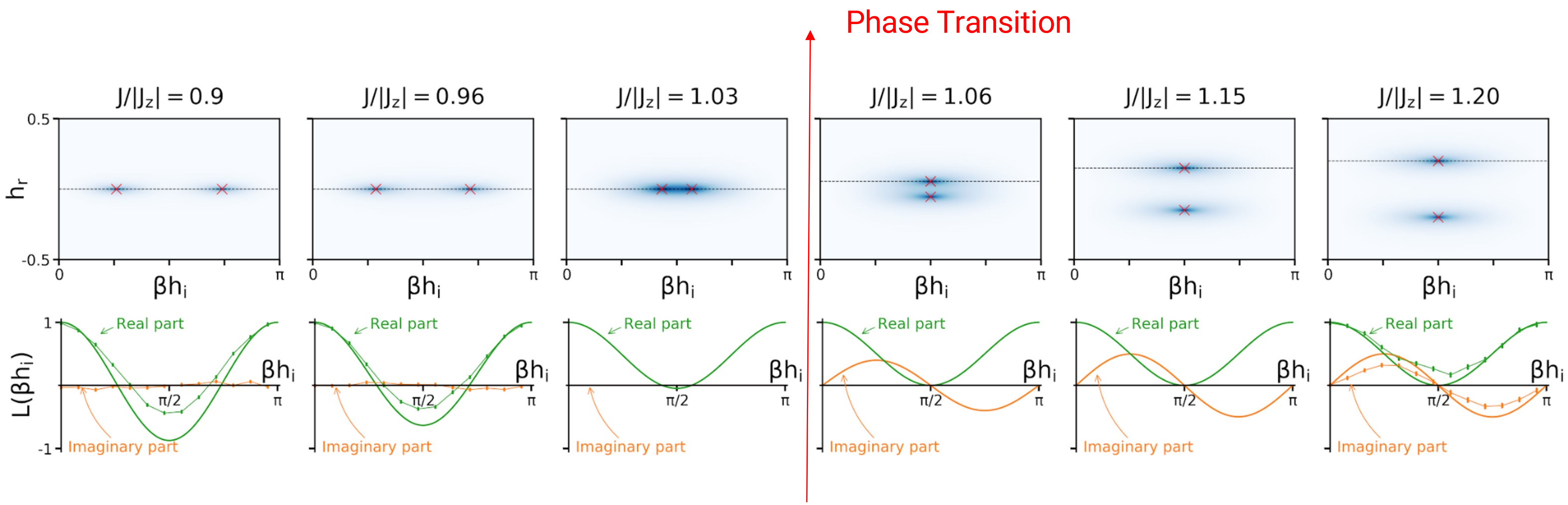
Measurement of L(t) for two-site system



The nature of zeros changes signaling a (Quantum) Phase Transition.

Science Advances Vol. 7, no. 34, eabf2447

Measurement of L(t) for two-site system



The nature of zeros changes signaling a (Quantum) Phase Transition.

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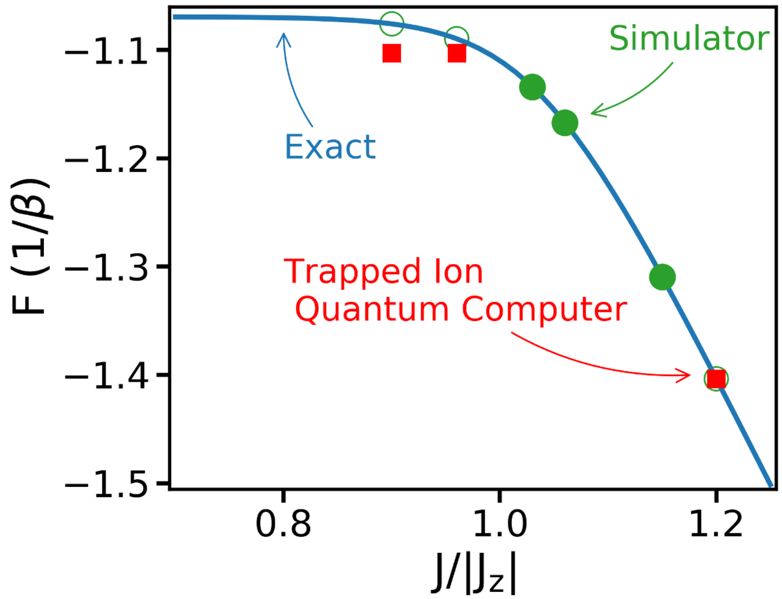
Reconstructing Partition function and Free Energy

Given the set of zeros measured from the quantum computer, we should now be able to reconstruct the partition function (and thus the free energy):

$$\mathcal{Z}(\beta, J, h) = c \prod_{h_0} (h - h_0)$$



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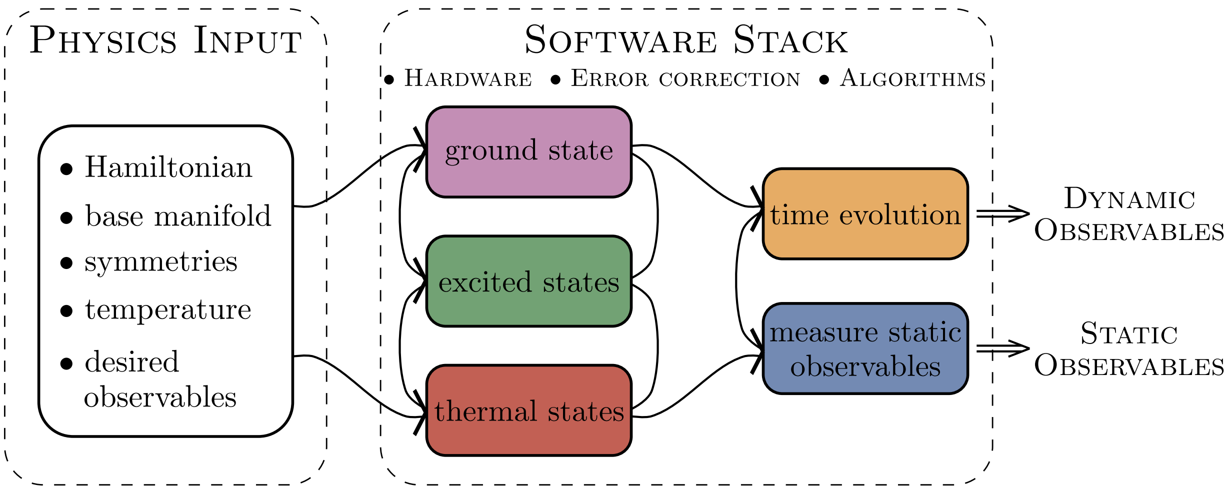
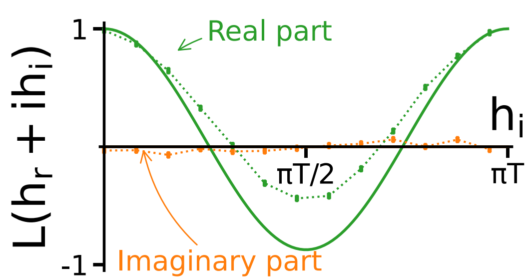
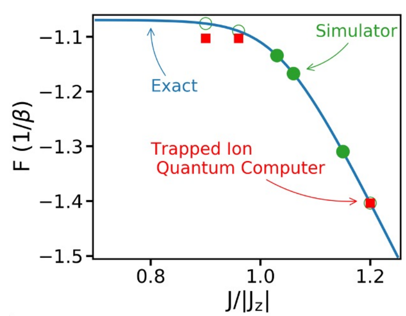
Quantum Matter meets Quantum Computing







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Emergence of topological matters (after 1980)

In 1980, the first ordered phase beyond symmetry breaking was discovered.

Electrons confined t
magnetic field show,
temperature, plateau
conductance" appea

$$\sigma_{xy} = n$$

How do we use quantum computers to determine topological properties?

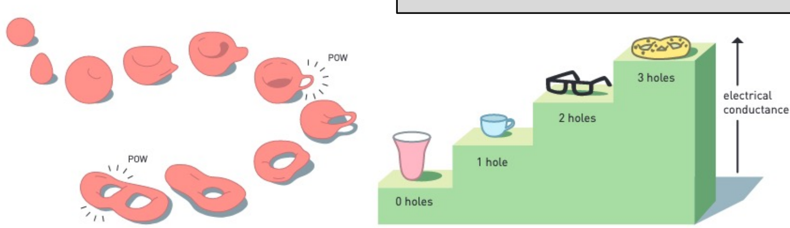
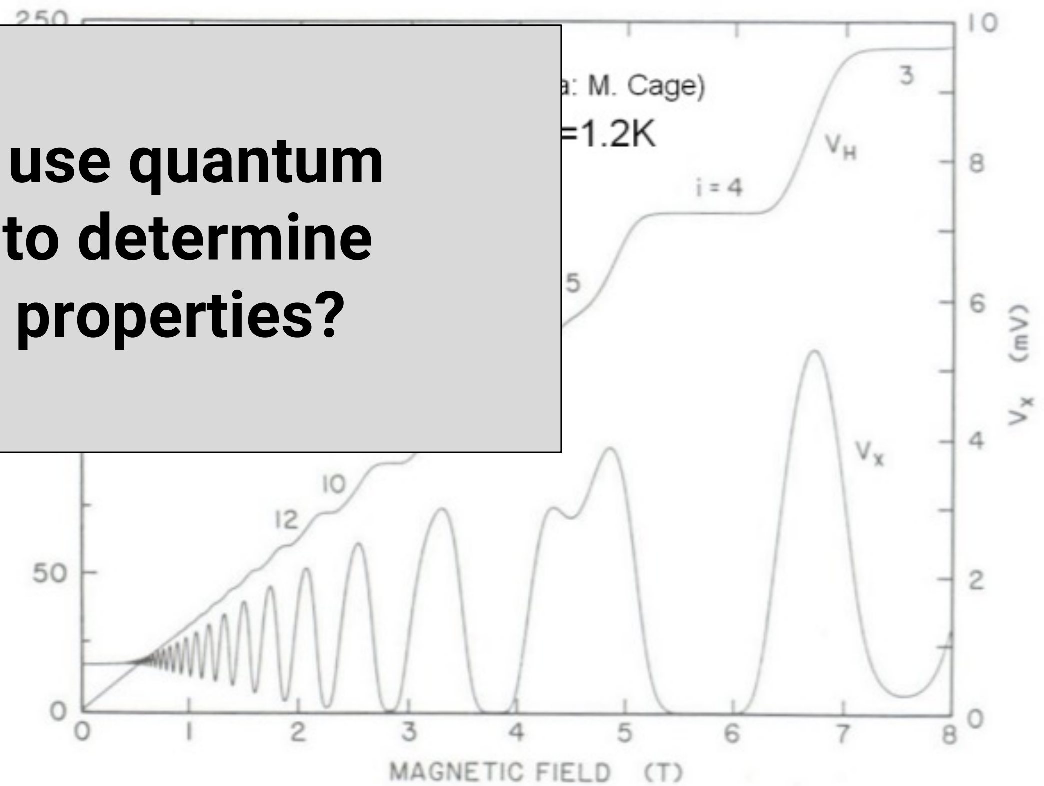


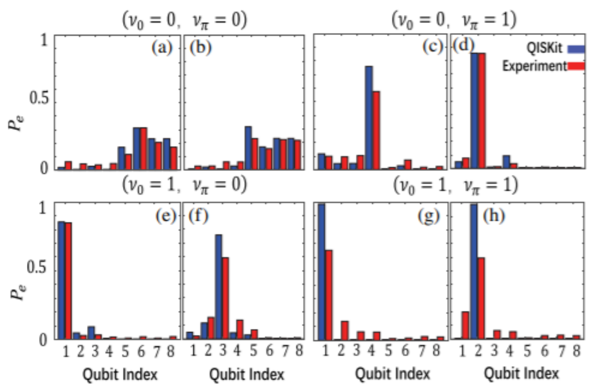
Fig 3. Topology. This branch of mathematics is interested in properties that change step-wise, like the number of holes in the above objects. Topology was the key to the Nobel Laureates' discoveries, and it explains why electrical conductivity inside thin layers changes in integer steps.

Nobel Prize in Physics 2016

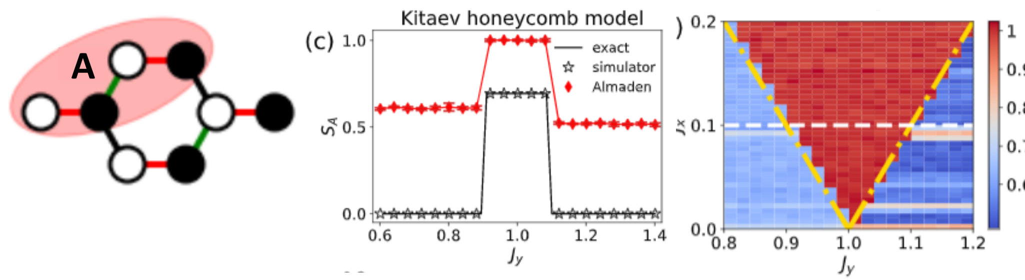


Topological states are robust… or are they?

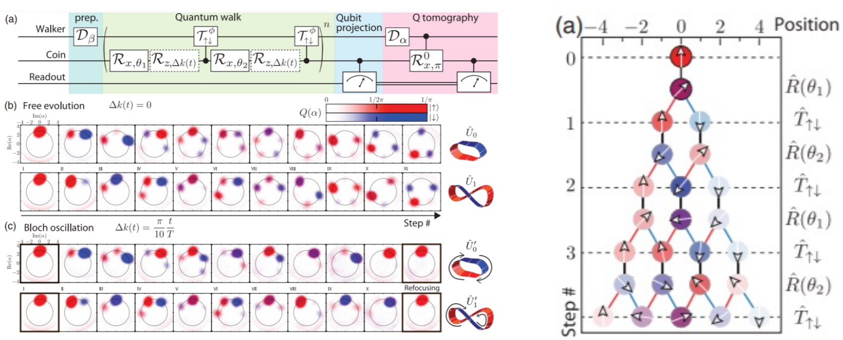
Floquet topological states, Mei et al (PRL 2020)



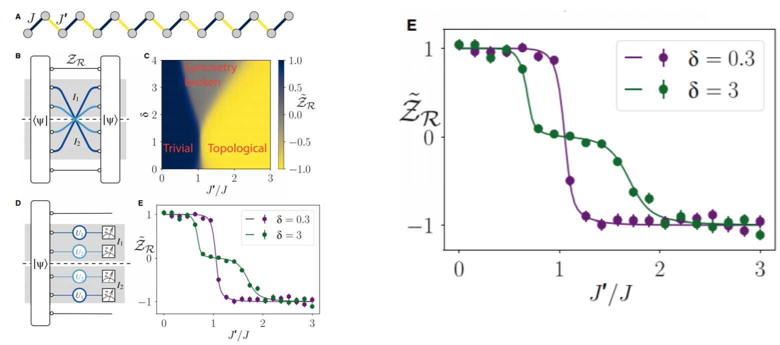
Kitaev Honeycomb Model, Xiao et al (arXiv:2006.05524)



1D topological quantum walk, Flurin et al (PRX 2017)



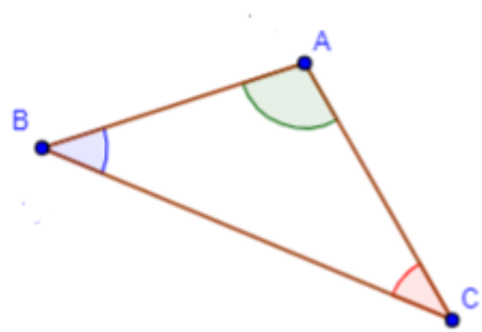
1D Symmetry Protected Topological (SPT) state, Elben (Sci Adv 2020)



A Brief Detour Into Geometry

The earth is round. [citation needed]

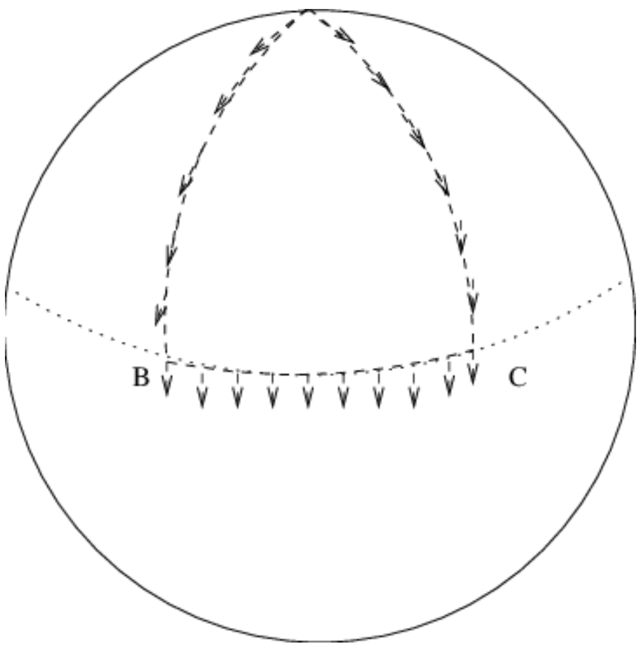
How can we tell?



$$\angle A + \angle B + \angle C = 180°$$

unless you're on a curved space...

A Brief Detour Into Geometry

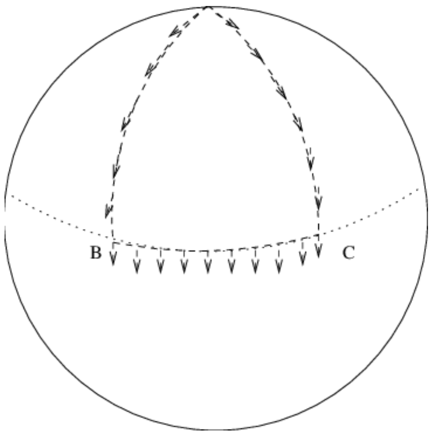


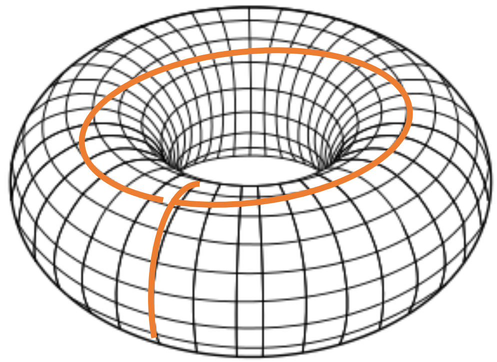
We could also use *parallel transport.*

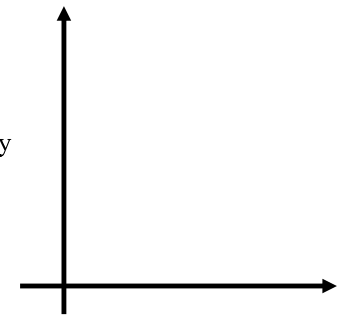
$$\frac{\partial}{\partial \vec{s}} \vec{v}$$

If you are on a curved space, as you make a loop your vector may point a different way than you started.

Quantum Geometry







$$\frac{\partial}{\partial \vec{s}}\vec{v} \quad \rightarrow \quad \langle \Psi_\Theta | \partial_\Theta | \Psi_\Theta \rangle$$

Q: If you walk a closed loop around the torus, what phase do you pick up?

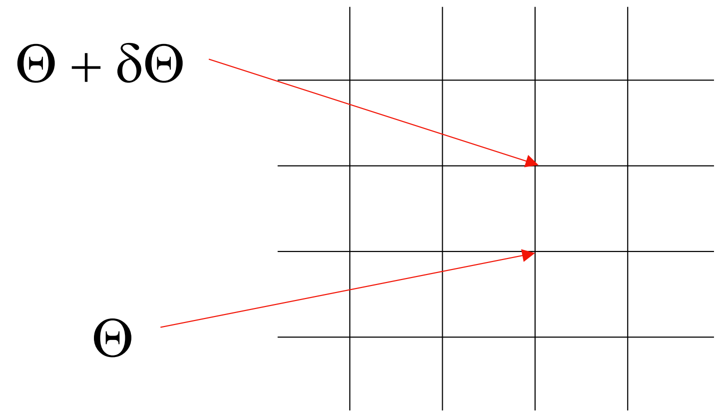
A: Some **integer** multiple of 2π

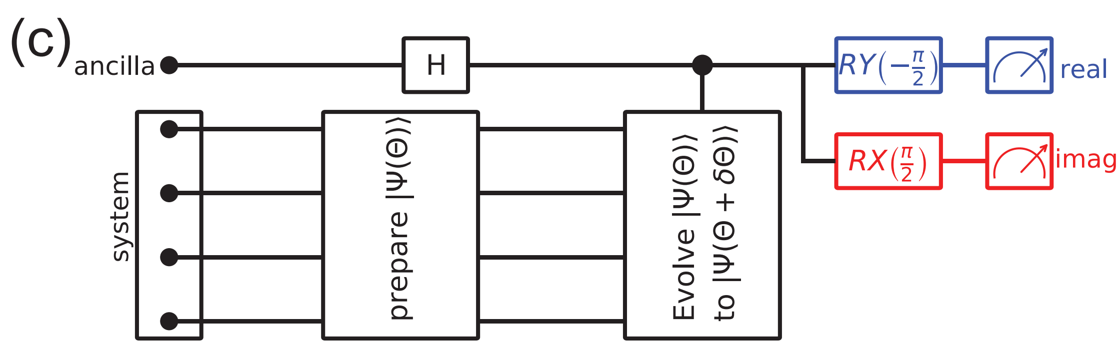
Quantum Geometry

How can we measure the topology of a wave function (bundle)?

$$\mathcal{C}_{Berry} = \langle \Psi_\Theta | \partial_\Theta | \Psi_\Theta \rangle$$

$$\delta\Theta \langle \Psi_\Theta | \partial_\Theta | \Psi_\Theta \rangle \approx \ln\left[1 + \delta\Theta \langle \Psi_\Theta | \partial_\Theta | \Psi_\Theta \rangle\right] \approx \ln \langle \Psi_\Theta | \Psi_{\Theta+\delta\Theta} \rangle$$



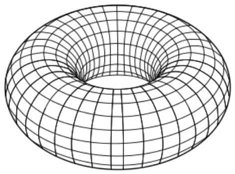


Quantum Geometry

Chiral *p*-wave superconductor

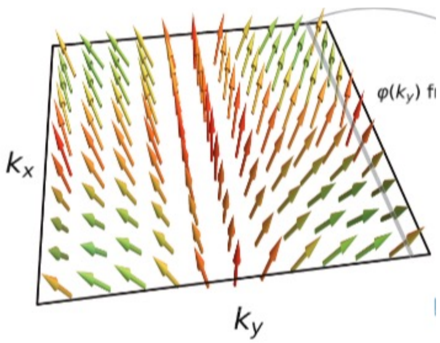
$$\mathcal{H}(\boldsymbol{k}) = \Delta(\sin k_y \sigma_x + \sin k_x \sigma_y) - \epsilon(\boldsymbol{k})\sigma_z$$

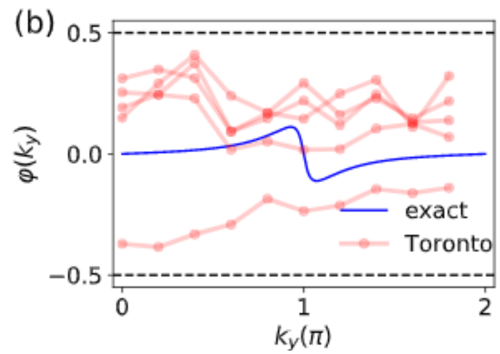
$$\epsilon(\boldsymbol{k}) = t(\cos k_x + \cos k_y) + \mu$$



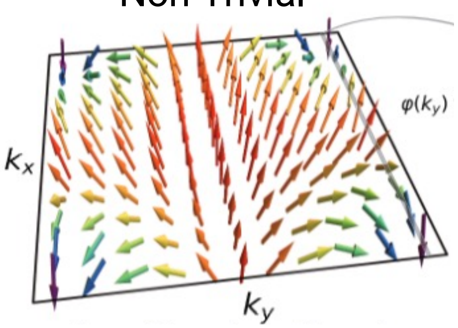
Phase: $2\pi\mathcal{C}$

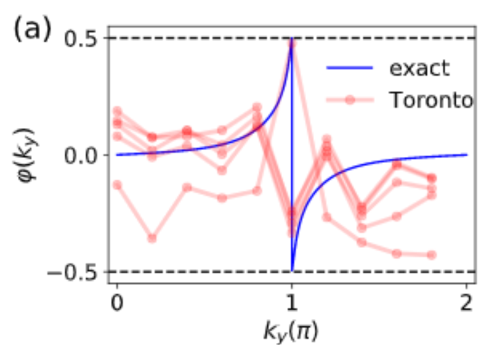
"Trivial"





"Non-Trivial"

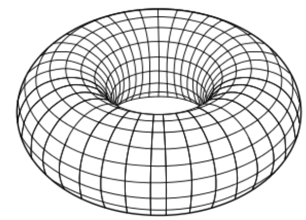




Chiral *p*-wave superconductor

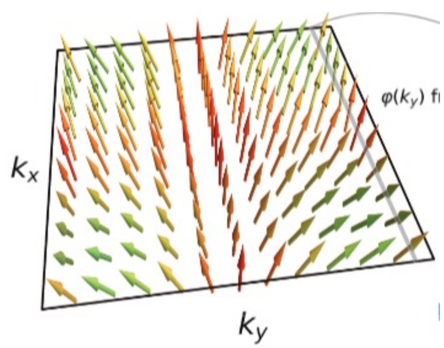
$$\mathcal{H}(\boldsymbol{k}) = \Delta(\sin k_y \sigma_x + \sin k_x \sigma_y) - \epsilon(\boldsymbol{k})\sigma_z$$

$$\epsilon(\boldsymbol{k}) = t(\cos k_x + \cos k_y) + \mu$$

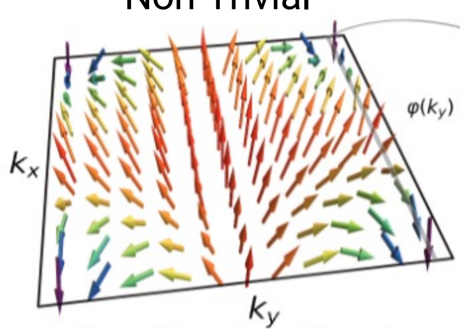


Phase: $2\pi\mathcal{C}$

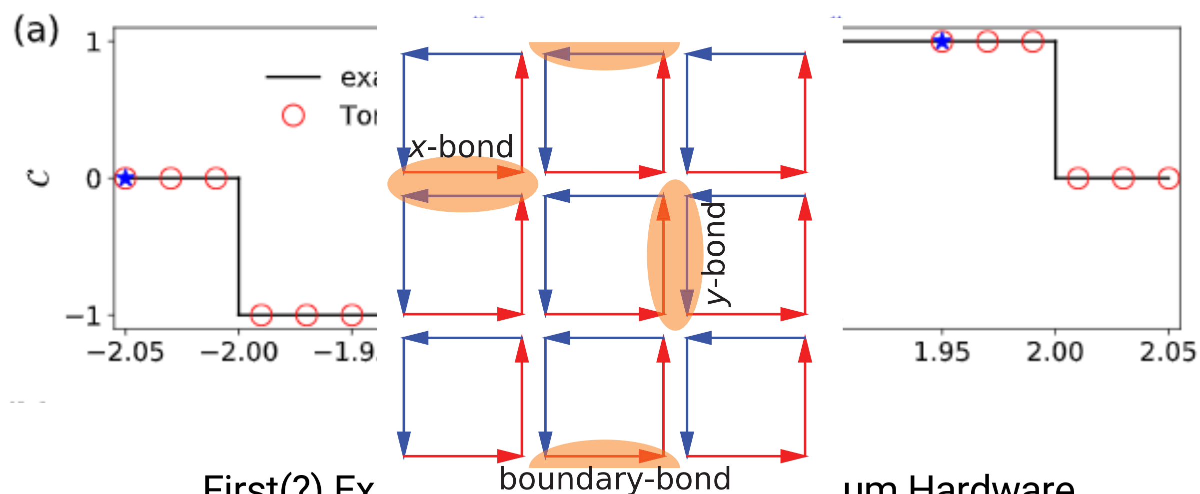
"Trivial"



"Non-Trivial"



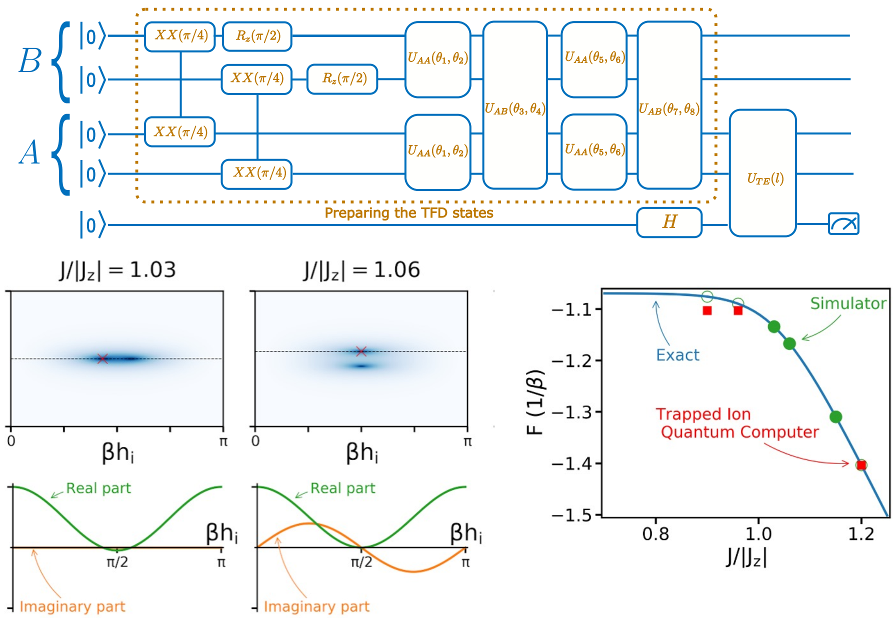
$$\mathcal{C} = \oint d\boldsymbol{k} \cdot \mathcal{A} = \int d^2k\, [\nabla \times \boldsymbol{A}(\boldsymbol{k})] \cdot \boldsymbol{n}_z = \int d^2k \mathcal{F}_{xy}(\boldsymbol{k}) \xrightarrow{discretize} \frac{1}{i2\pi} \sum_{\boldsymbol{k}} \mathcal{F}(\boldsymbol{k})$$



First(?) Ex ... um Hardware

Conclusion

- Thermodynamics on quantum computers using partition function zeros
- Examining topological physics on quantum computers



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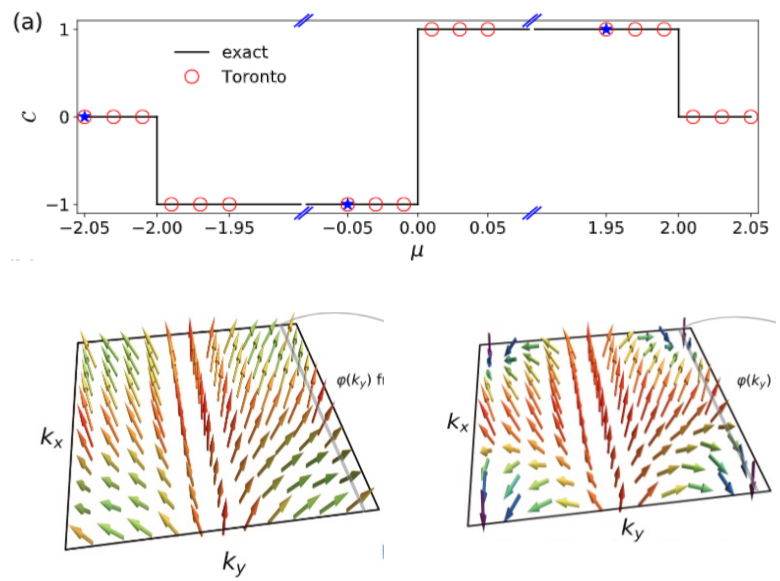
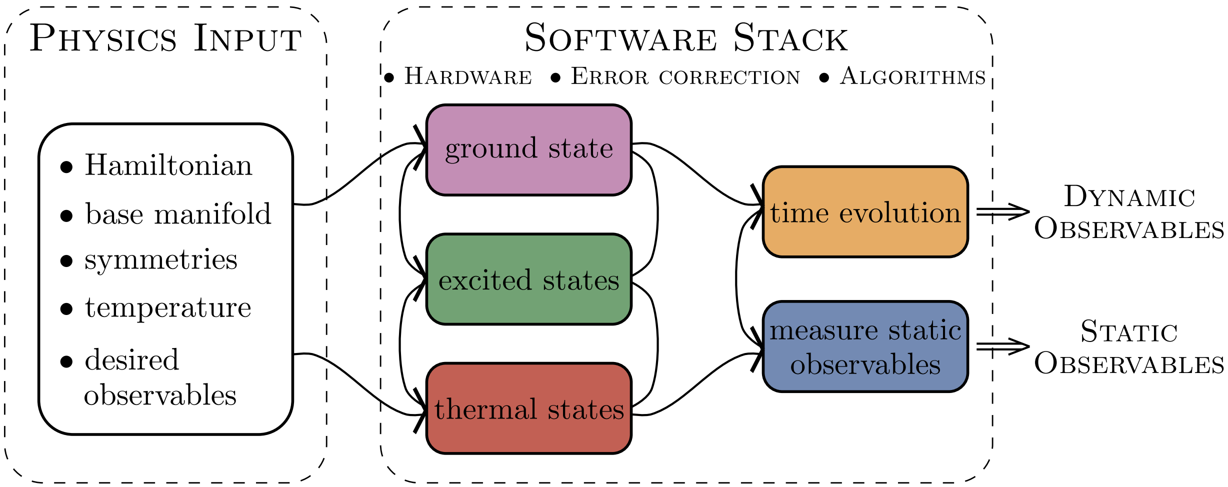
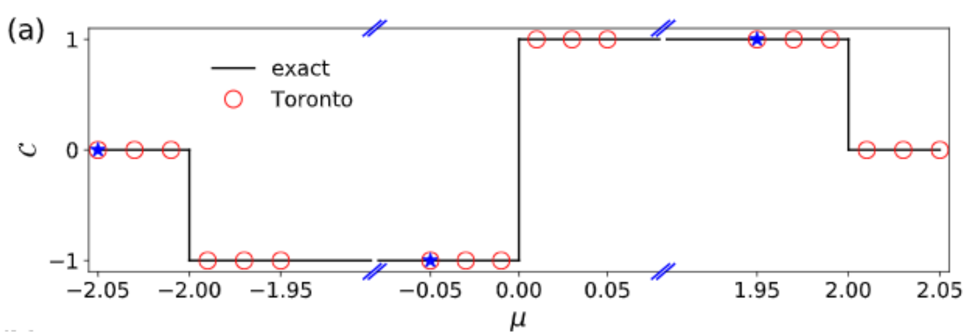


arXiv:2101.07283

Quantum Matter meets Quantum Computing





Exact measurement of Chern number on IBM quantum hardware:

2101.07283

- Measuring correlation functions
- Preparing/measuring topological states
- Modeling driven/dissipative systems
- Time evolution via Lie algebraic decomposition/compression
- Thermodynamics

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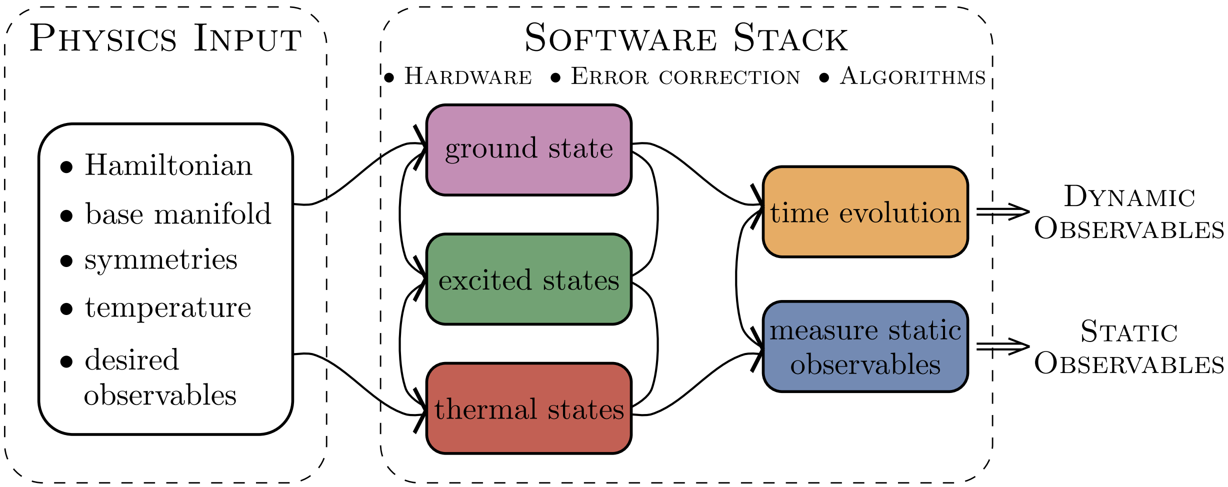
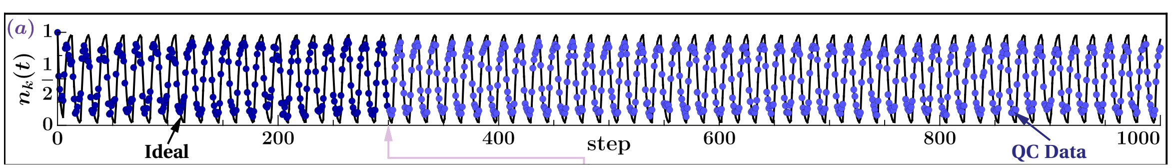
Quantum Matter meets Quantum Computing



1,000 Trotter steps of a driven/dissipative model on quantum hardware



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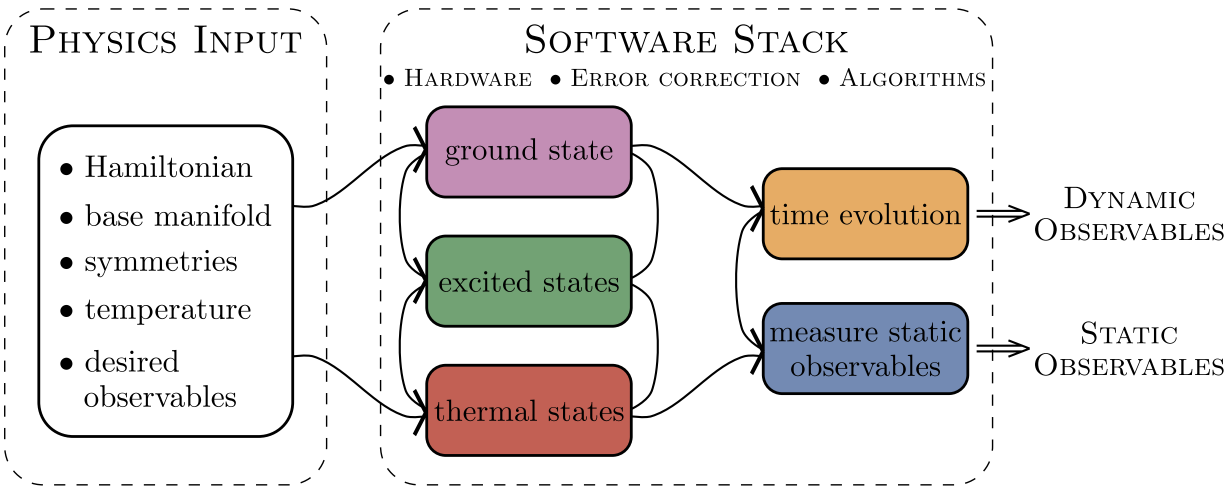

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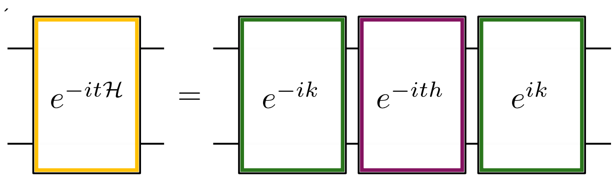
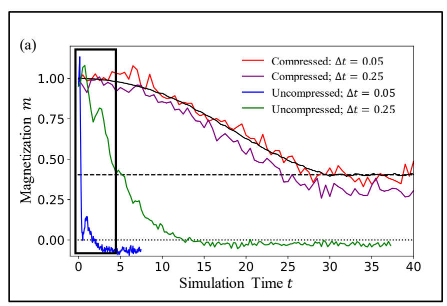
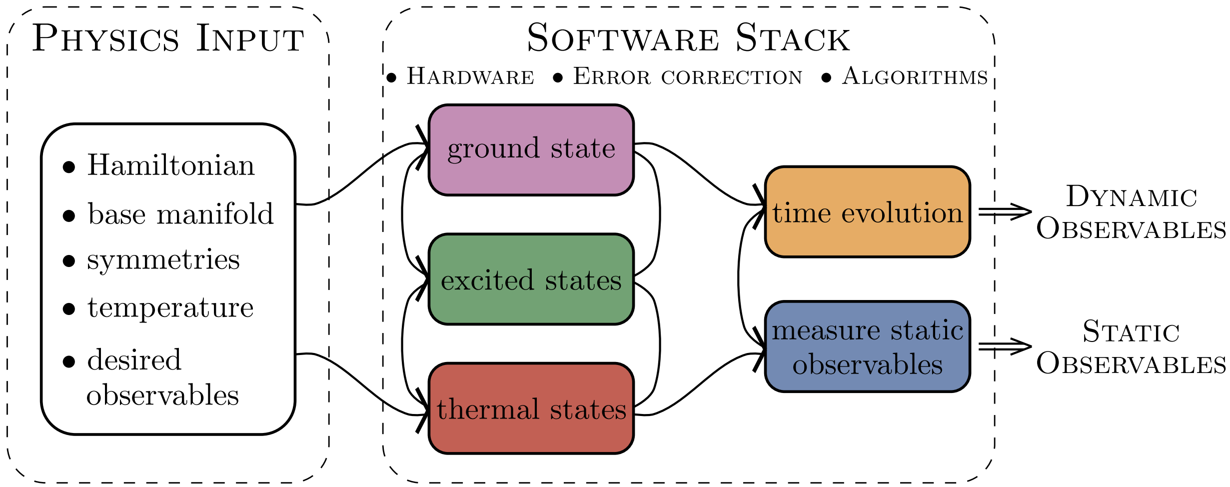
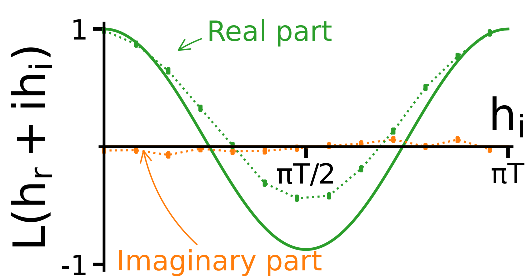


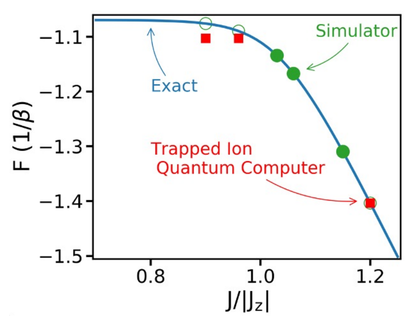
Building exact operator decompositions with Lie algebra



Quantum Matter meets Quantum Computing







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