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Quantum Computing Meets Condensed Matter Physics

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Alvarez Fellow Seminar
Lawrence Berkeley National Laboratory
04/05/2022

DARPA

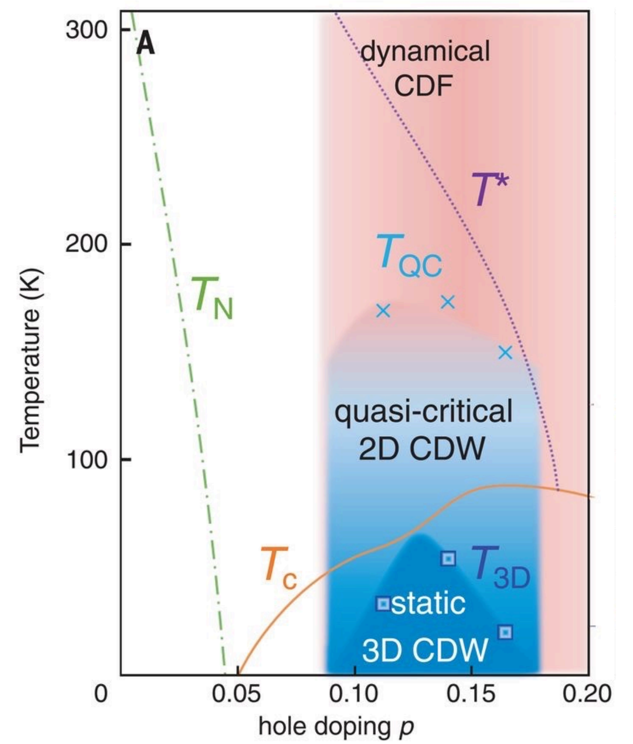
NSF DMR-1752713
PHY-1818914

DE-SC0019469

"It's not a cuprate talk unless it has a phase diagram…"

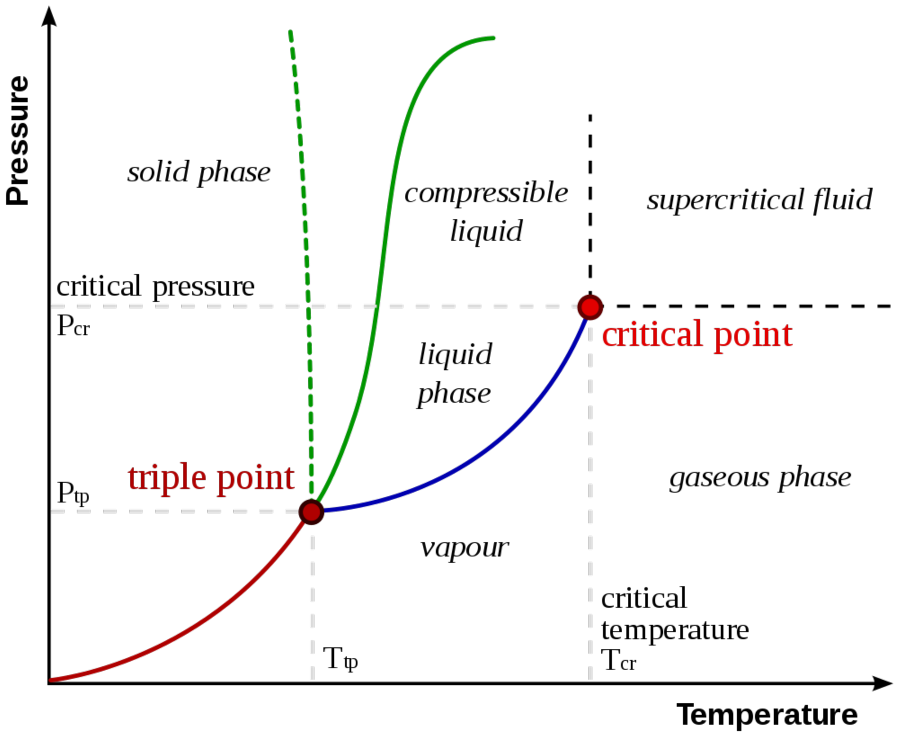
-- Overheard at APS March Meeting

$YBa_2Cu_3O_{7-x}$



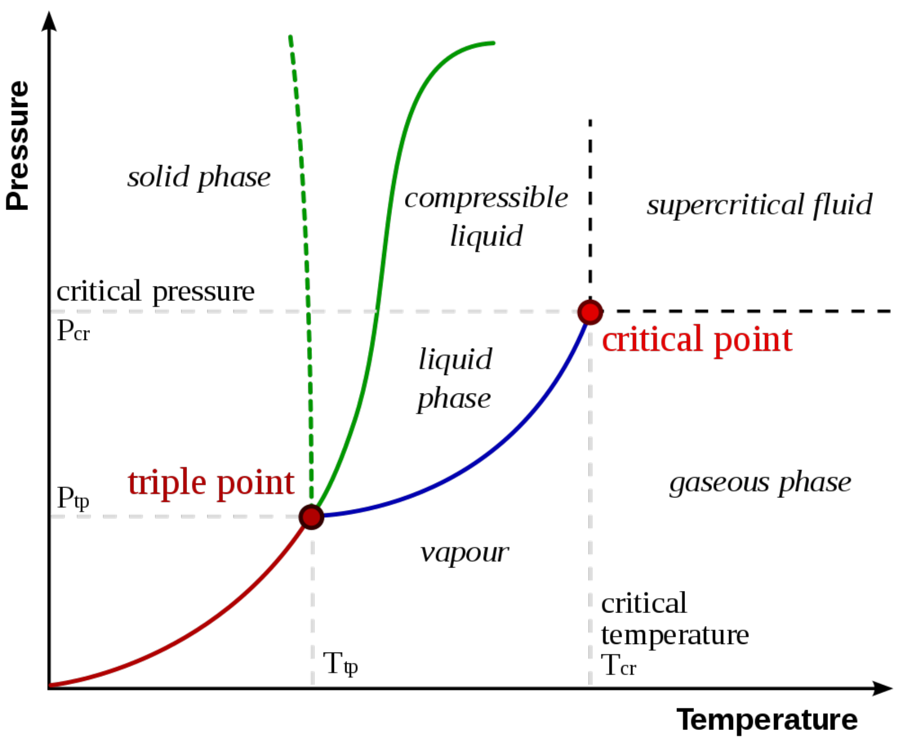
10.1126/science.aav1315

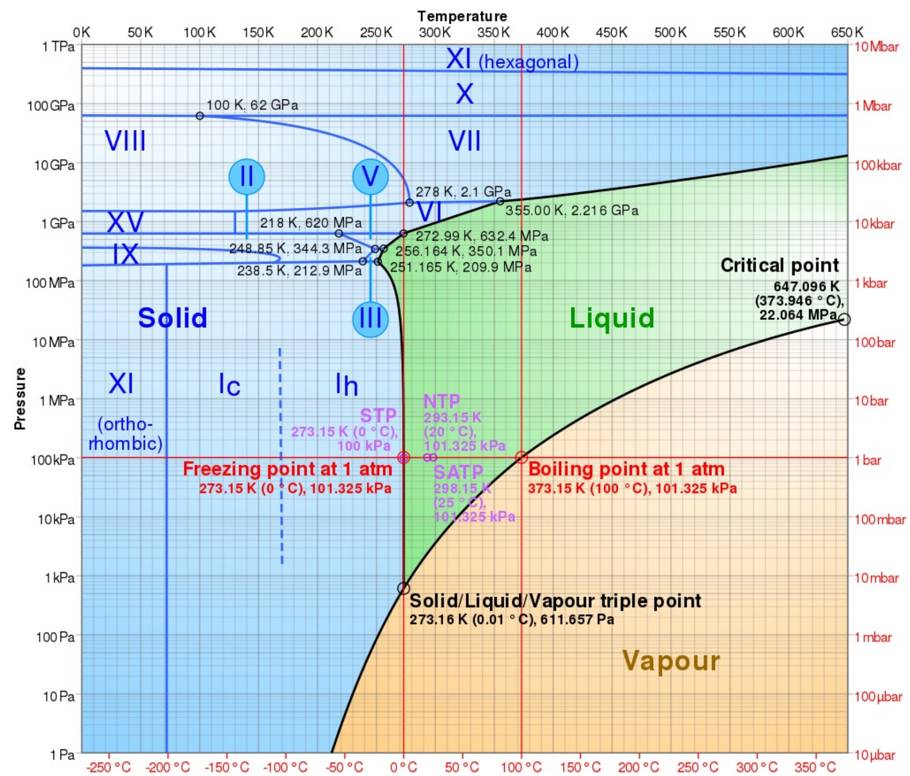
Phase diagrams and Phase transitions



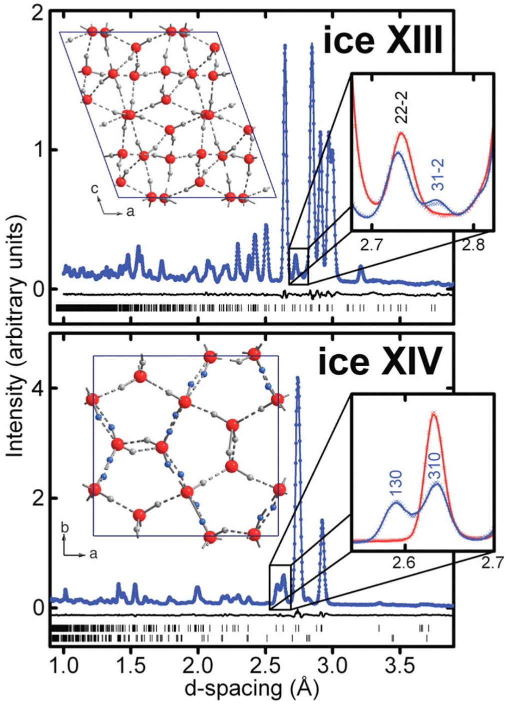
How many kinds (phases) of ice do we know about?

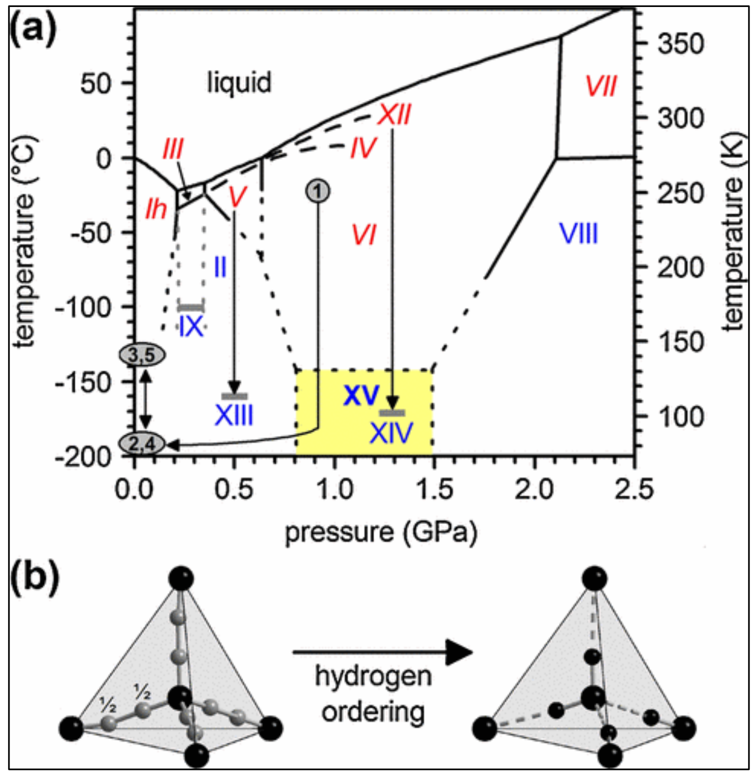
Phase diagrams and Phase transitions

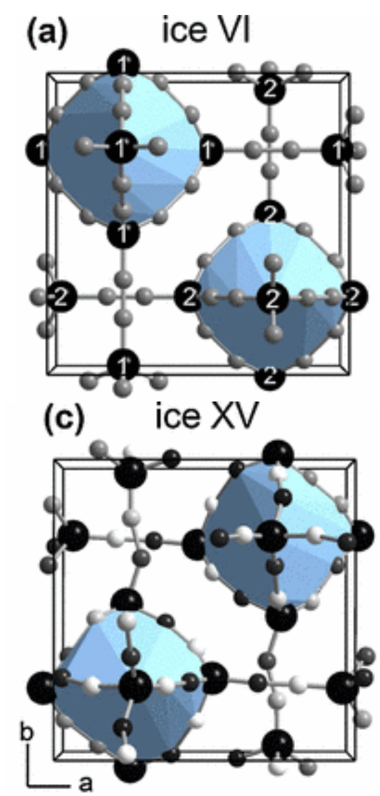




Phase diagrams and Phase transitions







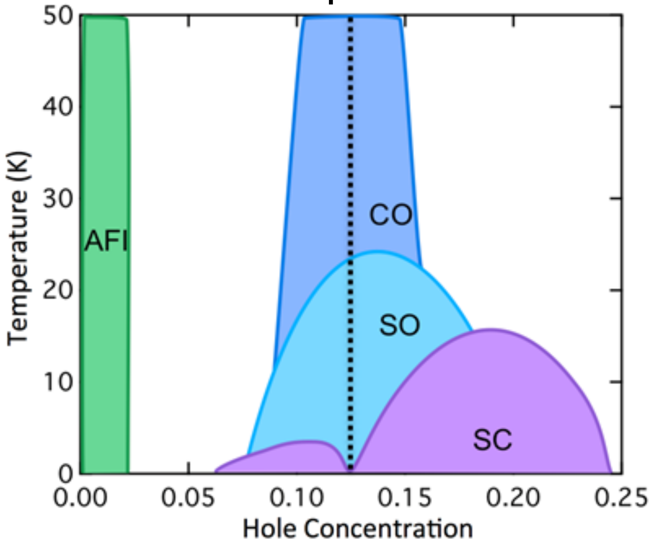
10.1126/science.1123896
10.1103/PhysRevLett.103.105701

Phase diagrams and Phase transitions

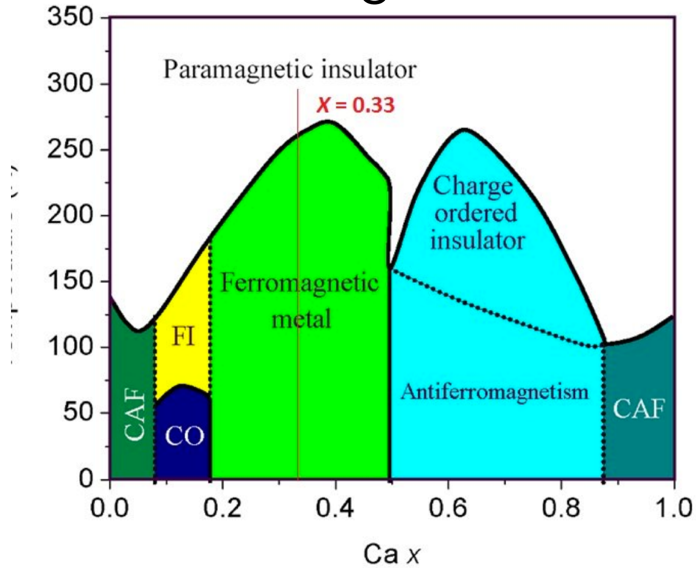
Group → / Period ↓	1	2	3		4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H																		2 He
2	3 Li	4 Be												5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg												13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc		22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y		40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	*	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	**	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Nh	114 Fl	115 Mc	116 Lv	117 Ts	118 Og
				*	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
				**	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

Sample phase diagrams from "hard" condensed matter

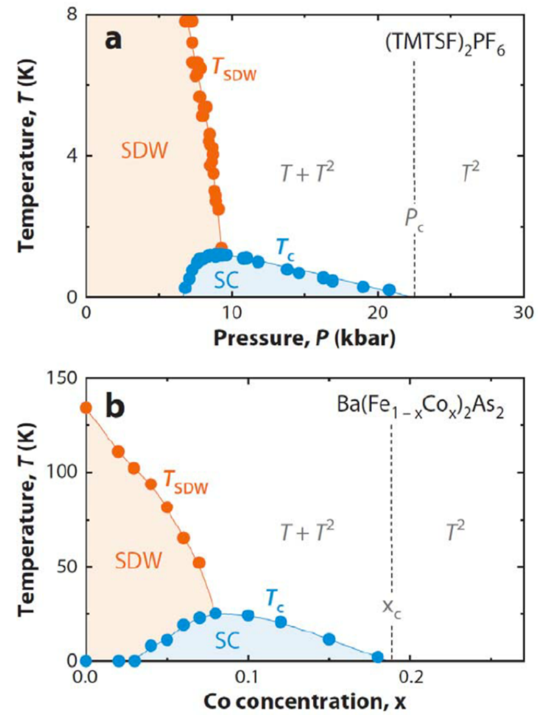
Cuprates



Manganites



Pnictides



10.1146/annurev-conmatphys-070909-104117

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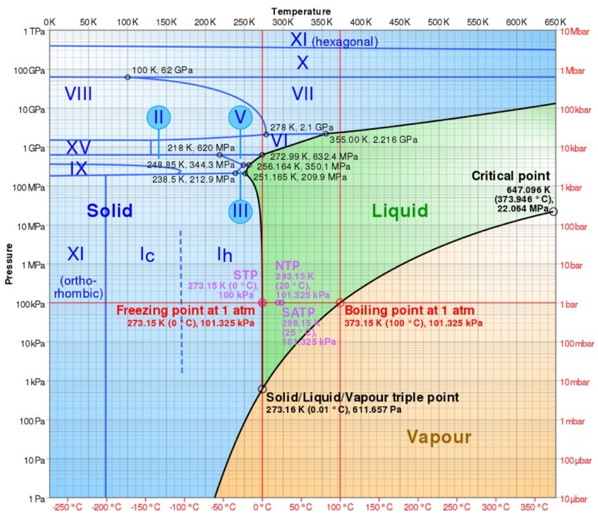
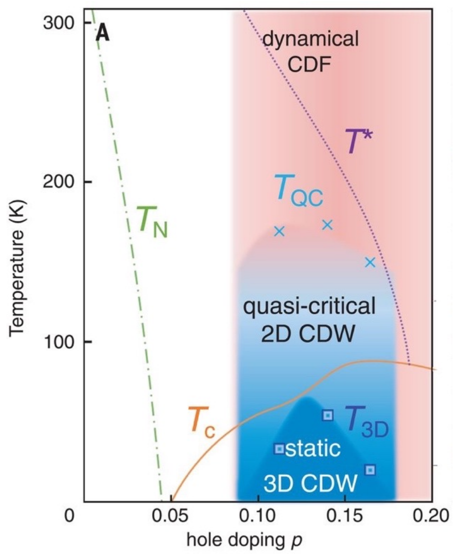
Why do we care about phase diagrams and transitions?

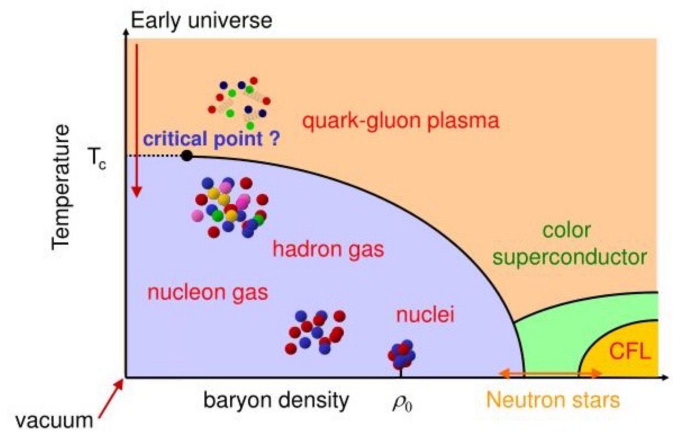
Fundamental science, of course!



Ice



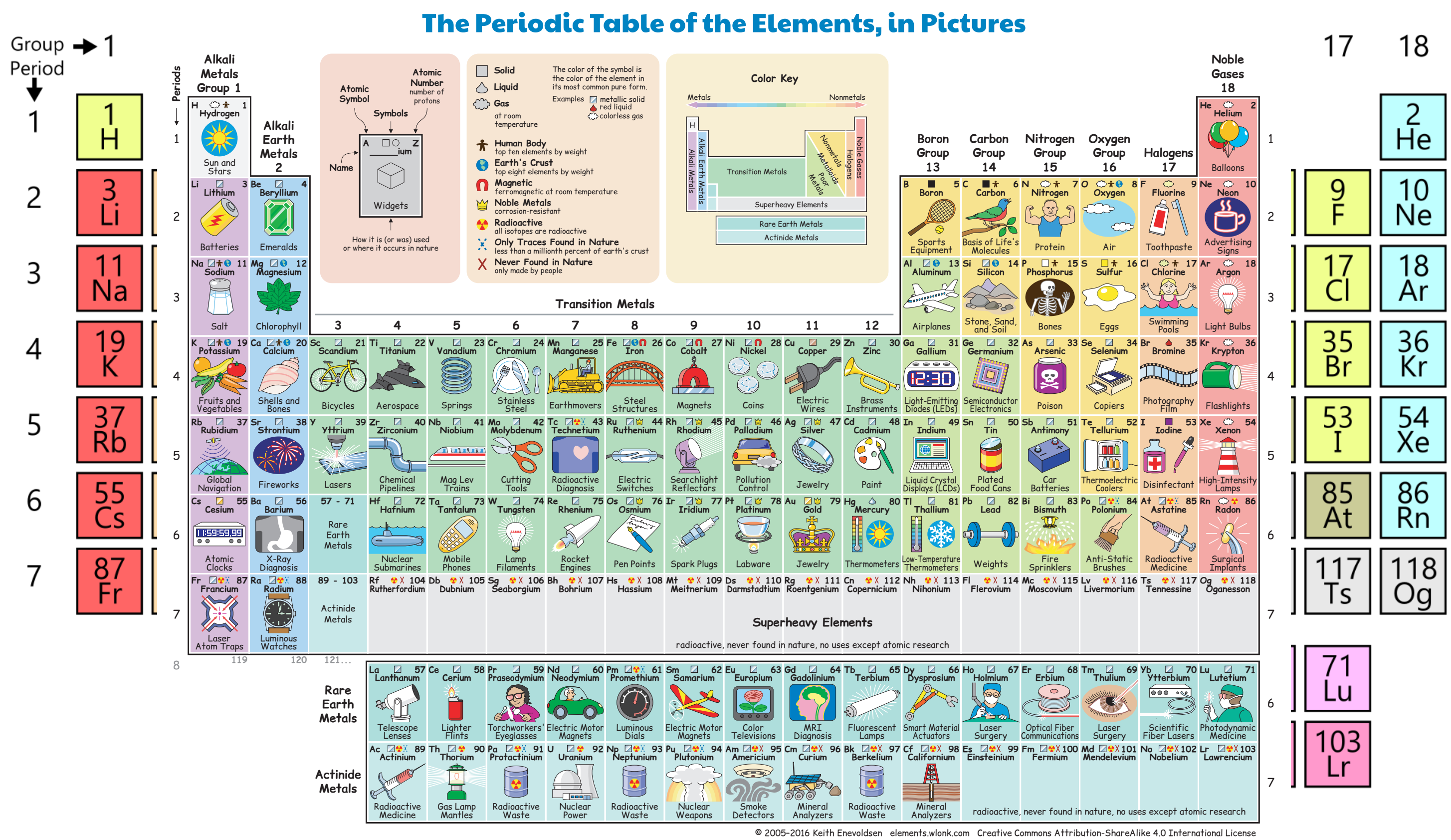
High-Tc cuprate superconductor



QCD

Why do we care about phase diagrams and transitions?

But also…



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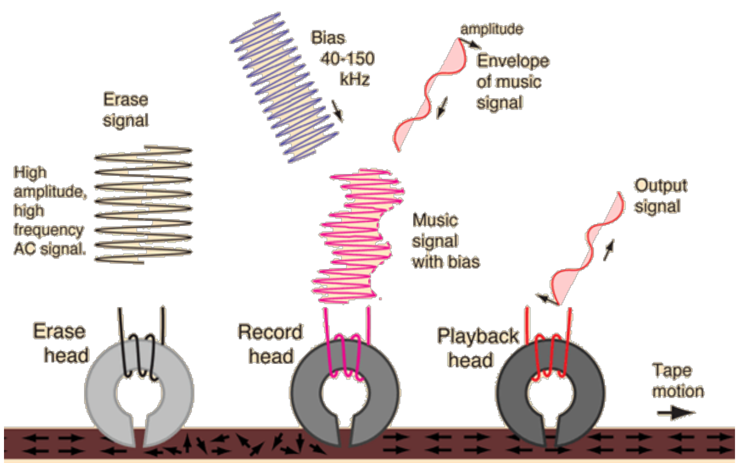
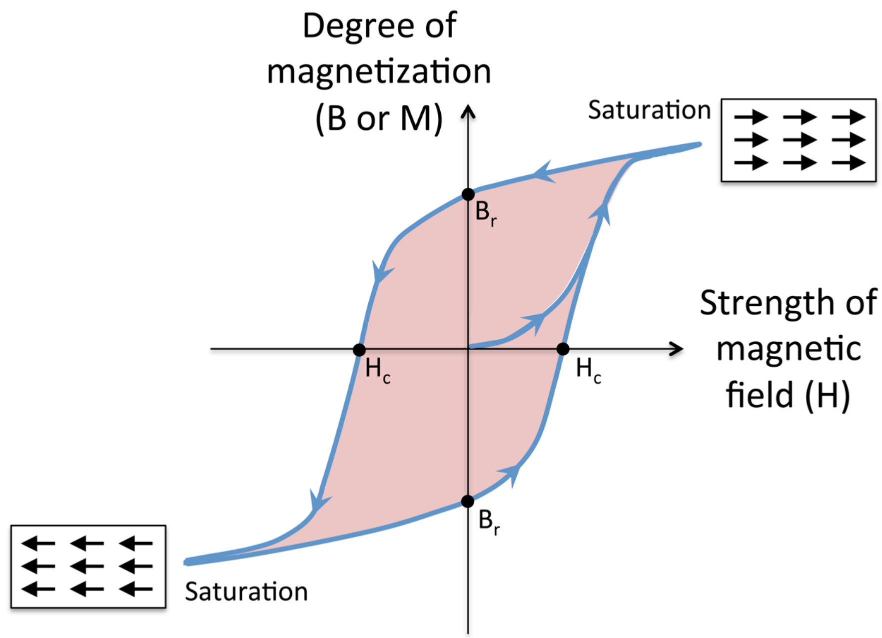
Why do we care about phase diagrams and transitions?





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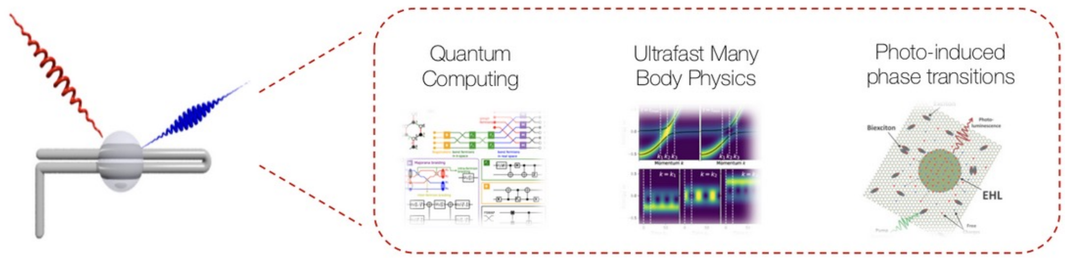
Why quantum computing for condensed matter?



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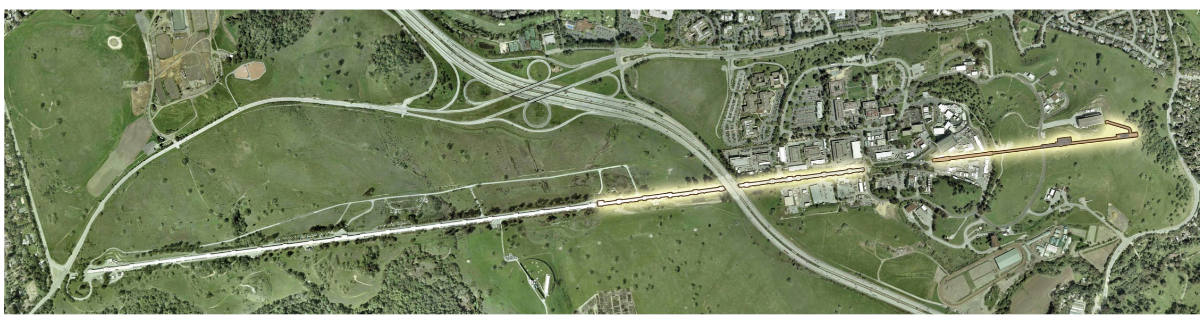
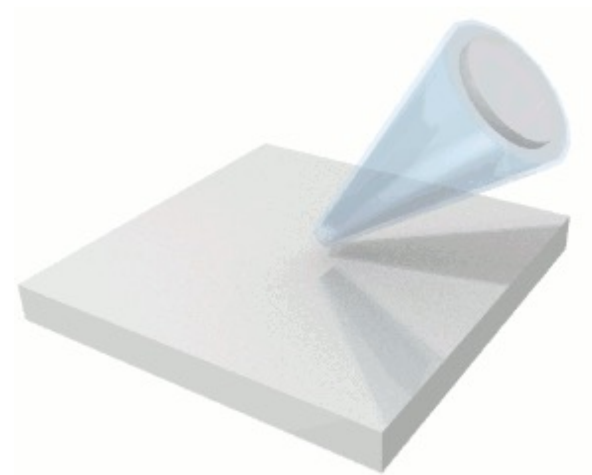
Quantum materials in and out of equilibrium.

Time-resolved experiments





Shen group (Stanford)

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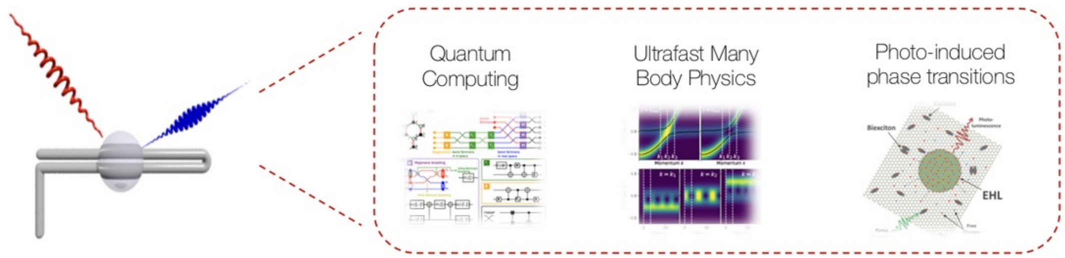

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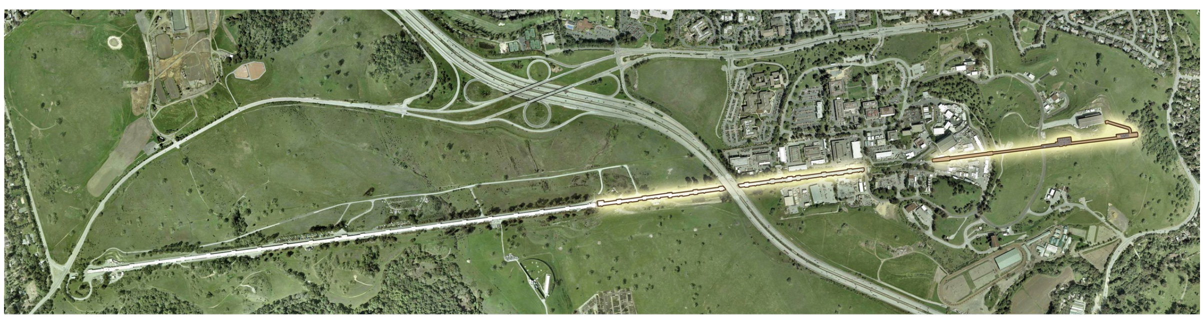
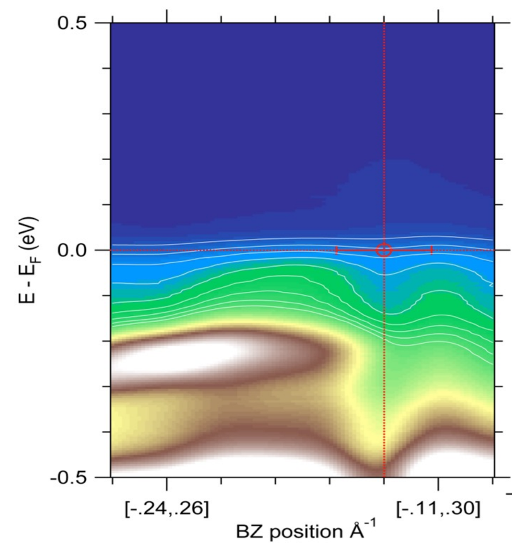


$ErTe_3$



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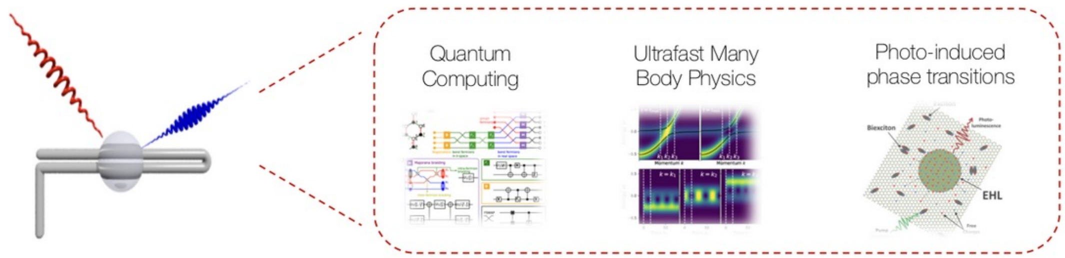

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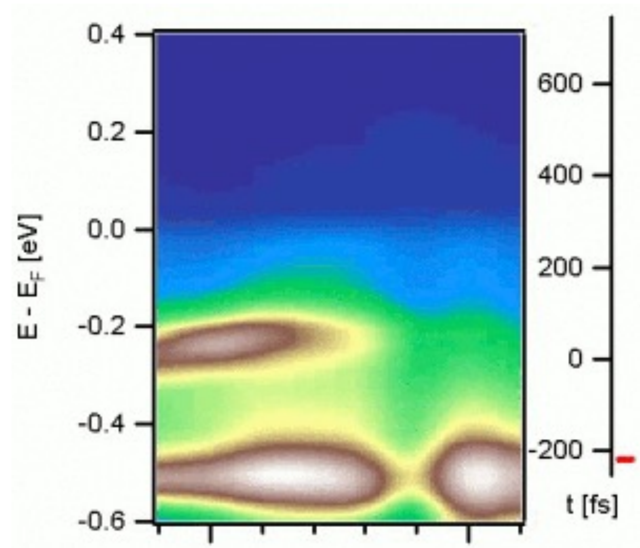
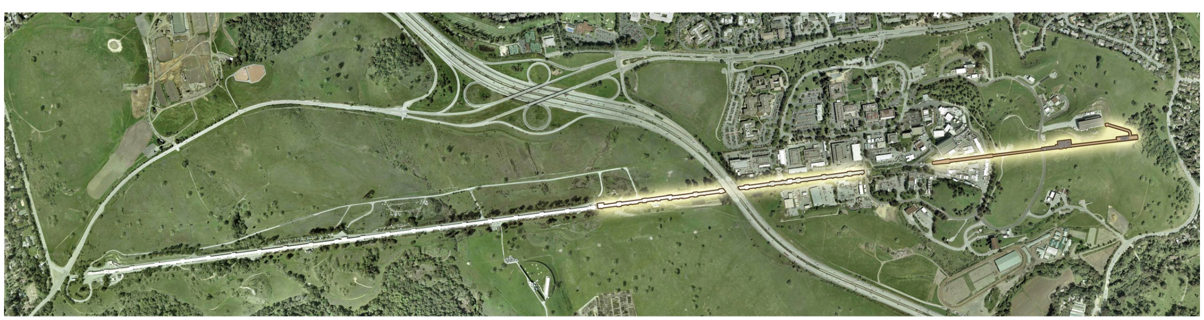


Time-resolved experiments



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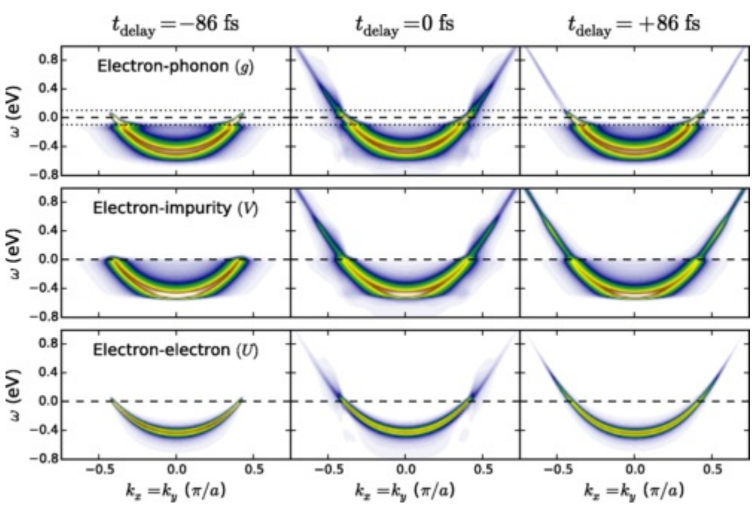
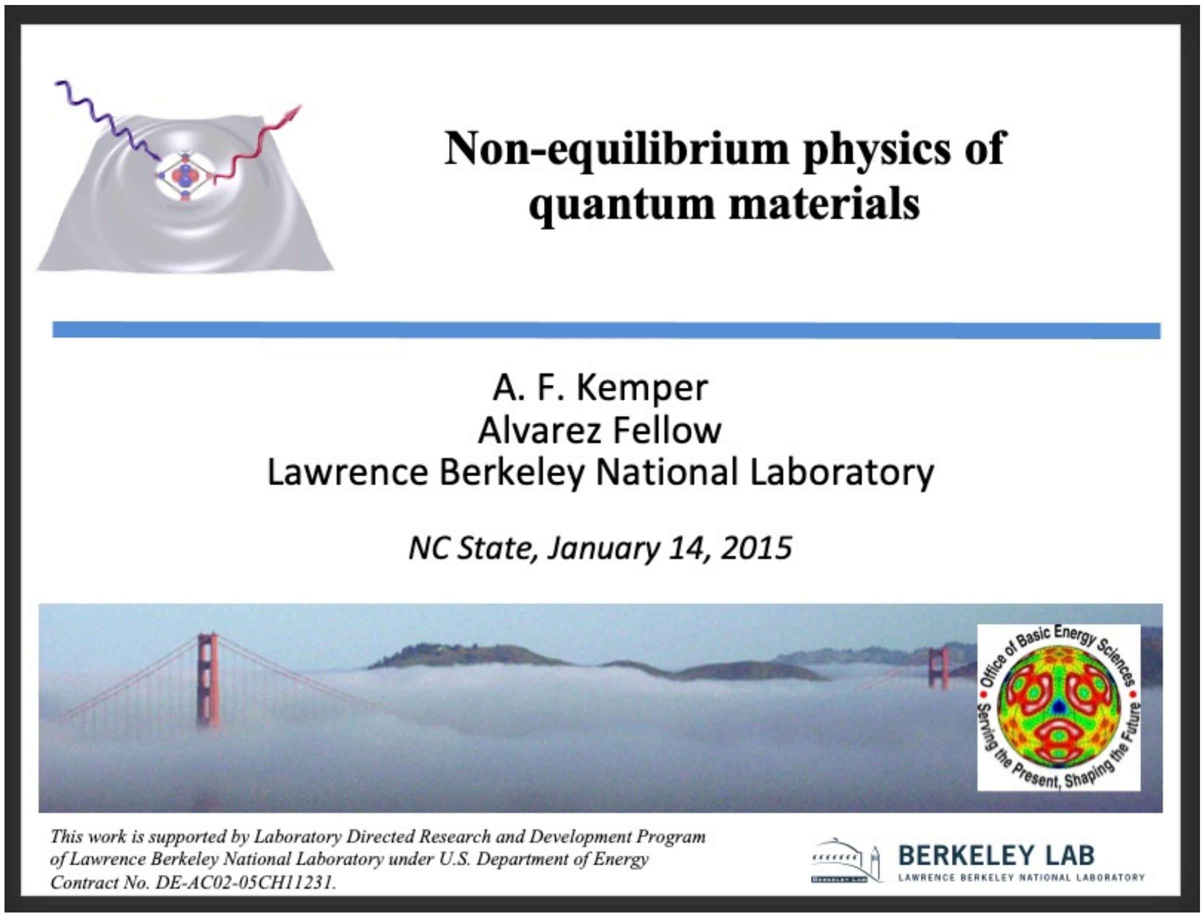


Non-Equilibrium Green's functions

Phys. Rev. X 8, 041009 (2018)


Non-equilibrium physics of quantum materials
A. F. Kemper
Alvarez Fellow
Lawrence Berkeley National Laboratory
NC State, January 14, 2015
Office of Basic Energy Sciences • Serving the Present, Shaping the Future •
This work is supported by Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC02-05CH11231.
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Theory background 2: Equations of motion

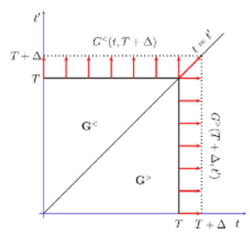
$$\left(i\partial_t - \varepsilon_{\mathbf{k}}\right)G_{\mathbf{k}}(t,t') = \delta(t-t') + \int d\bar{t}\,\Sigma(t,\bar{t})G_{\mathbf{k}}(\bar{t},t')$$

*Green's function for quantum state **k***

Interaction kernel, depends on $G_{\mathbf{k}}$

- Non-linear initial value problem
- Results depend on the history

Time stepping method:
A.Stan, N.E.Dahlen, R. van Leeuwen, J.Chem.Phys.130, 224101 (2009)

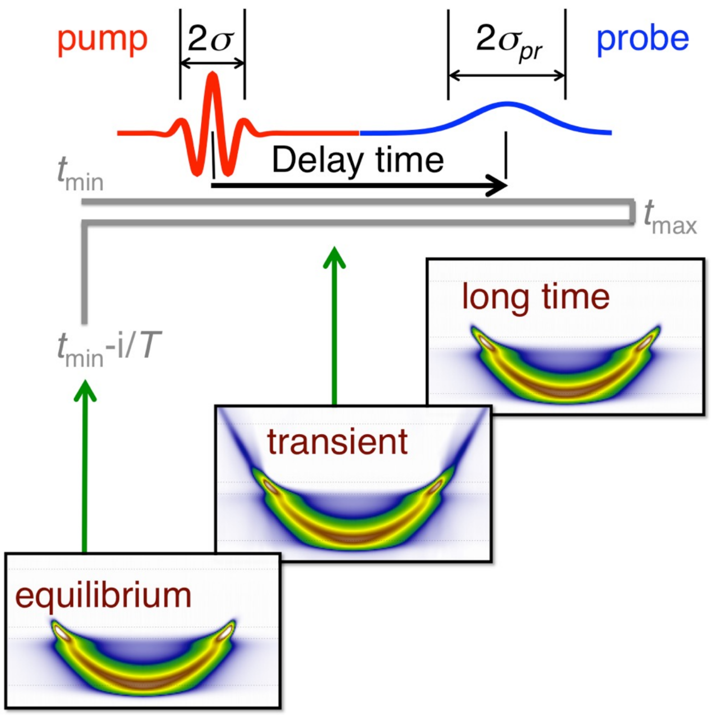


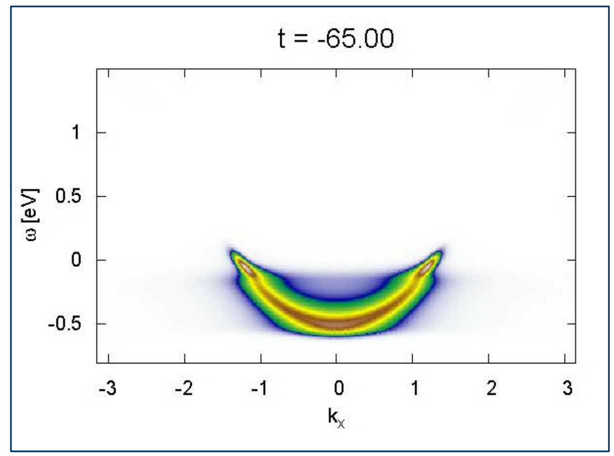
(Some) computational details

$$\left(i\partial_t - \varepsilon_{\mathbf{k}}\right)G_{\mathbf{k}}(t,t') = \delta(t-t') + \int d\bar{t}\,\Sigma(t,\bar{t})G_{\mathbf{k}}(\bar{t},t')$$

- 6,400 quantum ***k*** states are needed (somewhat reducible by symmetry)
- For each ***k***, the G matrix must be stored and one copy of Σ
  - Roughly 20 million unique entries
  - Entries are complex double 1x1 or 2x2 matrices (0.5 Gb or 2 Gb)
- Hybrid parallelism
  - MPI used to distribute set of G_k among MPI tasks
  - OpenMP used to parallelize integrations and other time loops

Pump-probe photoemission simulations

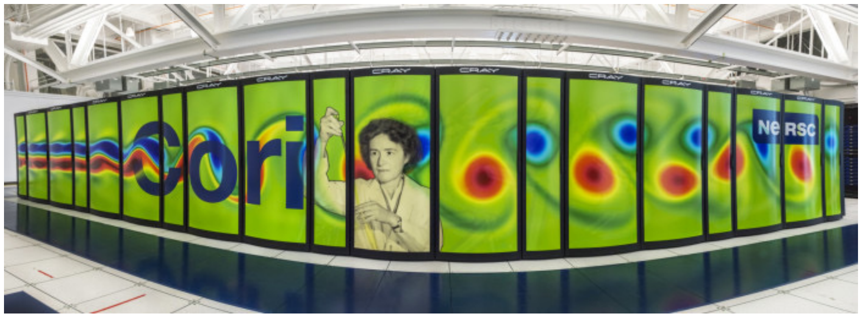


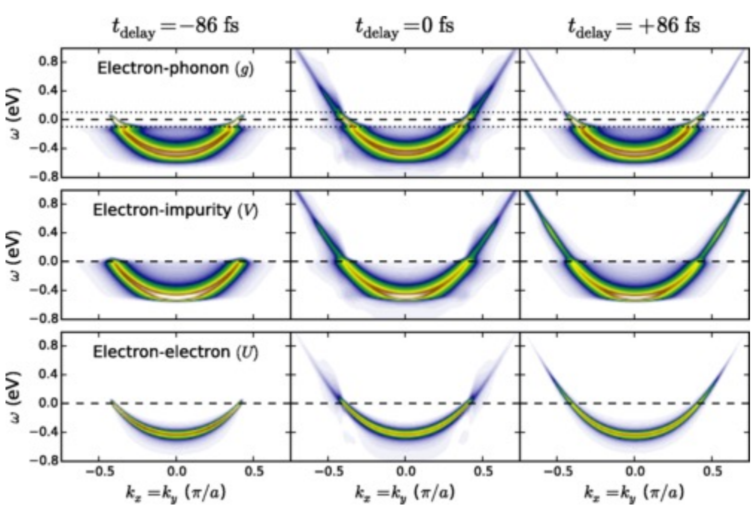


M. Sentef et al, PRX (2013)

$$A_{\mathbf{k}}(\omega, t_0) = \mathrm{Im}\ \frac{1}{2\pi\sigma^2}\int dt dt' \boxed{G^<_{\mathbf{k}}(t,t')}\boxed{e^{-(t-t_0)^2/2\sigma^2}e^{-(t'-t_0)^2/2\sigma^2}}e^{i\omega(t-t')}$$

Why quantum computing for condensed matter?





Non-Equilibrium Green's functions

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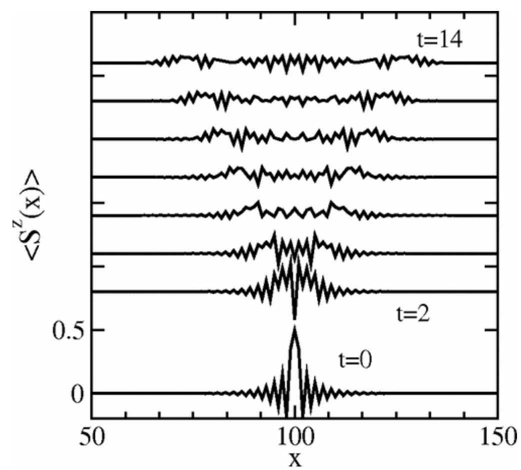
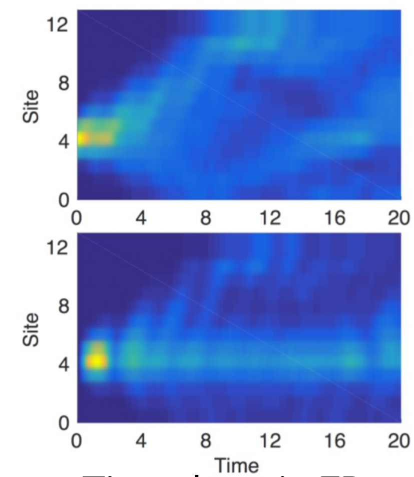


Time domain DMRG

Phys. Rev. Lett. 93, 076401 (2004)

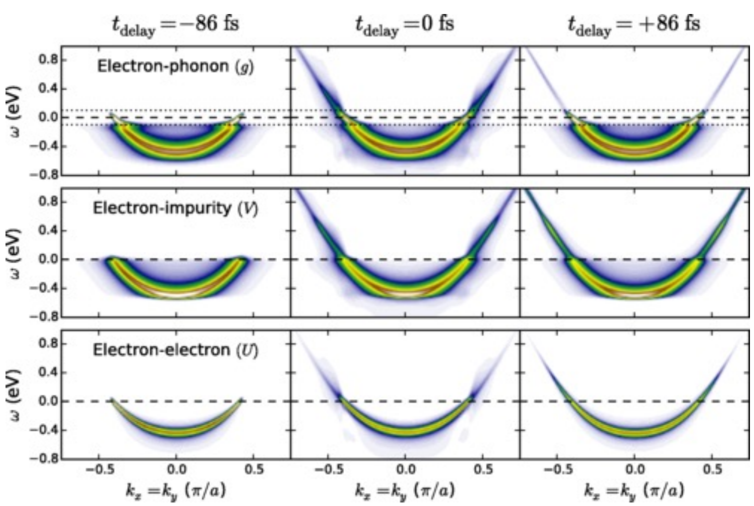


Time domain ED

Johnston & Kemper, unpublished

Why quantum computing for condensed matter?

All these techniques eventually reach a barrier.



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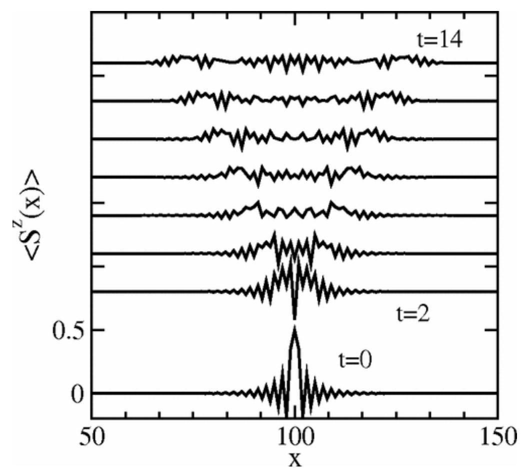

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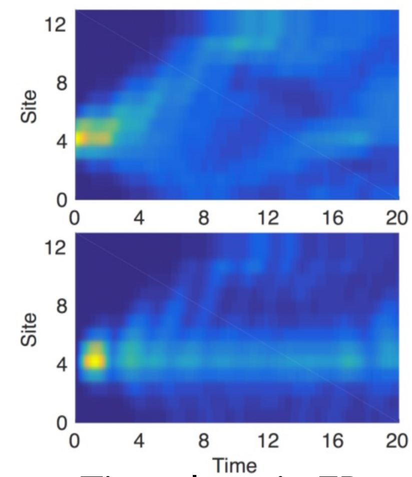

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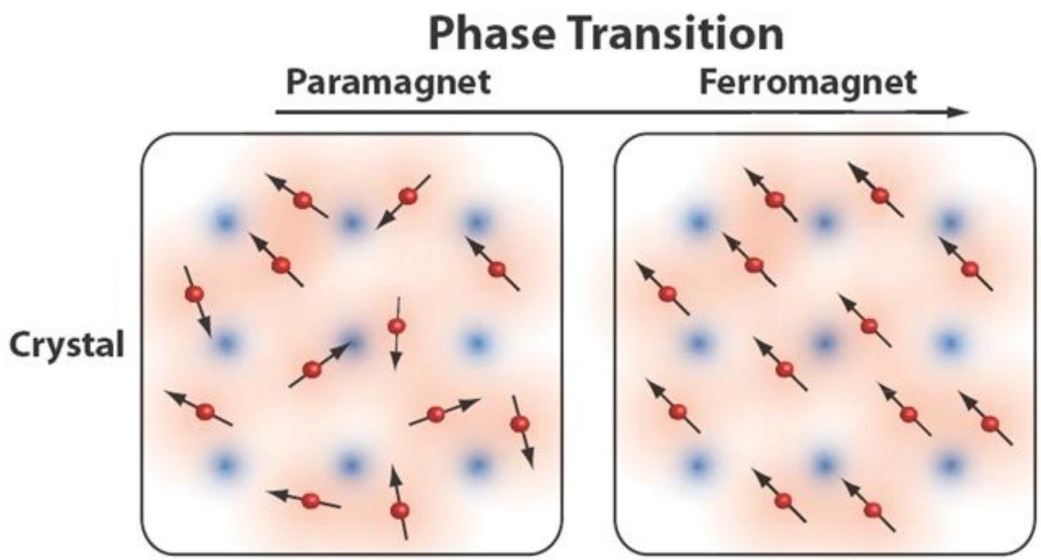
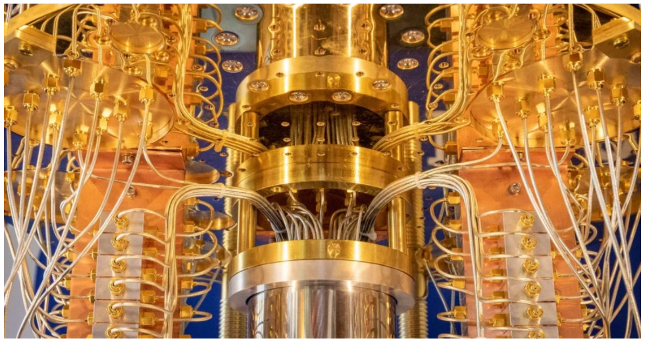
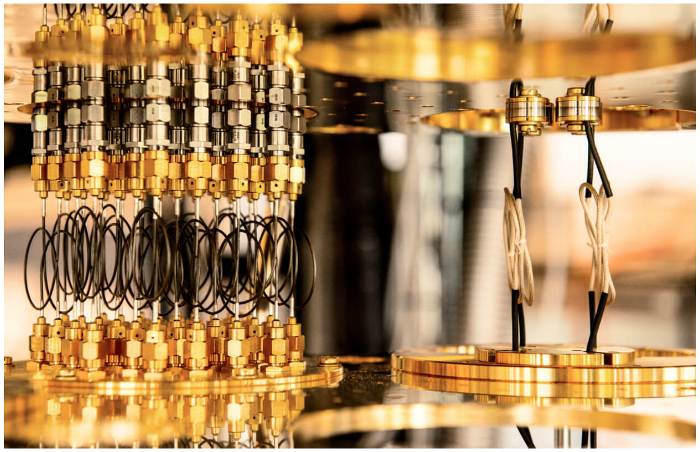


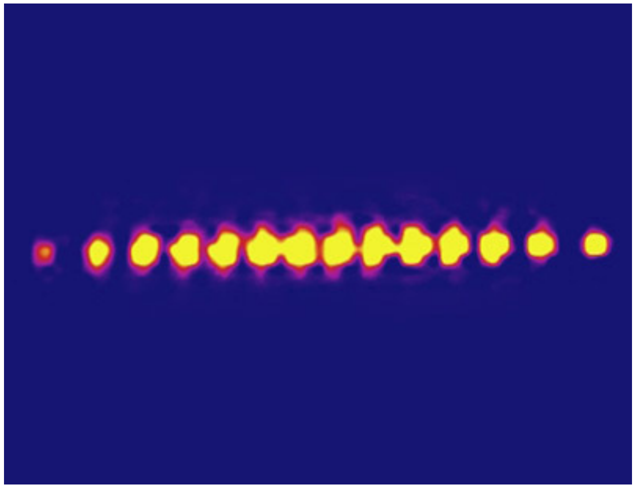
50 spins = 1,125,899,906,842,624 states

Quantum Computers

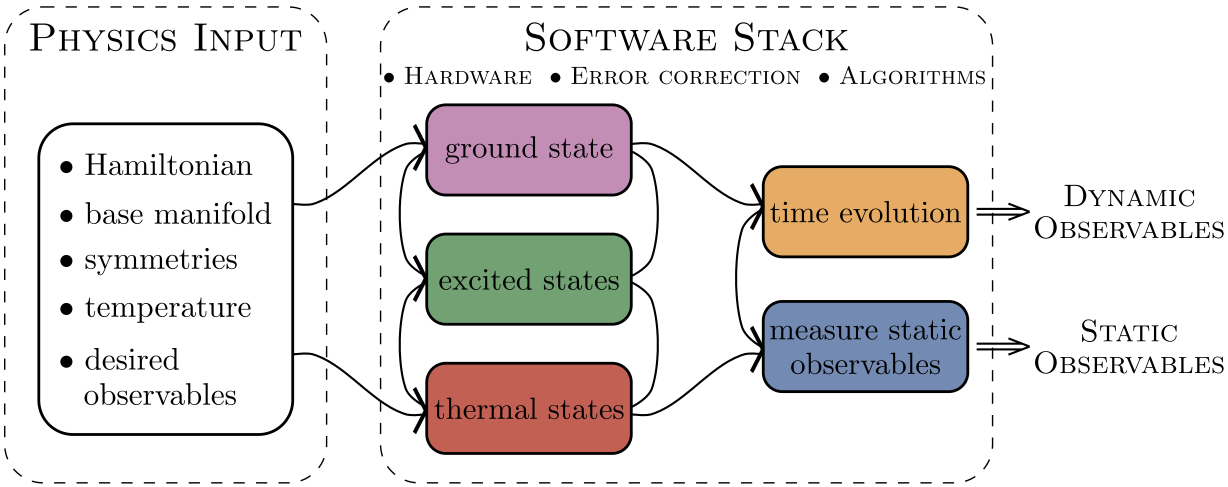
- Superconducting (IBM, Google)
- Ion (Ionq)
- Topological? (Microsoft)
- Photonic (Xanadu)







Quantum Matter meets Quantum Computing

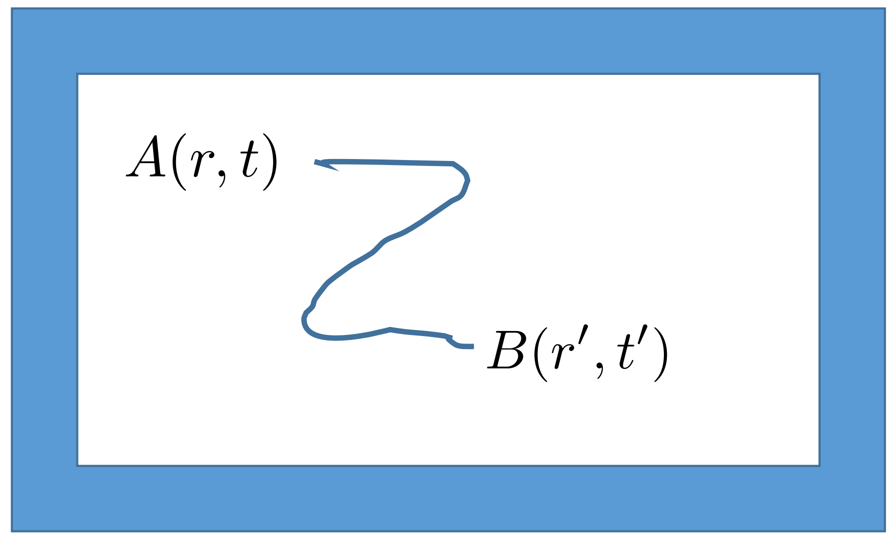


- Measuring correlation functions
- Preparing/measuring topological states
- Modeling driven/dissipative systems
- Time evolution via Lie algebraic decomposition/compression
- Thermodynamics

Low-energy excitations: correlation functions

$$\langle A(r,t)B(r',t')\rangle$$

Given some (observable) operator B at (r',t'), what is the likelihood of some (observable) operator A at (r,t)?



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Low-energy excitations: correlation functions

Conductivity

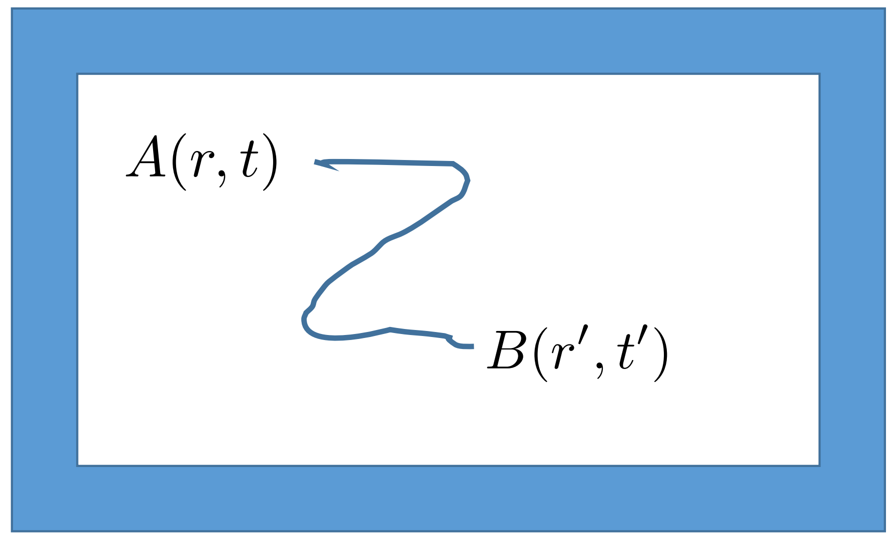
$$\langle j(r,t) j(r',t') \rangle$$

Single-particle spectra (ARPES)

$$\langle c(r,t) c^\dagger(r',t') \rangle$$

Spin-resolved neutron scattering

$$\sigma^{x,y,z}_{\alpha\beta} \langle S_\alpha(r,t) S_\beta(r',t') \rangle$$

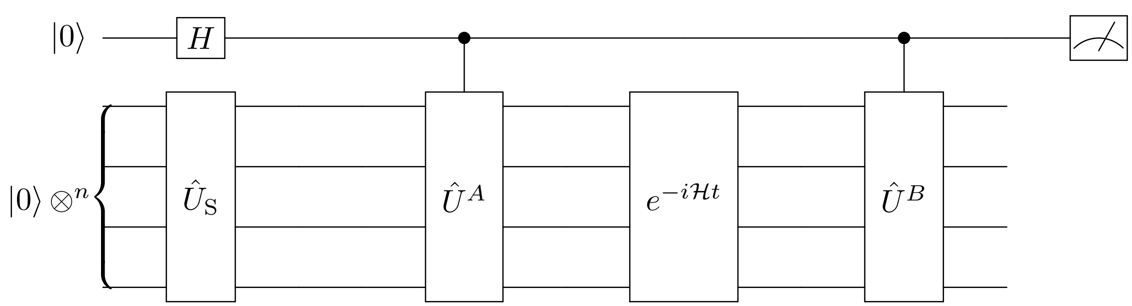


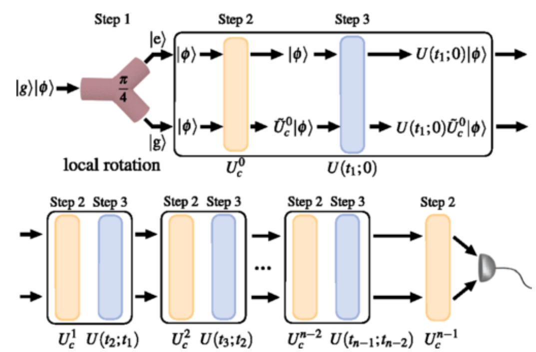
Low-energy excitations: correlation functions

Express the correlation function through the Lehmann representation:

$$C(t) = \langle \Phi | \hat{U}^B(t) \hat{U}^A(0) | \Phi \rangle = \sum_m e^{-i(E_m - E_0)t} \langle \phi_0 | U^B | m \rangle \langle m | U^A | \phi_0 \rangle \, .$$

Quantum circuit:

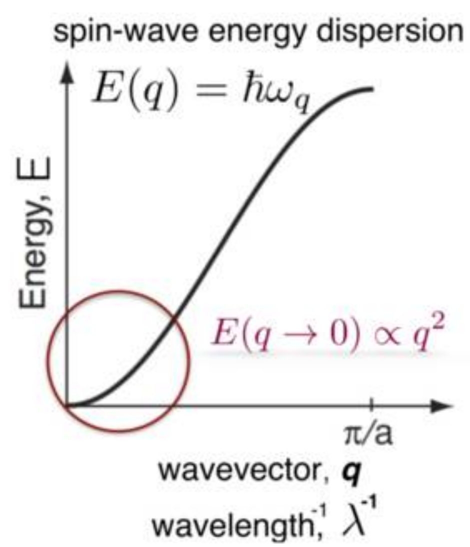




Low-energy excitations: 2-site magnons

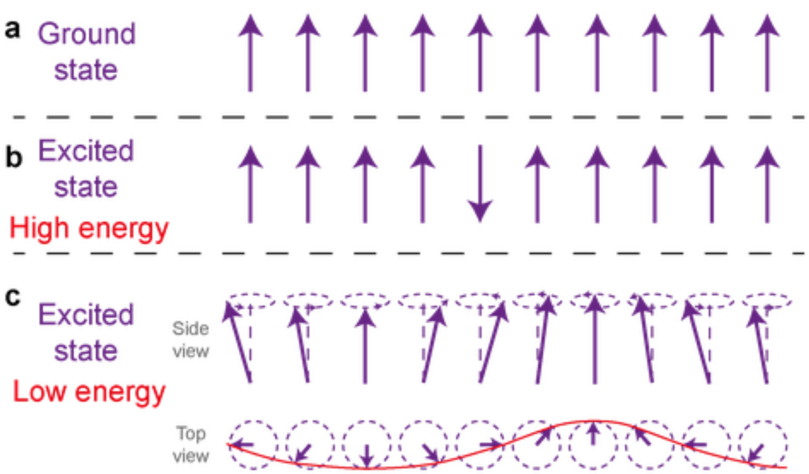
Spin-spin correlation function for periodic Heisenberg model: Magnons!

$$\mathcal{H} = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$



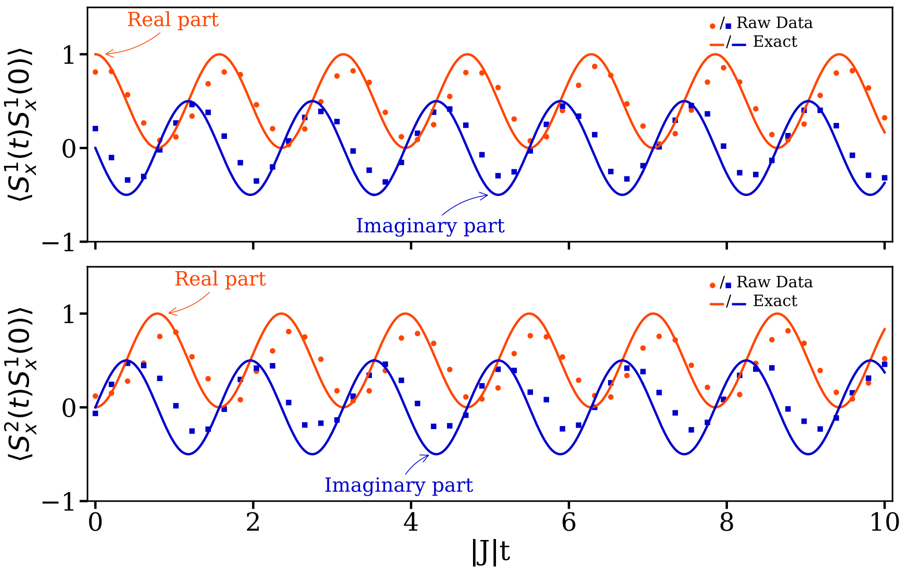
Etz, JPCM 27, 24 (2015)

Low-energy excitations: 2-site magnons

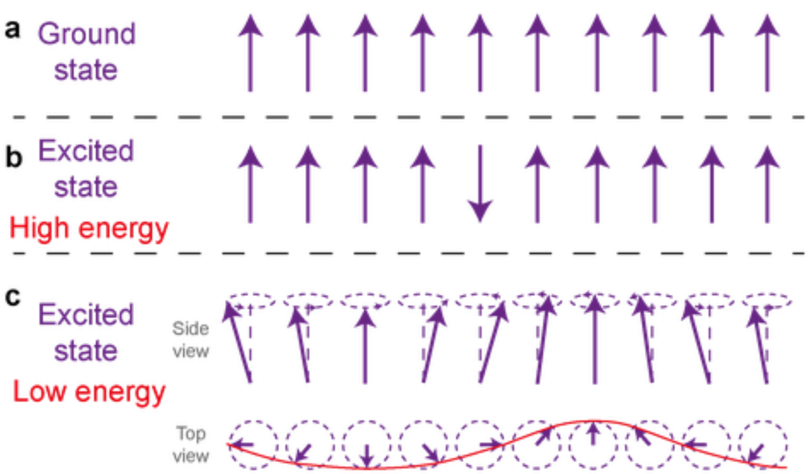


$$\hat{H} = 2SJ\sum_k (1-\cos(k))\hat{c}_k^\dagger \hat{c}_k$$

$$\uparrow\uparrow \quad \rightarrow \quad \uparrow\downarrow$$



Low-energy excitations: 4-site magnons



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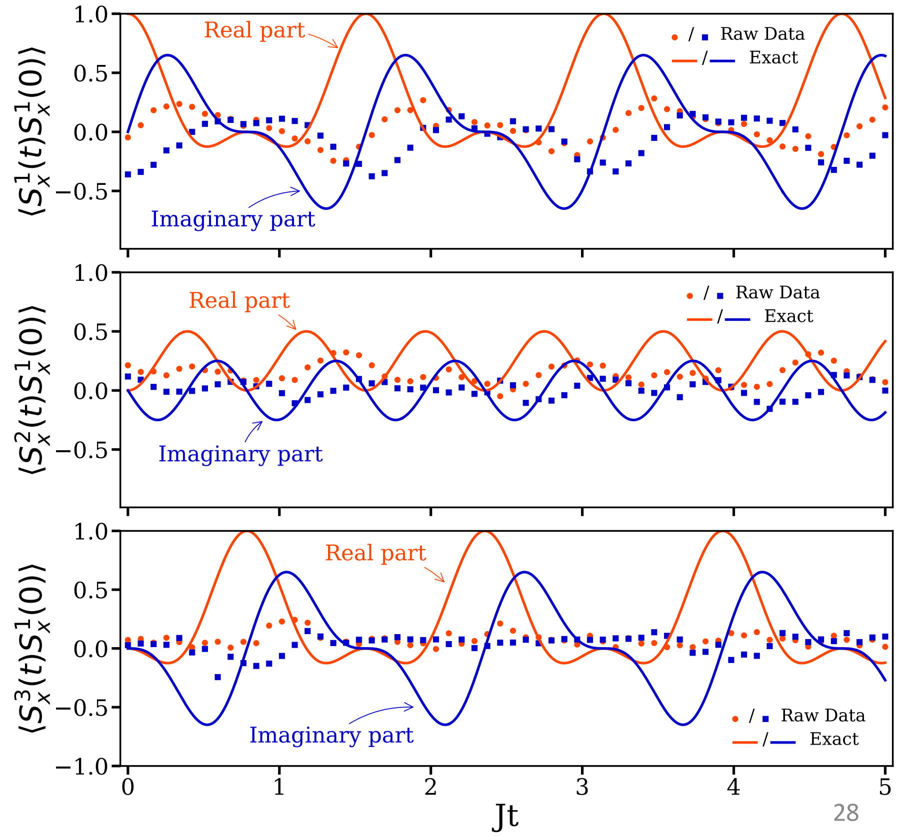

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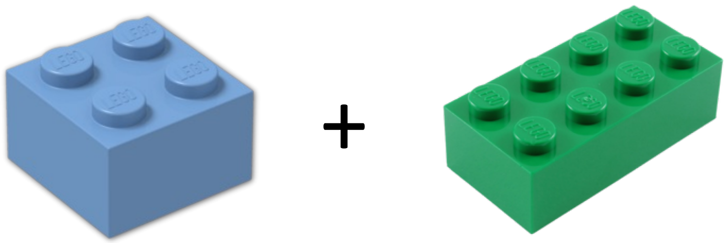
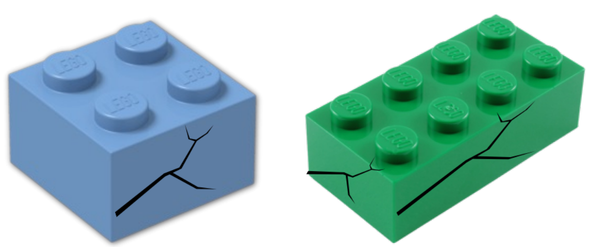


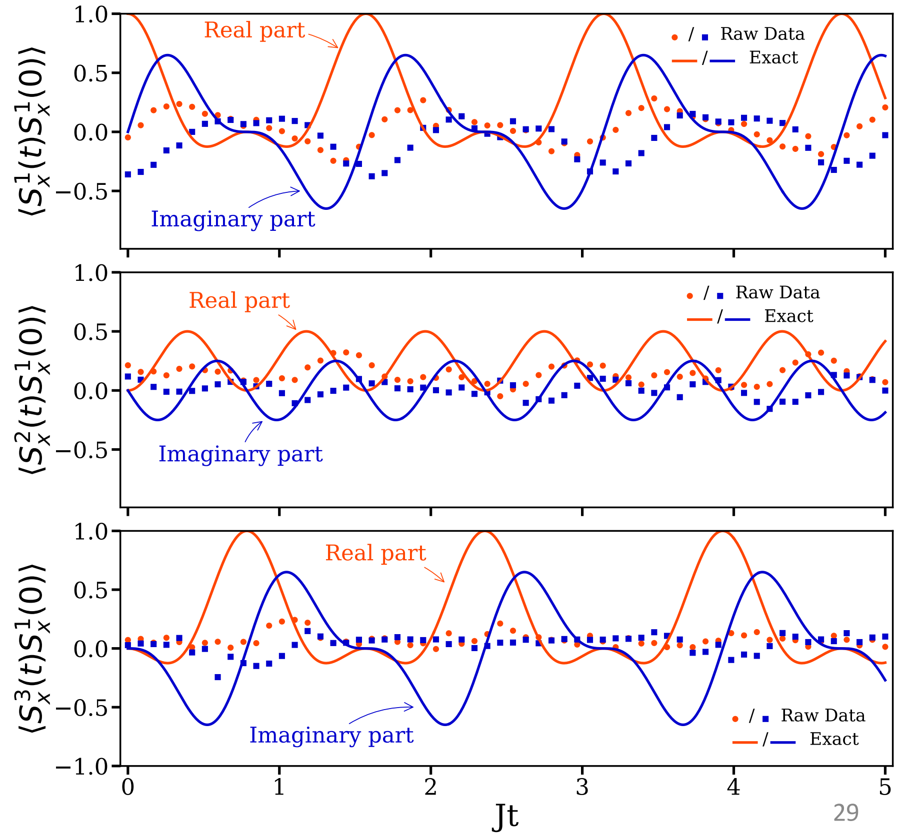
Single Qubit Gates + Two Qubit Gate

= Anything!*

*Actual Gates



$\uparrow\uparrow\uparrow\uparrow \rightarrow \uparrow\uparrow\uparrow\downarrow$



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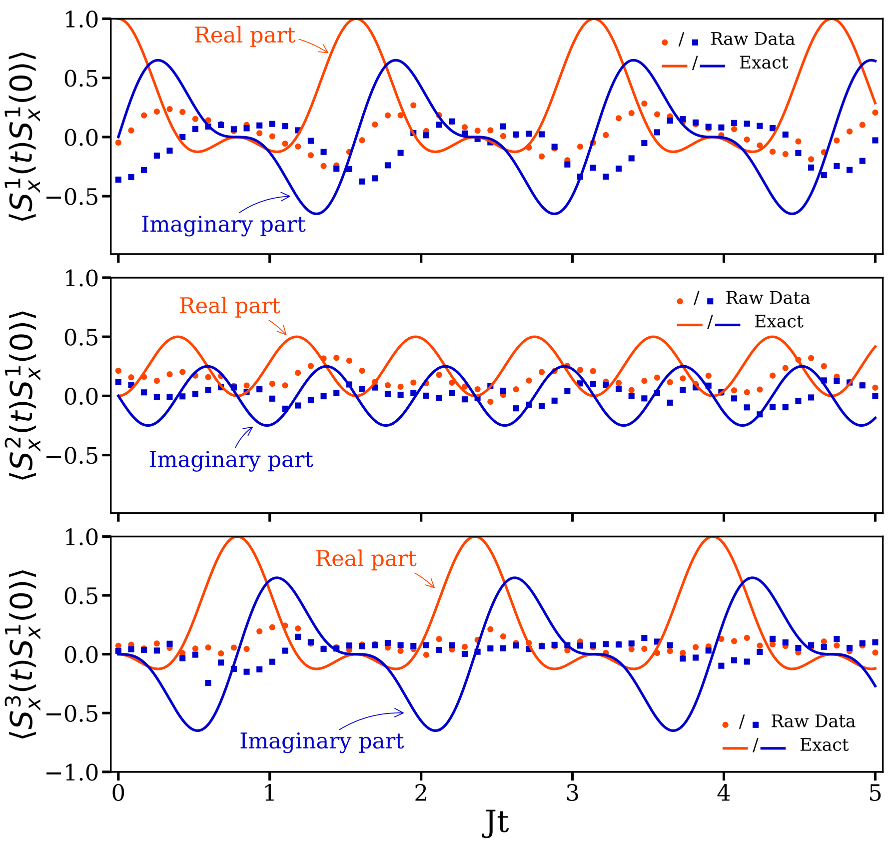
Low-energy excitations: 4-site magnons

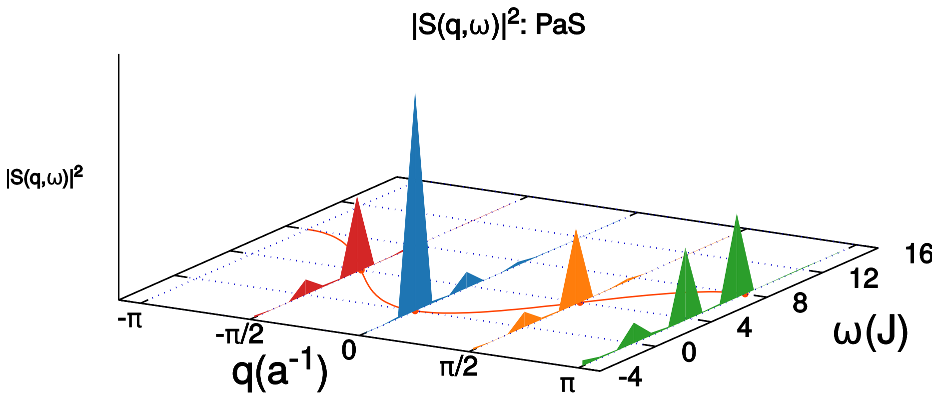
Error mitigation strategies:

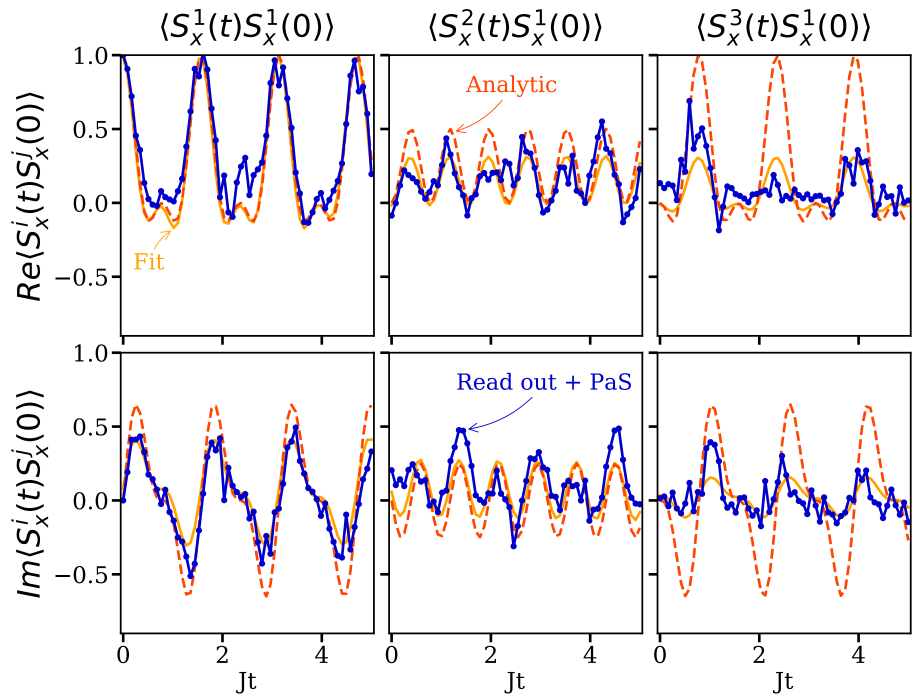
1. Read out error correction
2. Phase-and-scale
   - Multiply by complex number
3. Fourier fitting
   - Assume only 4 frequencies



Low-energy excitations: 4-site magnons

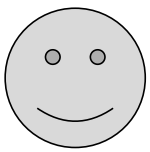
Spin-spin correlation function for periodic Heisenberg model: Magnons!



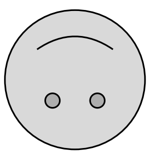


10.1103/PhysRevB.101.014411

Quantum computing for condensed matter?



Quantum computers are promising tools for solving problems in CMT…

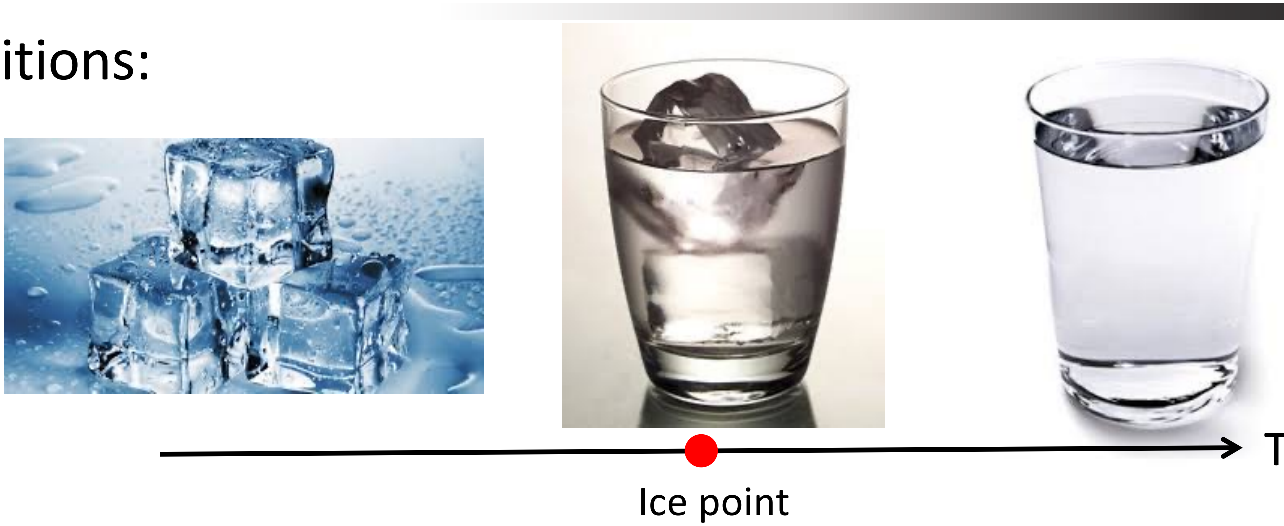


… but care needs to be taken to ameliorate their noisiness in the NISQ era.

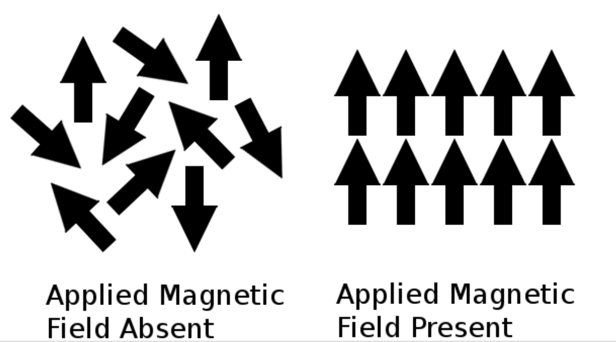
Noisy
Intermediate
Scale
Quantum

Quantum Phase Transition

Phase transitions:

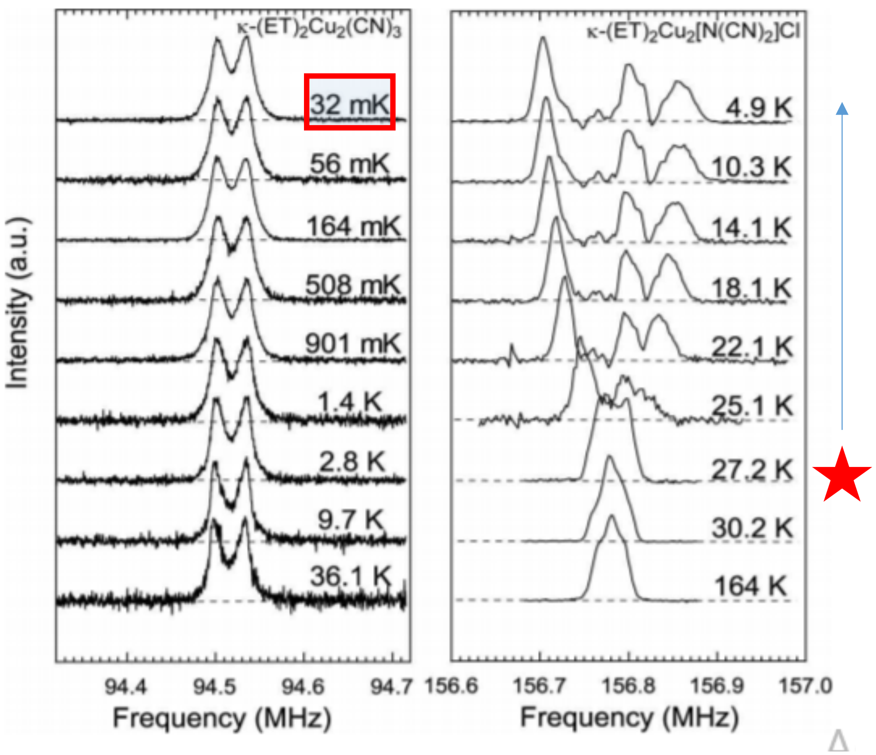


Quantum phase transitions: T=0, realized by quantum fluctuation controlled by physical quantities e.g. magnetic fields:



Topological Quantum Phase Transitions

The important feature of topological quantum phase transition is **featureless** in the sense that there is **no local order parameter** and no symmetry breaking.



Spin Liquid State in an Organic Mott Insulator with a Triangular Lattice

Y. Shimizu, K. Miyagawa, K. Kanoda, M. Maesato, and G. Saito
Phys. Rev. Lett. **91**, 107001 – Published 4 September 2003

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?

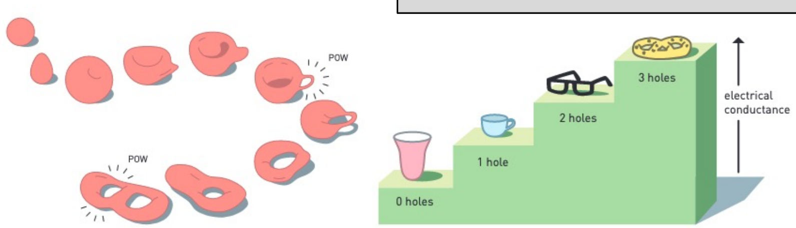
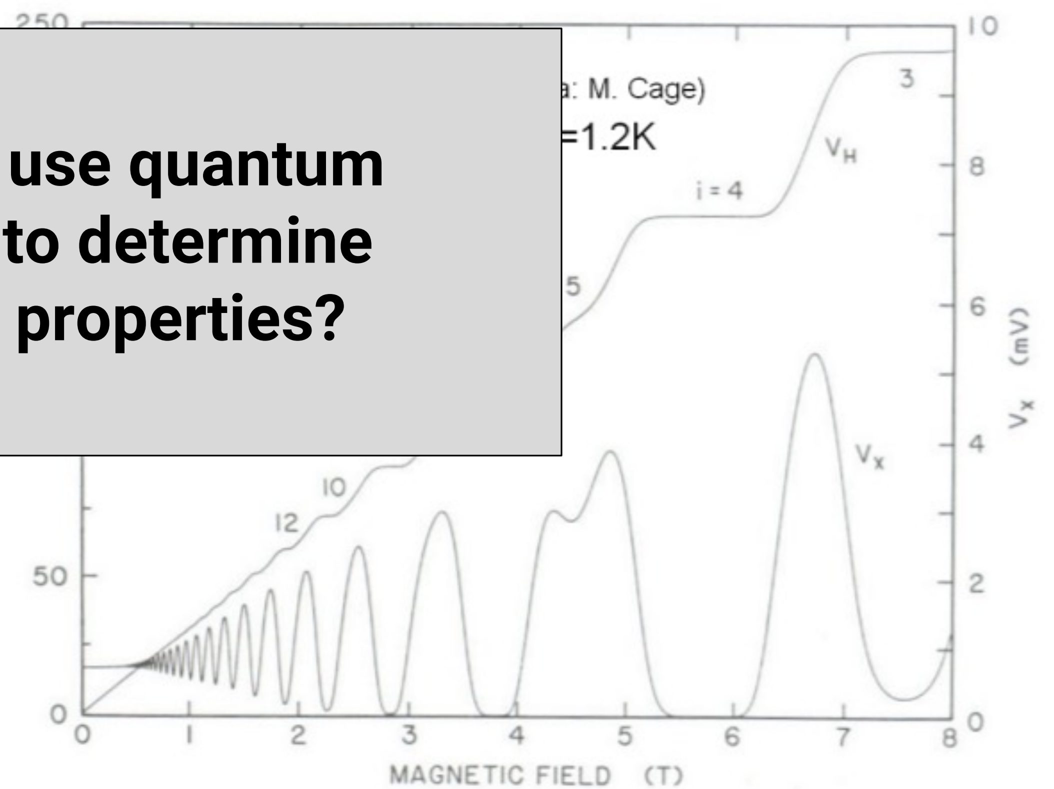


Fig 3. Topology. This branch of mathematics is interested in properties that change step-wise, like the number of holes in the above objects. Topology was the key to the Nobel Laureates' discoveries, and it explains why electrical conductivity inside thin layers changes in integer steps.

Nobel Prize in Physics 2016

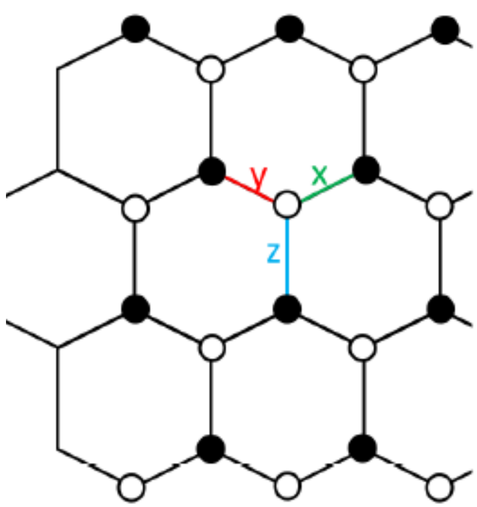


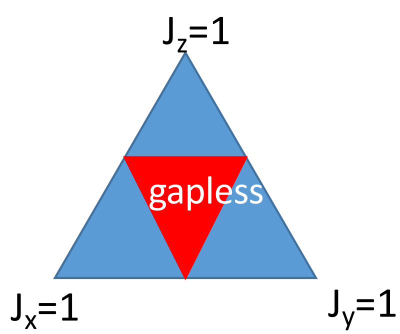
The Kitaev model

PHYSICAL REVIEW B **95**, 045112 (2017)

Kitaev honeycomb tensor networks: Exact unitary circuits and applications

Philipp Schmoll and Román Orús
Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany





No local order parameter!

Topological QPT

Spins
→ Jordan-Wigner →
Fermions
→ Majorana braiding →
Fermions(r) + Gauge fields
→ Fourier →
Fermions(k) + Gauge fields
→ Bogoliubov →
Bogoliubons(k) + Gauge fields

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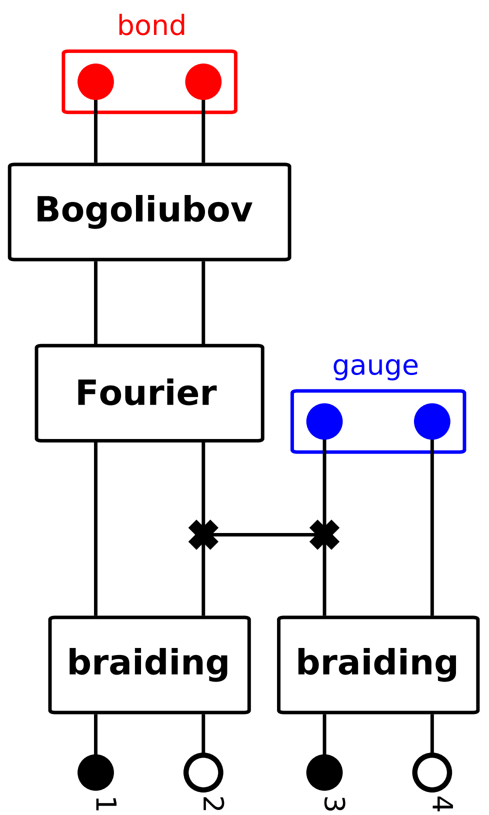
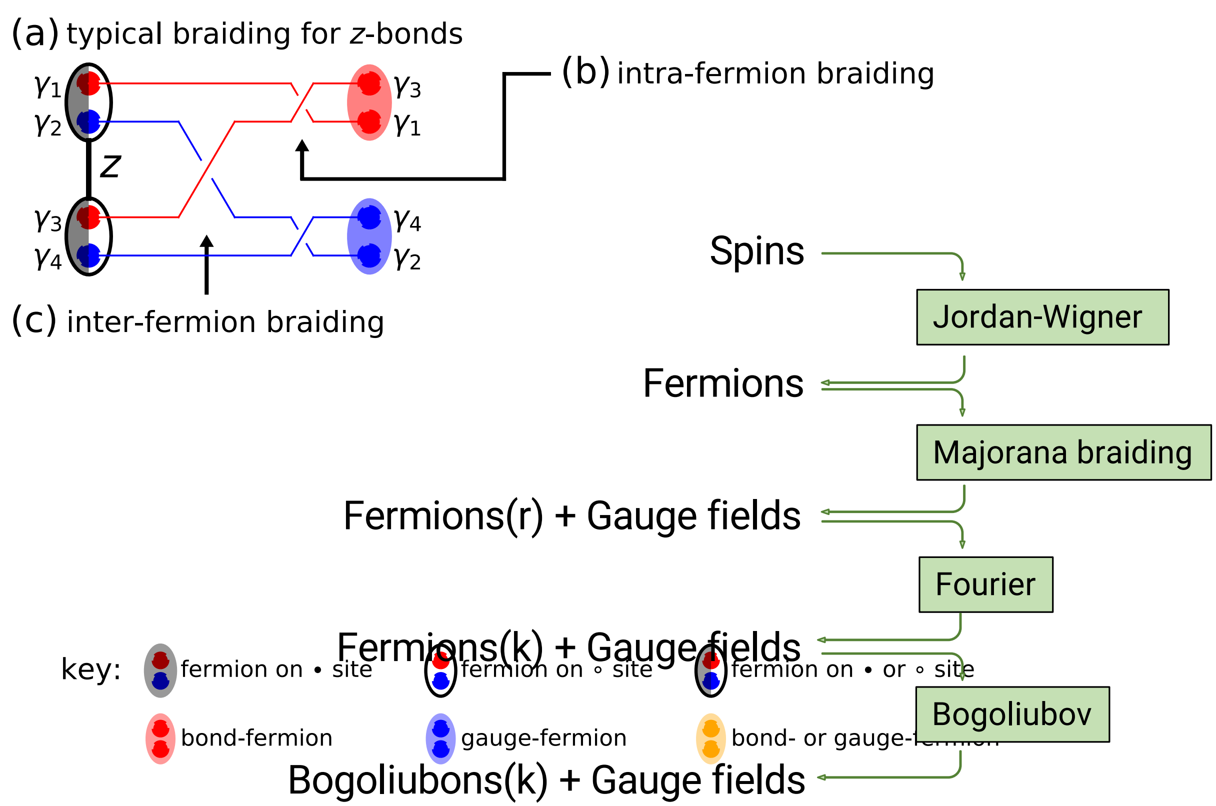
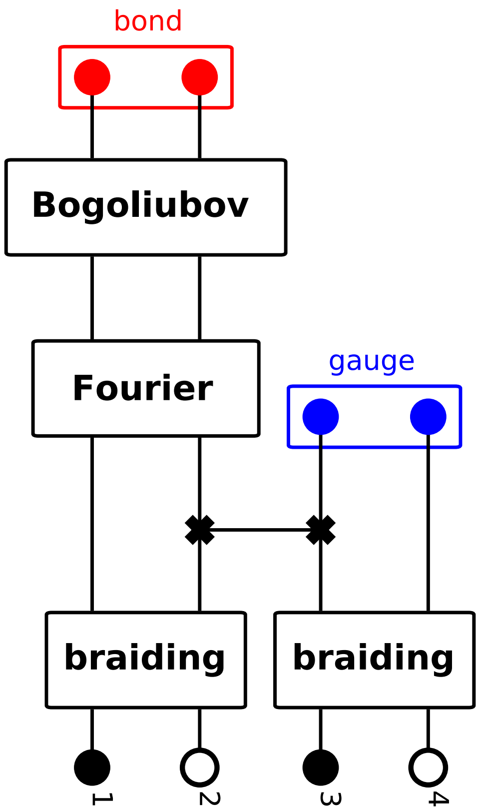
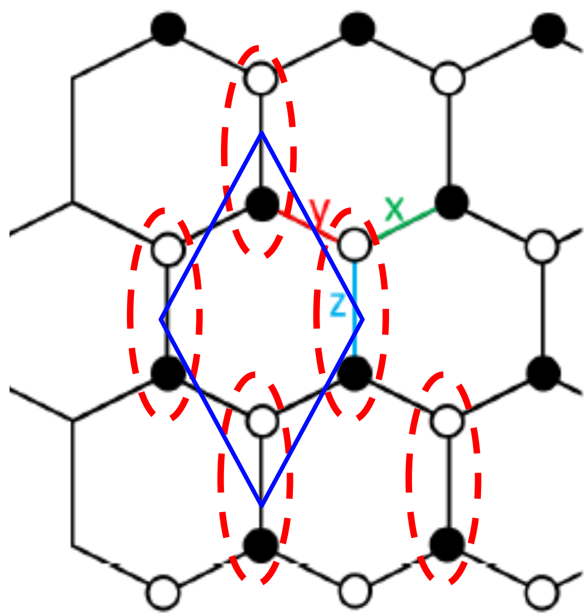
Majorana Braiding



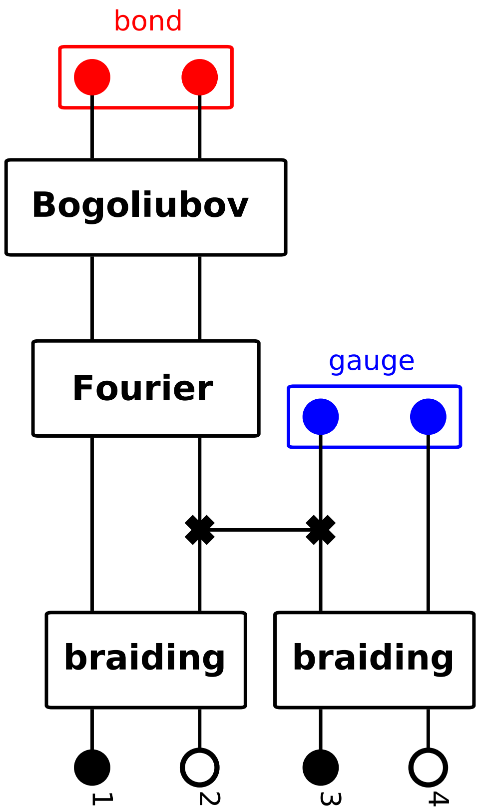


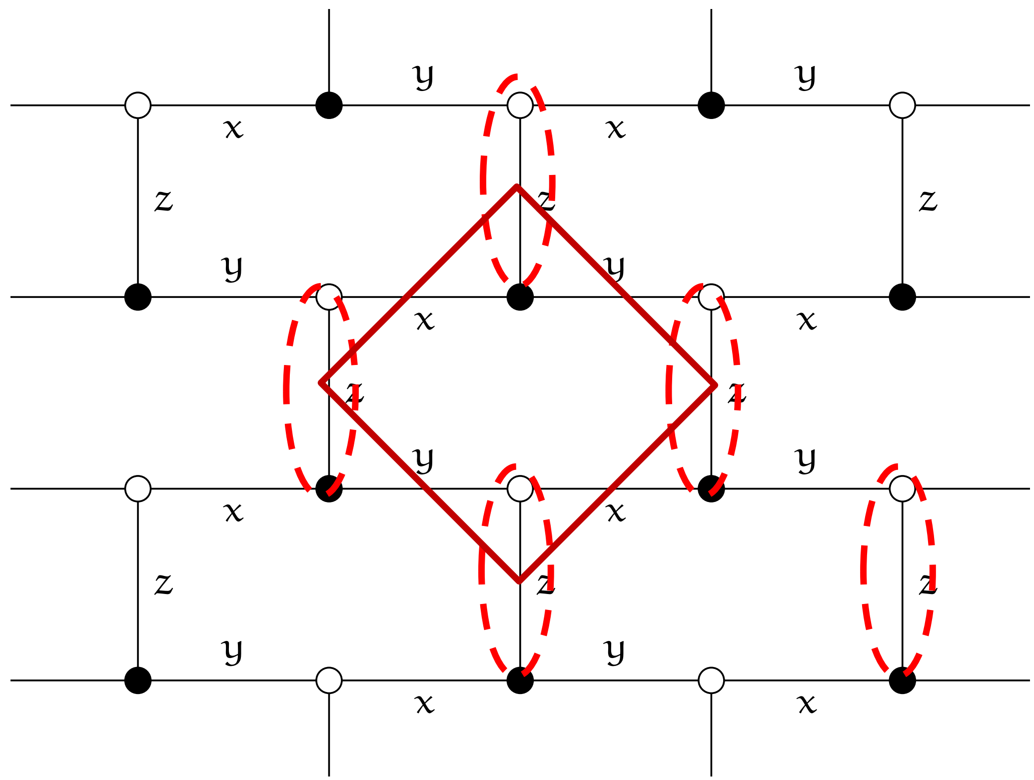
Majorana Braiding





Majorana Braiding





The Kitaev model

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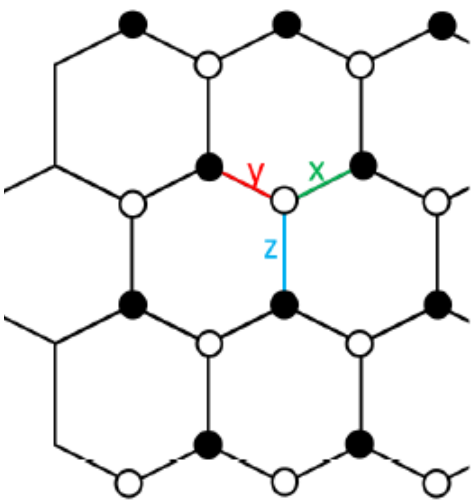
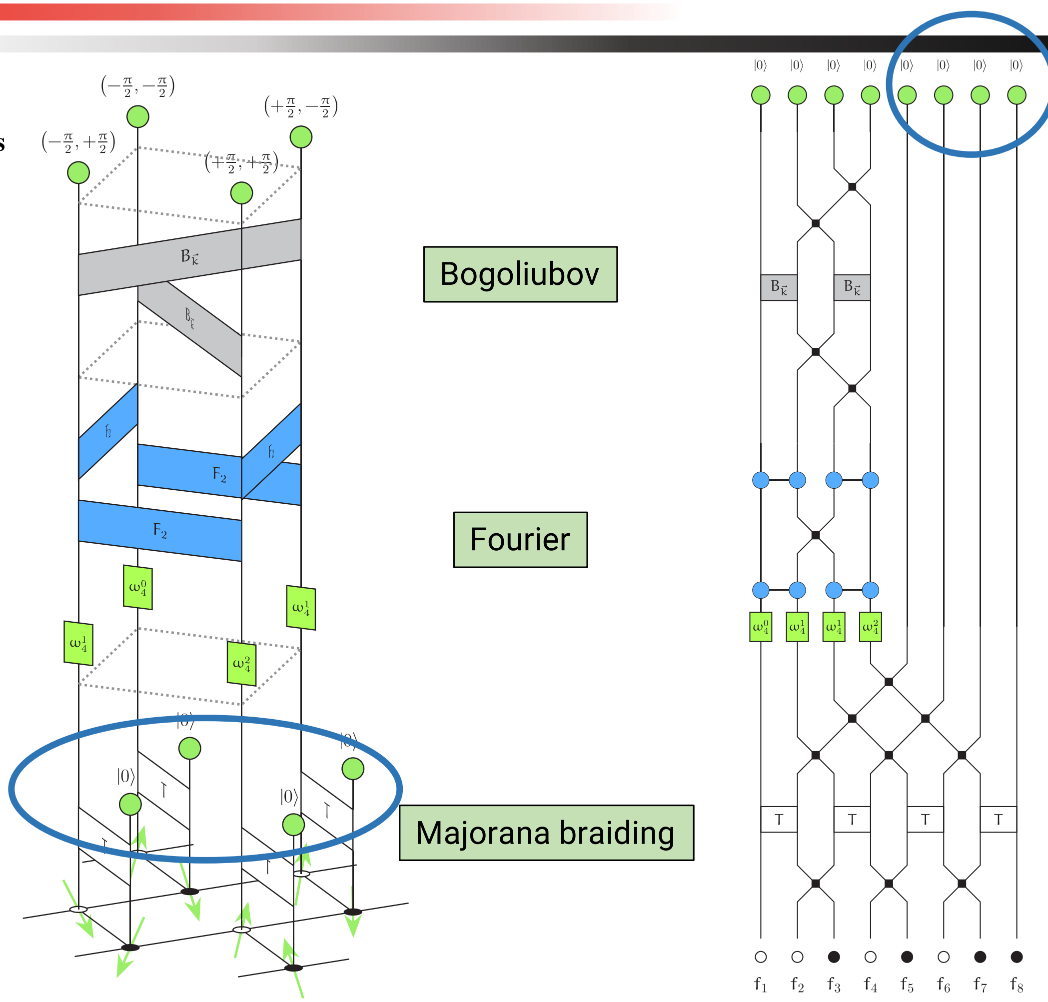
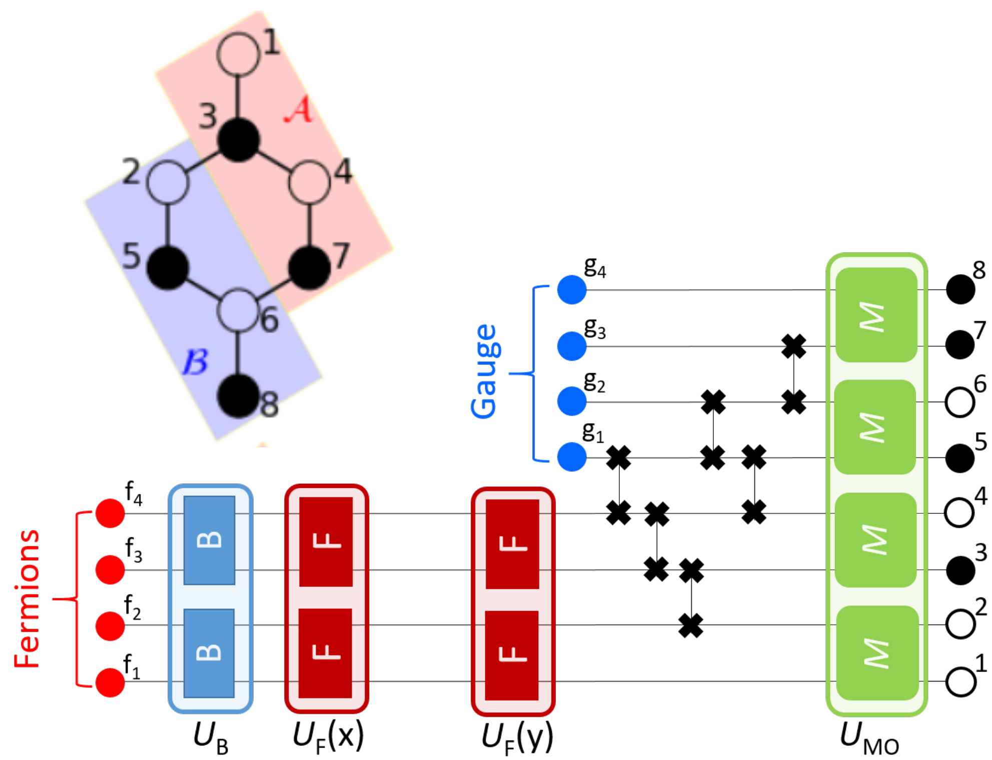
Kitaev honeycomb tensor networks: Exact unitary circuits and applications

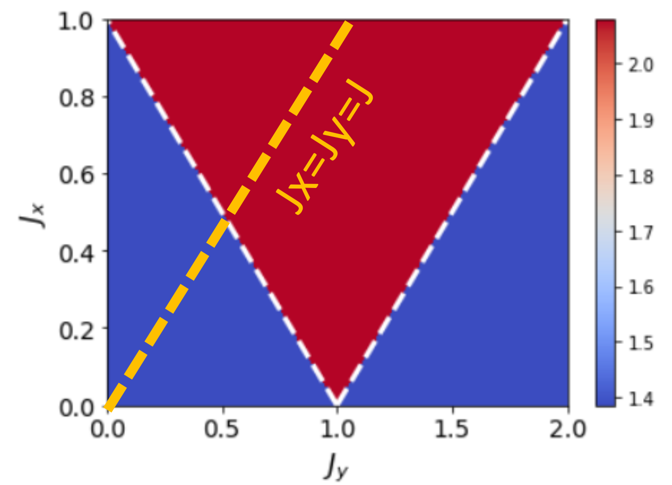
Philipp Schmoll and Román Orús
Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

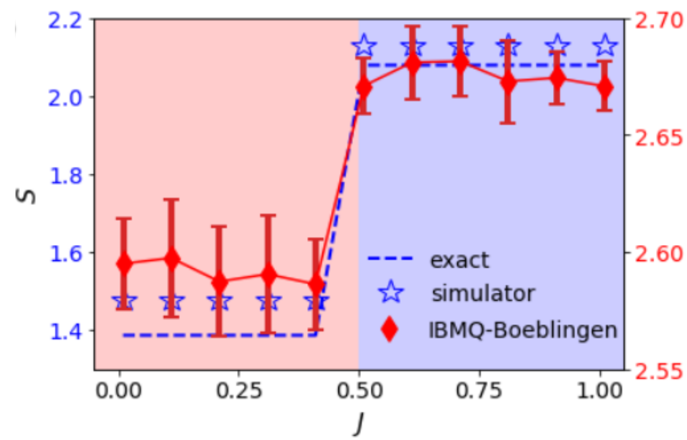




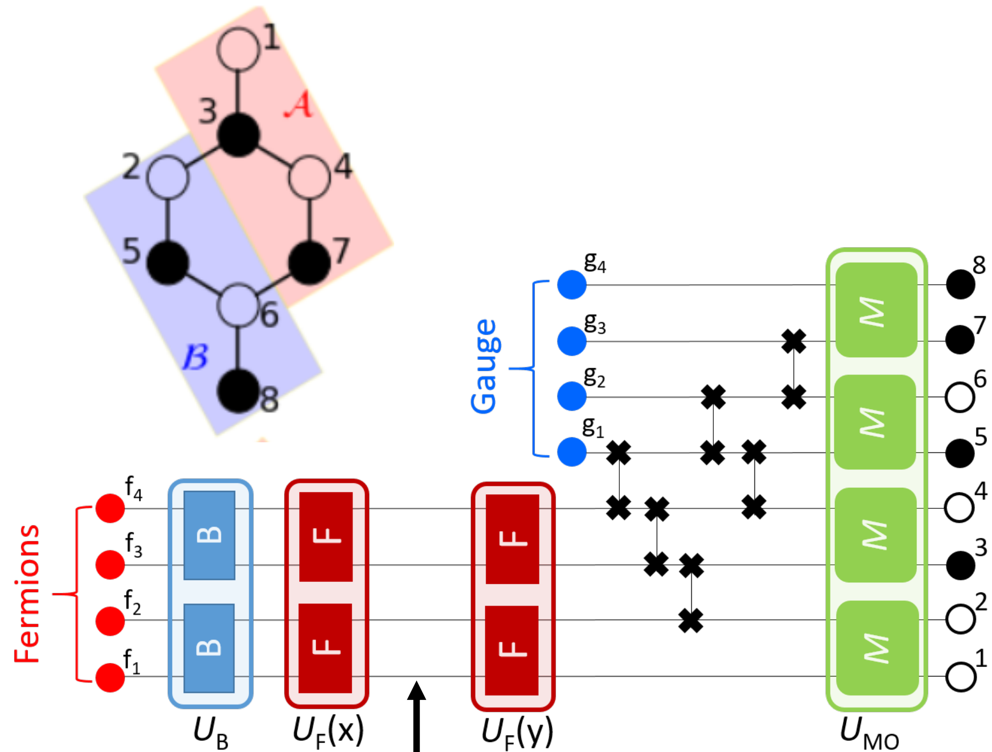
Characterize QPT of Kitaev spin model by quantum computer

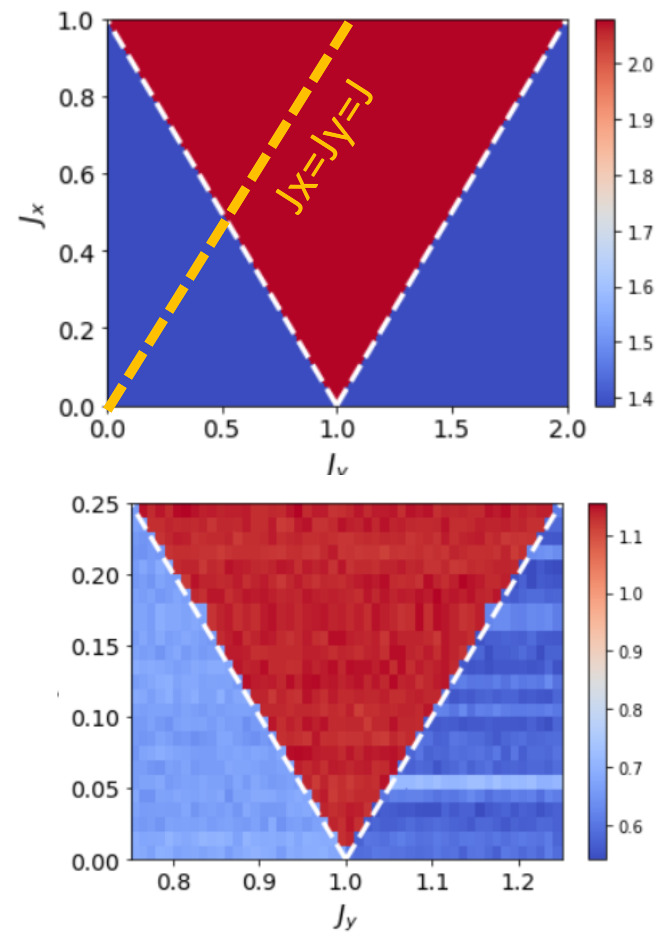






Characterize QPT of Kitaev spin model by quantum computer

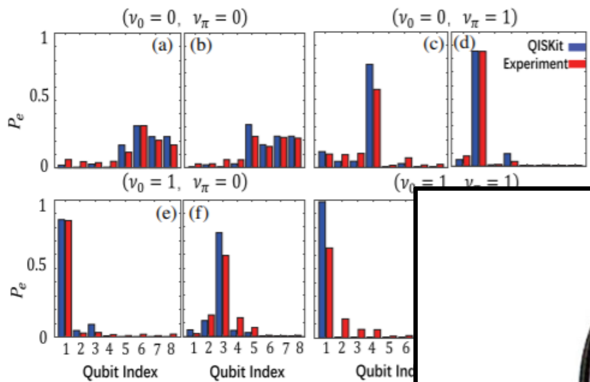




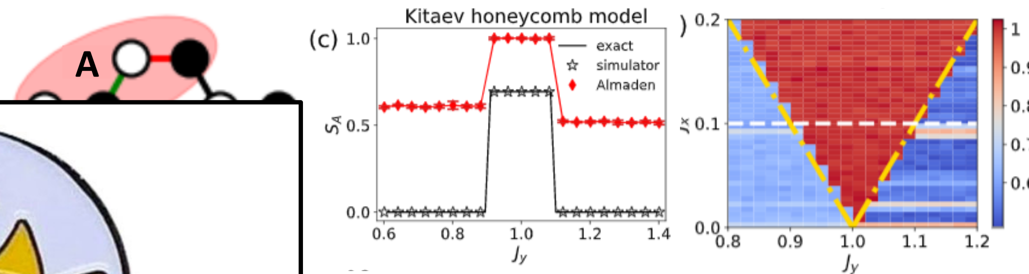
But we can do better! The gauge part has a trivial contribution, so we can instead compute a correlation function $\langle \eta_x(-k_y)\eta_{x'}(k_y)\rangle$

Topological states are robust… or are they?

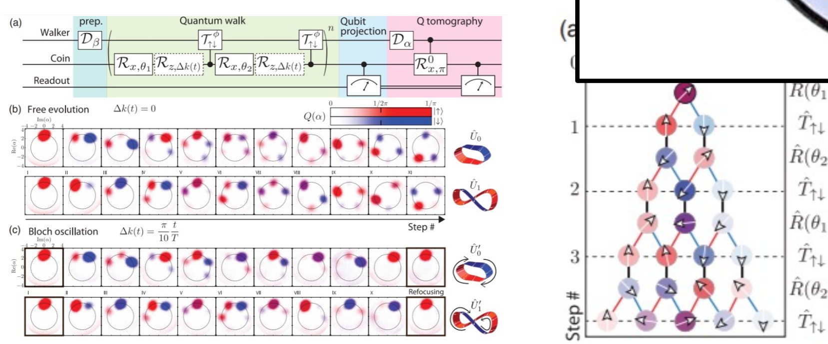
Floquet topological states, Mei et al (PRL 2020)



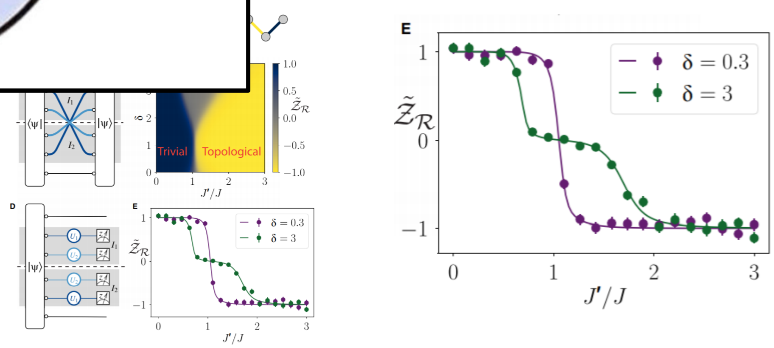
Kitaev Honeycomb Model, Xiao et al (arXiv:2006.05524)



1D topological quantum walk, Flurin



…ed Topological (SPT) state, Elben (Sci Adv 2020)



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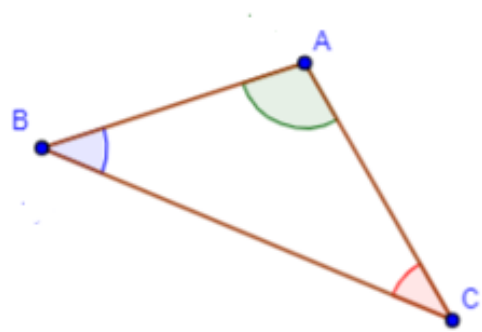
A Brief Detour Into Geometry

The earth is round. [citation needed]

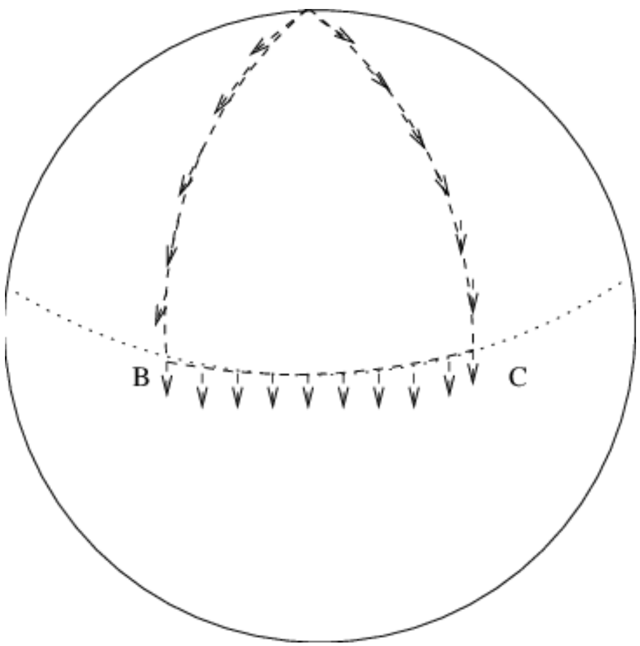
How can we tell?



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

unless you're on a curved space...

A Brief Detour Into Geometry

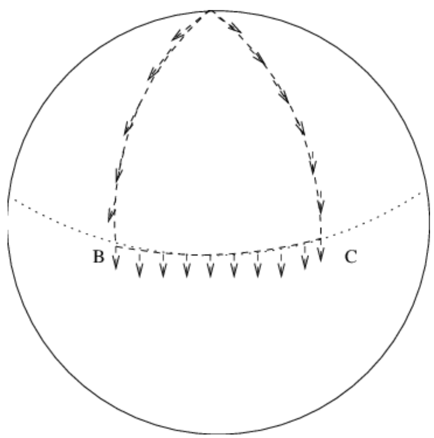


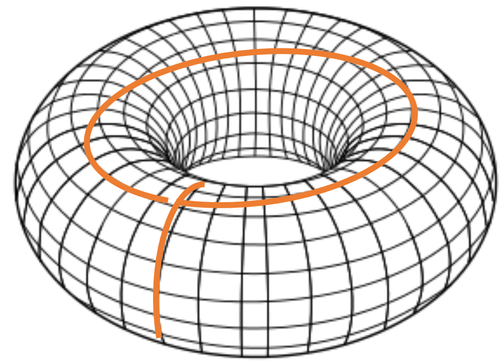
We could also use *parallel transport*.

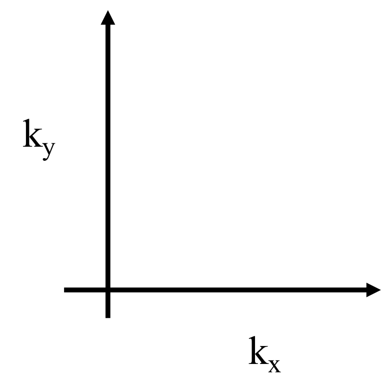
$$\frac{\partial}{\partial \vec{s}}\vec{v}$$

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

Quantum Geometry







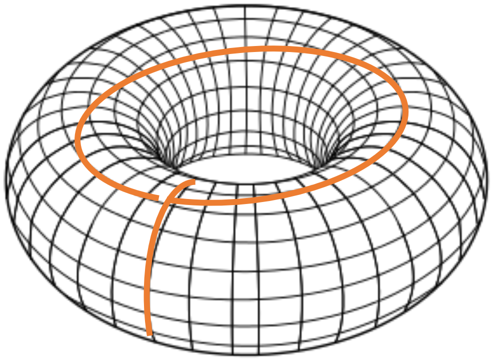
$$\frac{\partial}{\partial \vec{s}}\vec{v}$$

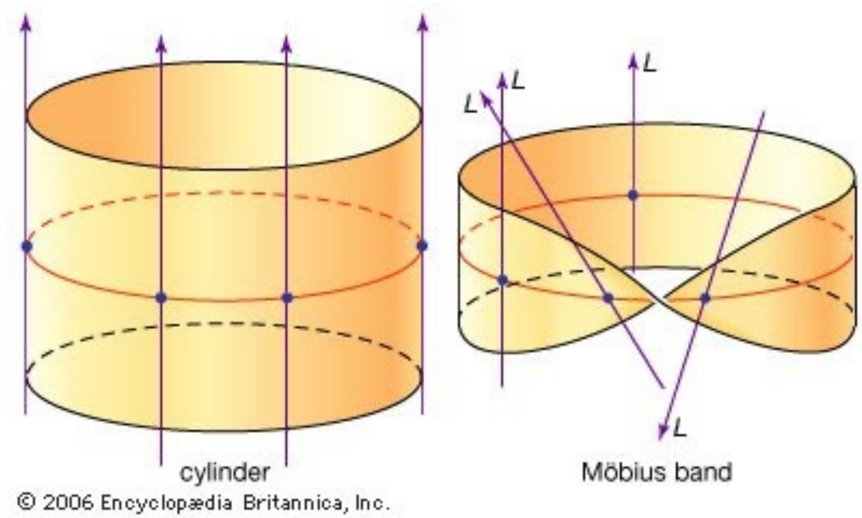
$$\langle \Psi_\Theta | \partial_\Theta | \Psi_\Theta \rangle$$

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

A: Some **integer** multiple of 2π

Quantum Geometry





$$\langle \Psi_\Theta | \partial_\Theta | \Psi_\Theta \rangle$$

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

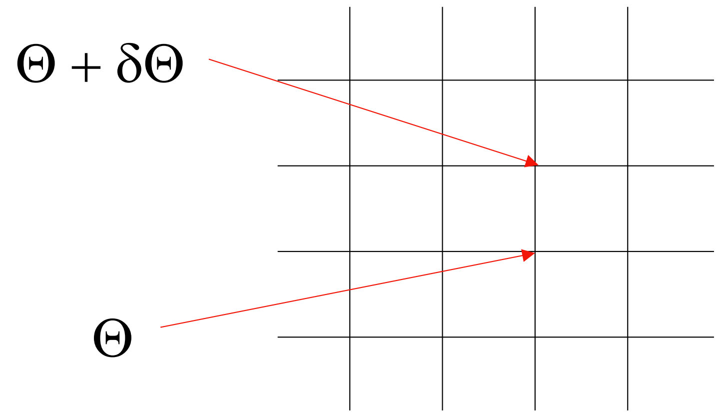
A: Some **integer** multiple of 2π

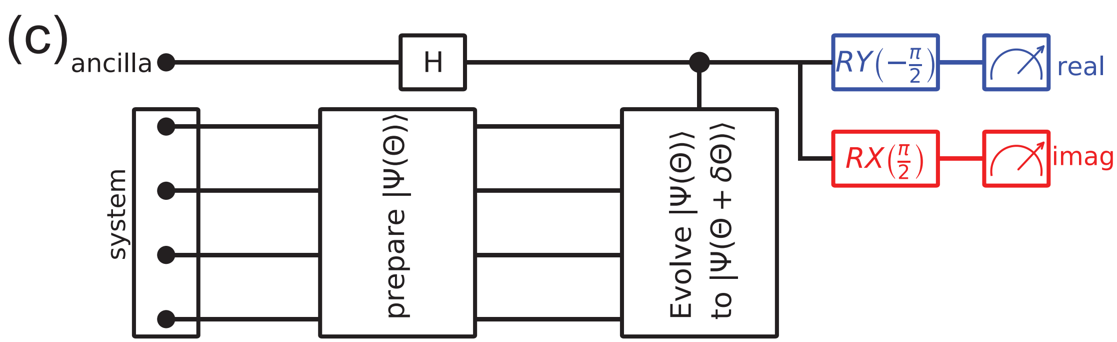
Quantum Geometry

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

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

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



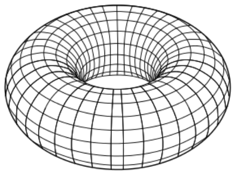


Quantum Geometry

Chiral p-wave superconductor

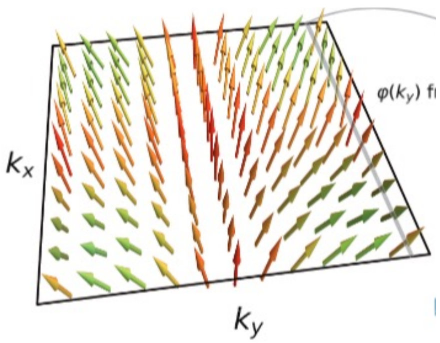
$$\mathcal{H}(\boldsymbol{k}) = \Delta(\sin k_y \sigma_x + \sin k_x \sigma_y) - \epsilon(\boldsymbol{k})\sigma_z$$

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

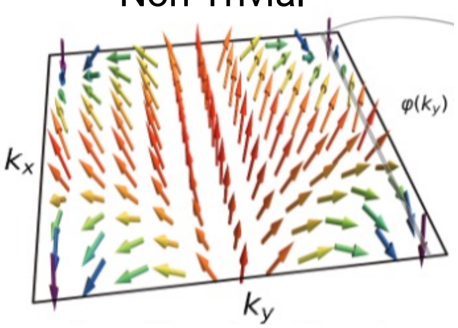


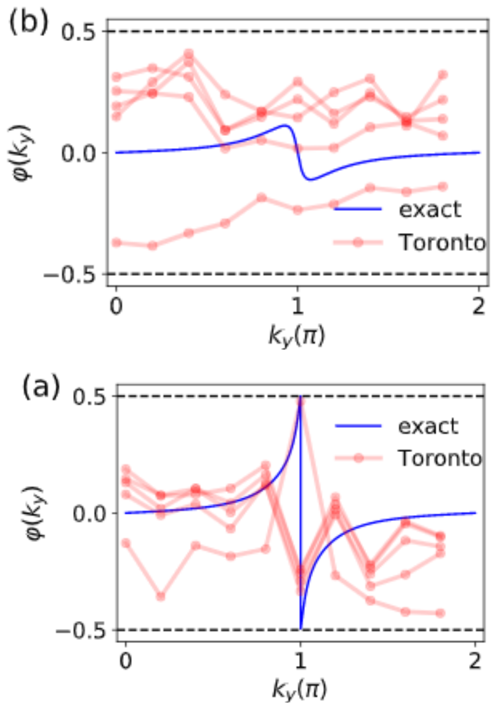
Phase: $2\pi\mathcal{C}$

"Trivial"

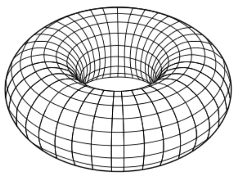


"Non-Trivial"

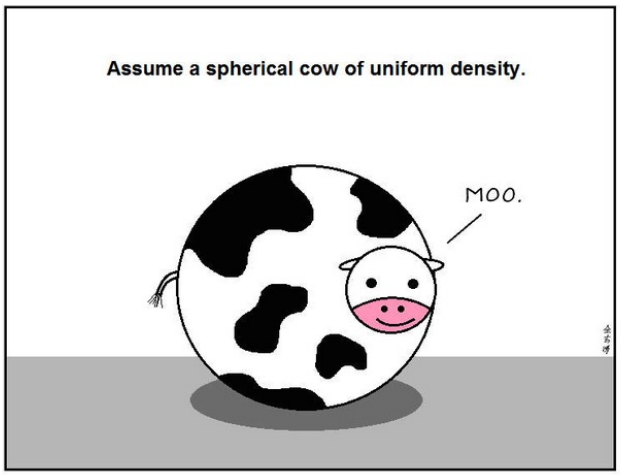




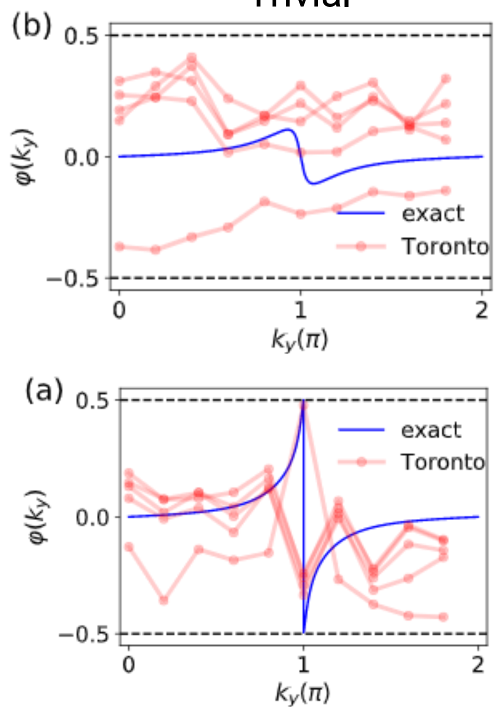
Quantum Geometry



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



"Trivial"



"Non-Trivial"

Solution: Rather than taking lines across the manifold, consider the whole manifold.

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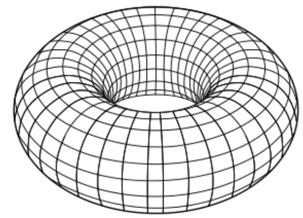
Quantum Geometry

Chiral *p*-wave superconductor

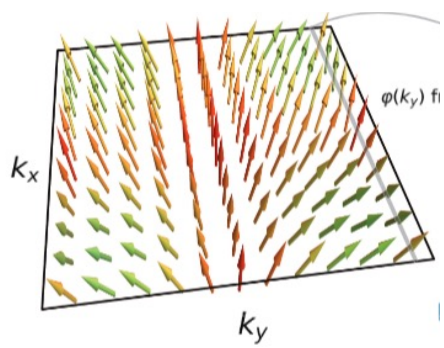
$$\mathcal{H}(\boldsymbol{k}) = \Delta(\sin k_y \sigma_x + \sin k_x \sigma_y) - \epsilon(\boldsymbol{k})\sigma_z$$

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

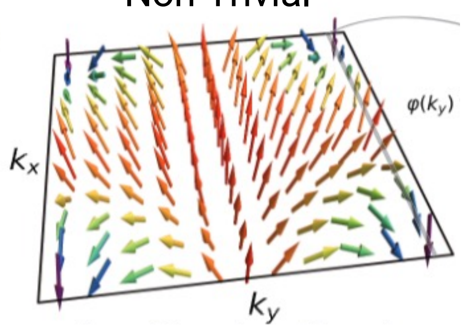


Phase: $2\pi\mathcal{C}$

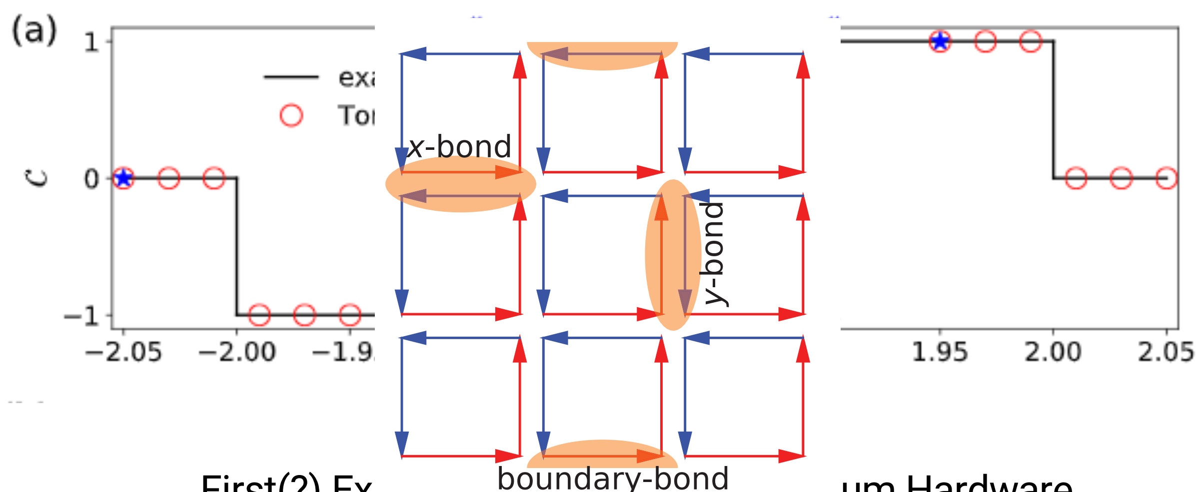
"Trivial"



"Non-Trivial"

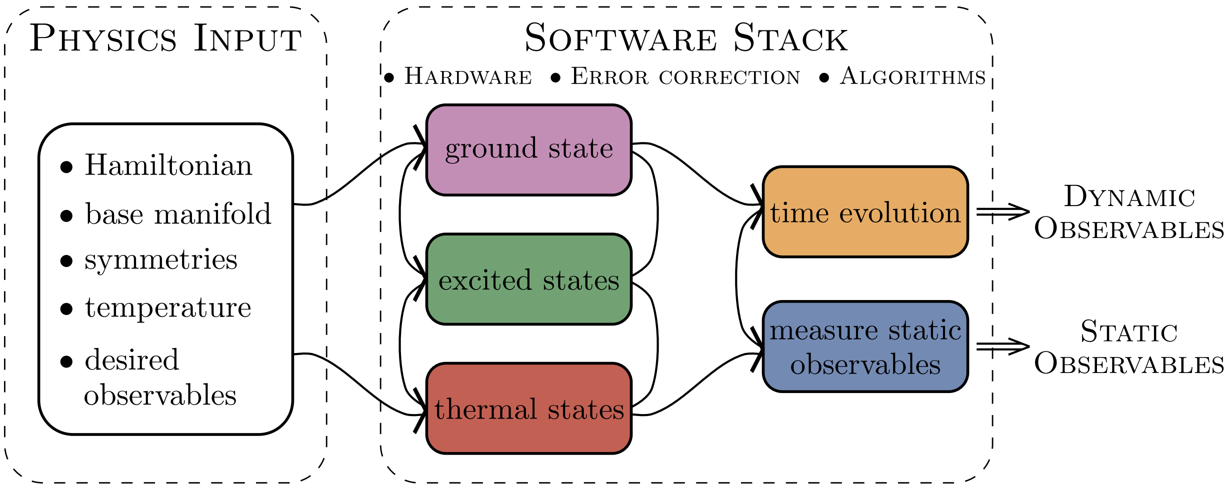


$$\mathcal{C} = \oint d\boldsymbol{k} \cdot \mathcal{A} = \int d^2k\, [\nabla \times \boldsymbol{A}(\boldsymbol{k})] \cdot \boldsymbol{n}_z = \int d^2k \mathcal{F}_{xy}(\boldsymbol{k}) \xrightarrow{discretize} \frac{1}{i2\pi} \sum_{\boldsymbol{k}} \mathcal{F}(\boldsymbol{k})$$



First(?) Ex ... um Hardware

Quantum Matter meets Quantum Computing



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

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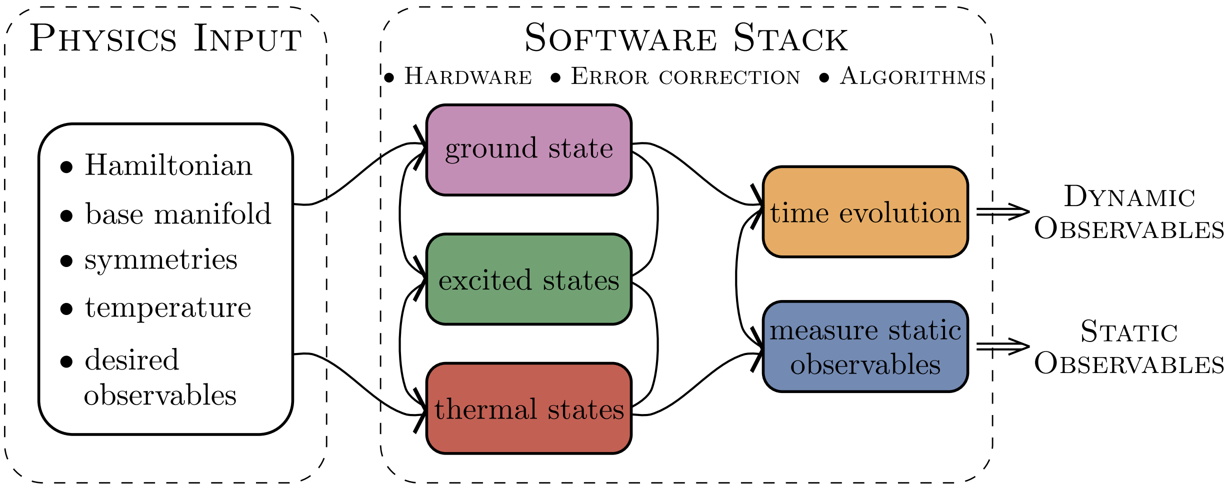
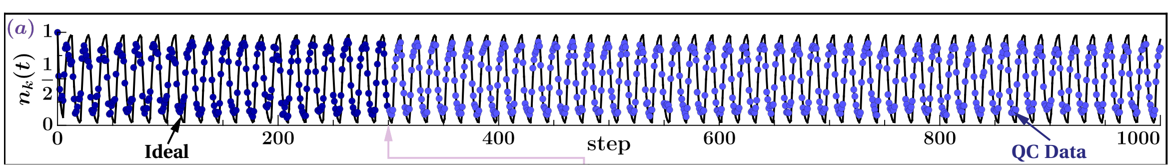
Quantum Matter meets Quantum Computing



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



- Measuring correlation functions
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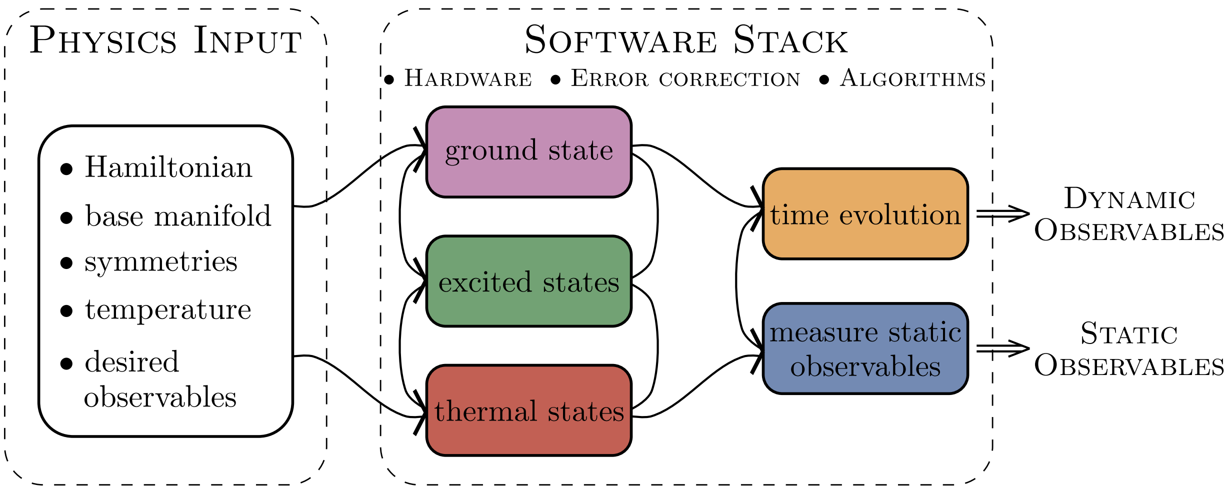
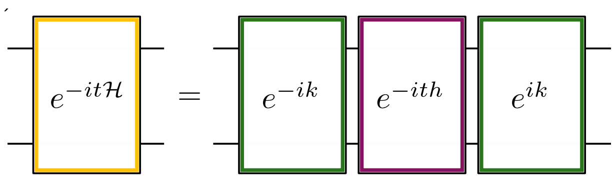
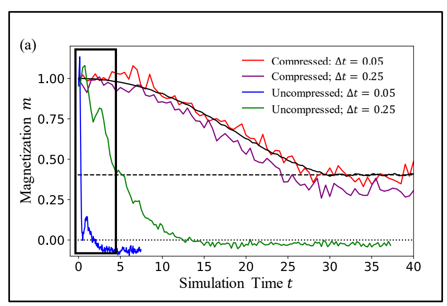
Quantum Matter meets Quantum Computing



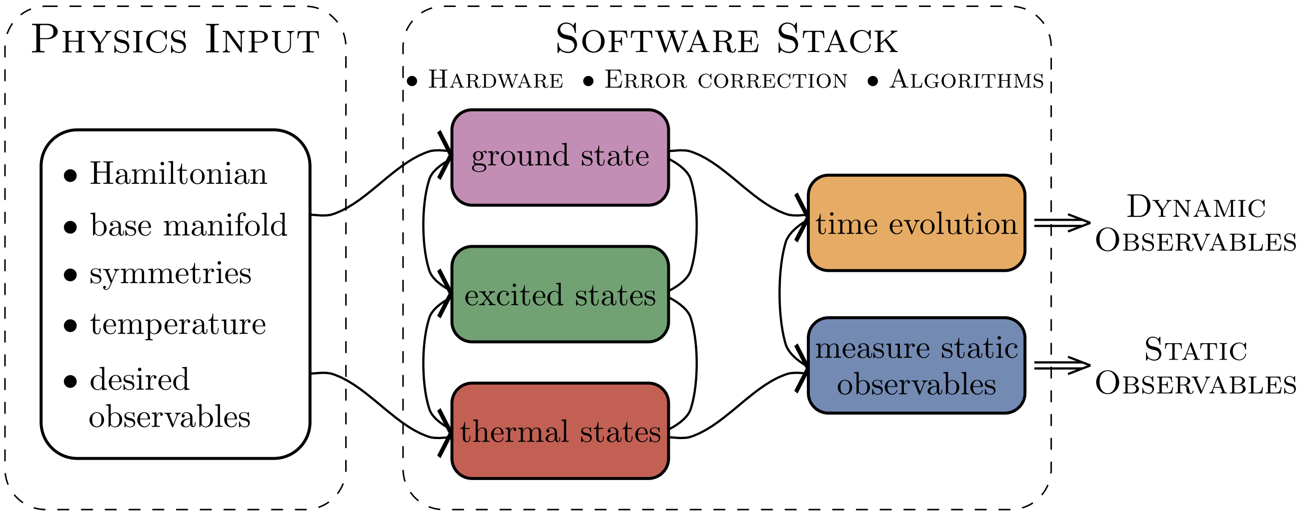


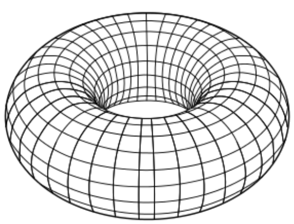
Building exact operator decompositions with Lie algebra

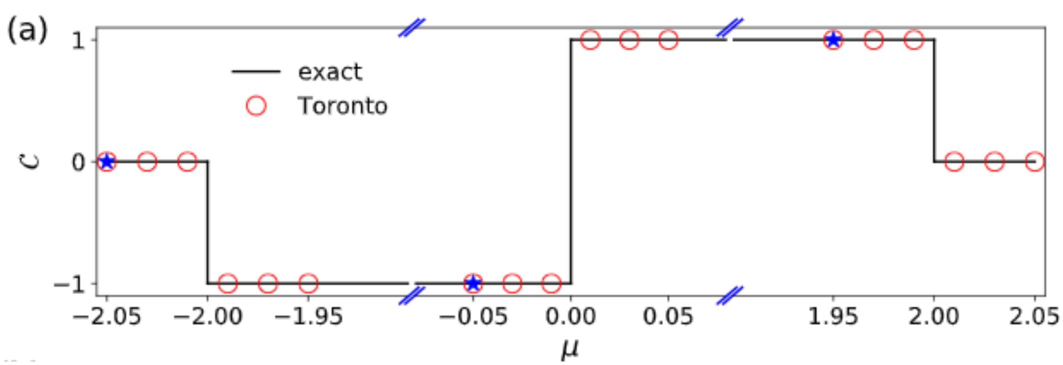


- Measuring correlation functions
- Preparing/measuring topological states
- Modeling driven/dissipative systems
- Time evolution via Lie algebraic decomposition/compression
- Thermodynamics

Conclusion







Topological physics on QC
- Quantum 5, 553 (2021)
- arXiv:2101.07283

Thermodynamics on QC
- Science Advances Vol. 7, no. 34, eabf2447
- arXiv:2112.05688

Exact Time Evolution
- arXiv:2104.00728
- Phys. Rev. A 105, 032420 (2022)
- arXiv:2108.03283

Computing Spectra
- 10.1103/PhysRevB.101.014411

Quantum Matter on QC Review
- Quantum Sci. Technol. 6 043002