Title: A QMC study of the Rydberg phase diagram

Speakers: Anna KnÃ¶rr

Collection: Machine Learning for Quantum Many-Body Systems

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A QMC study of the Rydberg phase diagram

Anna Knörr

Supervised by Roger Melko

Based on my master's defence (last week!)
& an internship with QuEra Computing Inc.

June 2023

PERIMETER
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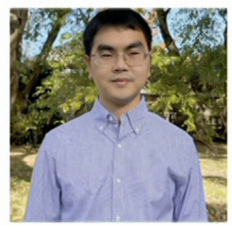
- Machine learning? Nope.
- Quantum many body physics? Definitely.
- Techniques used?
  - Stochastic Series Expansion Quantum Monte Carlo (SSE QMC)
    - based on SSE-QMC code by Ejaaz Merali & Isaac de Vlugt
    - internship & continuing collaboration with QuEra (Milan Kornjaca & Fangli Liu)

Ejaaz Merali

Milan Kornjaca



Fangli Liu

Jonathan Wurtz

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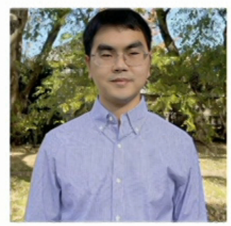
  - Experimental data from QuEra's 256 qubit processor *Aquila*
    - provided by Fangli Liu & Jonathan Wurtz (QuEra Computing Inc.)


Ejaaz Merali


Milan Kornjaca


Fangli Liu


Jonathan Wurtz

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The second quantum revolution is being powered both by theoretical understanding as well as **exquisite quantum control**, down to the level of single atoms.

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The second quantum revolution is being powered both by theoretical understanding as well as **exquisite quantum control**, down to the level of single atoms.

Big shout out to experimentalists!

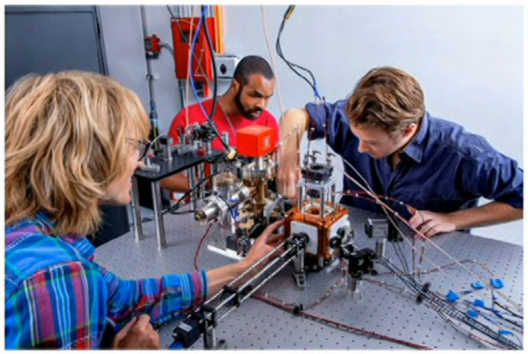


Figure: Niki, Julian and Connor building a quantum processor. Photo credits: QuEra Computing Inc.

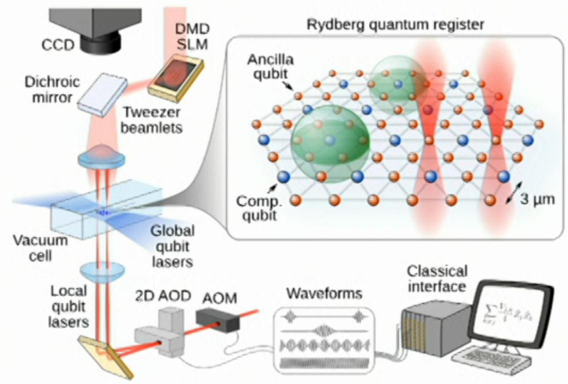
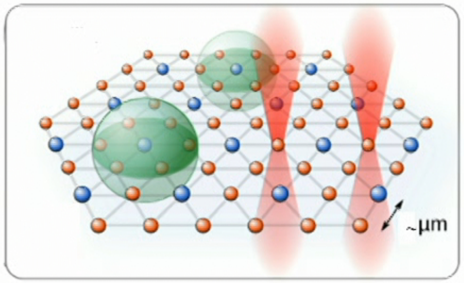


Figure: Reproduced from Browaeys et al. (2020) [1].

Synthetic quantum matter: Atom arrays

"One approach to [quantum computing] was suggested by Richard Feynman and consists in building a ***synthetic quantum system in the lab****, implementing a model of interest for which no other way to solve it is known. The model may be an approximate description of a real material, but it can also be a purely abstract one. In this case, its implementation leads to the construction of an* ***artificial many-body system, which becomes an object of study in its own****."* Browaeys *et al. (2020)*



Source (quote + figure): Browaeys et al. (2020) [1].

Describing atom arrays

Our protagonist: The Rydberg Hamiltonian

$$\frac{H_{Ryd}(t)}{\hbar} = \frac{\Omega(t)}{2}\sum_i \left(|g_i\rangle\langle r_i| + |r_i\rangle\langle g_i|\right) - \Delta(t)\sum_i n_i + \sum_{i<j} V_{ij} n_i n_j,$$

where $|g_i\rangle$ and $|r_i\rangle$ describe the ground and an excited Rydberg state of the i-th atom and n_i is its occupation operator measuring whether an excitation is present.

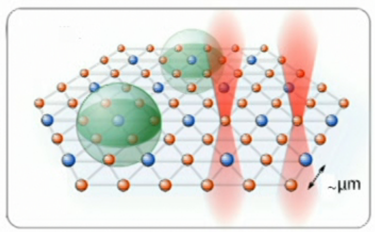


Figure: Reproduced from Browaeys et al. (2020) [1].

Global detuning

The Rydberg Hamiltonian

$$\frac{H_{Ryd}(t)}{\hbar} = \frac{\Omega(t)}{2}\sum_i (|g_i\rangle\langle r_i| + |r_i\rangle\langle g_i|) - \Delta(t)\sum_i n_i + \sum_{i<j} V_{ij} n_i n_j$$

Detuning of the Rabi drive by Δ.

Useful analogy in many-body picture: similar effect to a **chemical potential**.

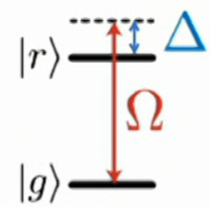


Figure: Reproduced from Ebadi et al. (2020) [2].

The building block: Rydberg states

Atomic states with electrons excited close to ionization limit (i.e. high principal quantum number $n \gtrsim 10$) exhibiting **exaggerated properties**.

Property	n dependence
Binding energy	n^{-2}
Energy between adjacent n states	n^{-3}
Orbital radius	n^2
Geometric cross section	n^4
Dipole moment $\langle nd\|er\|nf\rangle$	n^2
Polarizability	n^7
Radiative lifetime	n^3
Fine-structure interval	n^{-3}

Figure: Scaling relations of Rydberg atoms, reproduced from Gallagher (1994) [3]. The scaling of the dipole moment $\propto n^2$ is crucial to using Rydberg atoms as qubits.

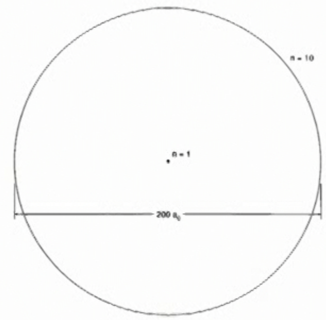


Figure: Visualization of orbital radius scaling $\propto n^2$. Reproduced from Gallagher (1994) [3].

Atom-atom interactions

Leading electrostatic interaction (at interatomic distances $r_{jk} > a_0$): **dipole-dipole interaction**,

$$V_{dd}(R) \propto \frac{\mu_j \mu_k}{R^3},$$

where μ_j and μ_k denote the transition dipole moment operators for the j-th and k-th atom.

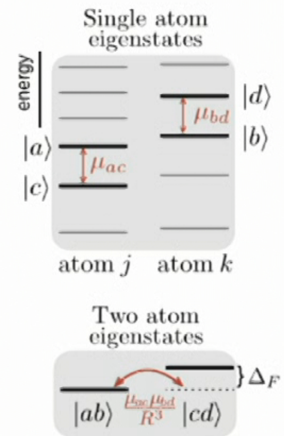


Figure: Reproduced from Morgado et al. (2021) [4].

Atom-atom interactions: van der Waals

Leading electrostatic interaction (at interatomic distances $r_{jk} > a_0$): **dipole-dipole interaction**,

$$V_{dd}(R) \propto \frac{\mu_j \mu_k}{R^3},$$

where μ_j and μ_k denote the transition dipole moment operators for the j-th and k-th atom.

In a certain limit ($\Delta_F > |\mu_{ac}\mu_{bd}|$), second-order perturbation theory in the low energy subspace yields the following diagonal term,

$$\hat{H}_{int} = -\frac{C_6}{R^6} |ab\rangle \langle ab| ,$$

where the van der Waals coefficient is given by $C_6 = \frac{|\mu_{ac}|^2 \mu_{bd}|^2}{\Delta_F}$.

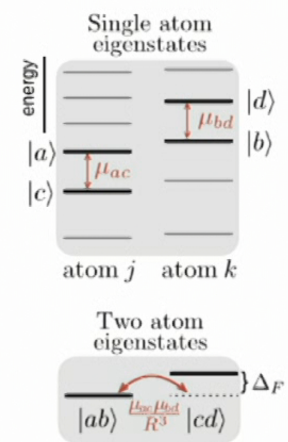


Figure: Reproduced from Morgado et al. (2021) [4].

Blockade effect

Blockade condition:

$$R << R_b \Longleftrightarrow \hbar\Omega << C_6/R^6,$$

i.e. the **blockade radius** is defined as $R_b = (C_6/\hbar\Omega)^{1/6}$.

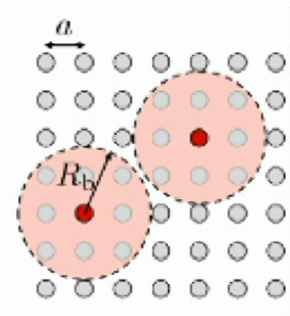


Figure: Reproduced from Browaeys et al. (2020) [1]

Intuition: Within one blockade radius, only one atom is excited.

The Rydberg phase diagram

$$\frac{H_{Ryd}(t)}{\hbar} = \frac{\Omega(t)}{2}\sum_i(|g_i\rangle\langle r_i| + |r_i\rangle\langle g_i|) - \Delta(t)\sum_i n_i + \sum_{i<j}\frac{C_6}{r_{ij}^6}n_i n_j.$$

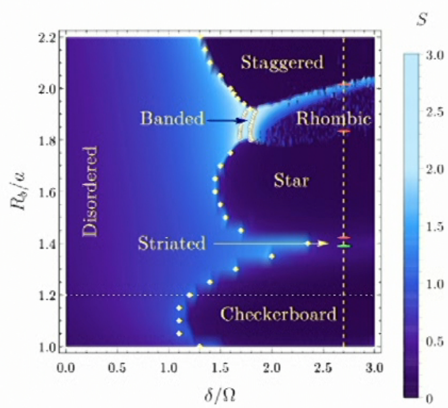
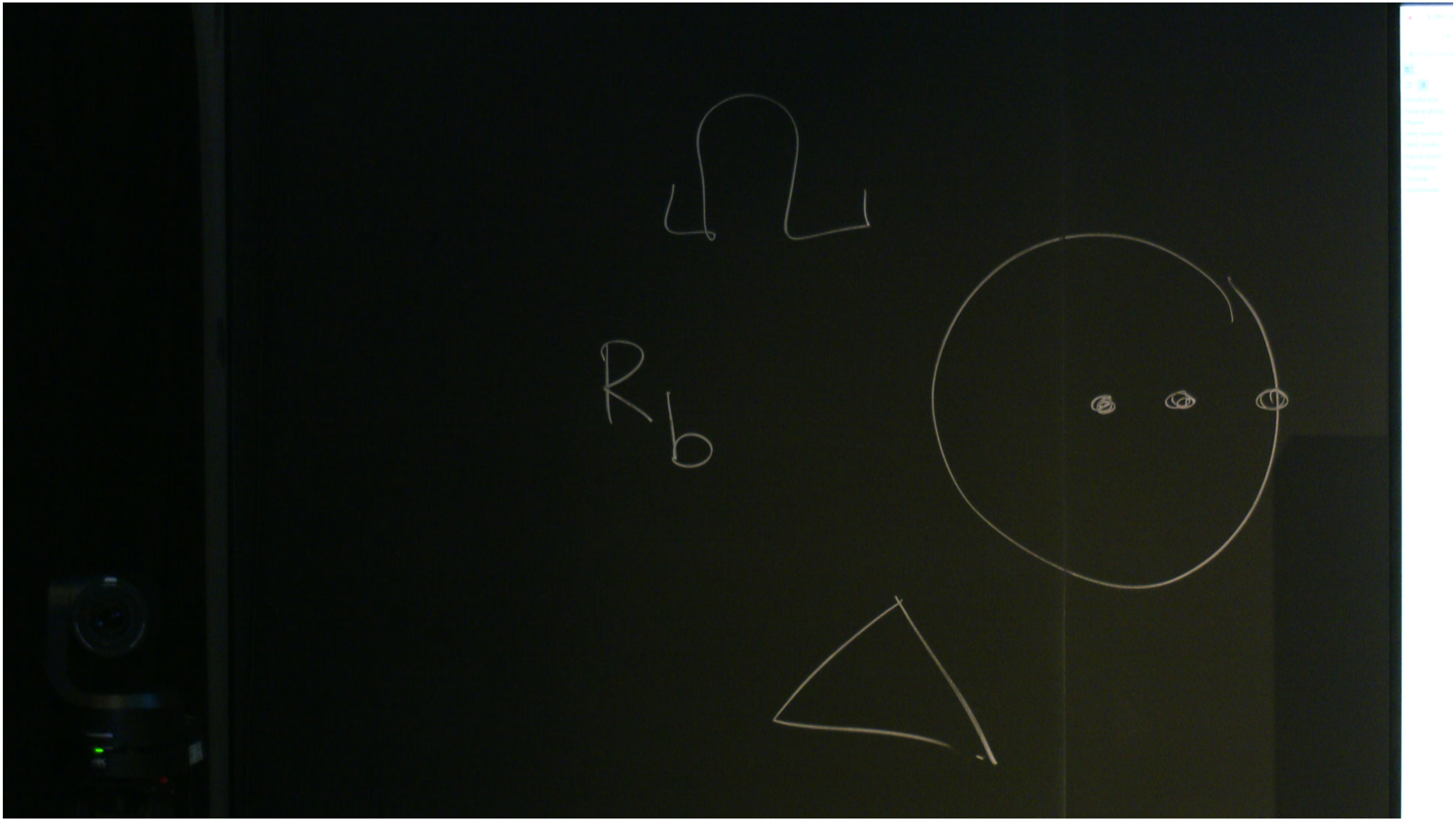


Figure: Reproduced from Samajdar et al. (2020) [5]. δ is equivalent to Δ in our notation, a is the lattice spacing between individual atoms.

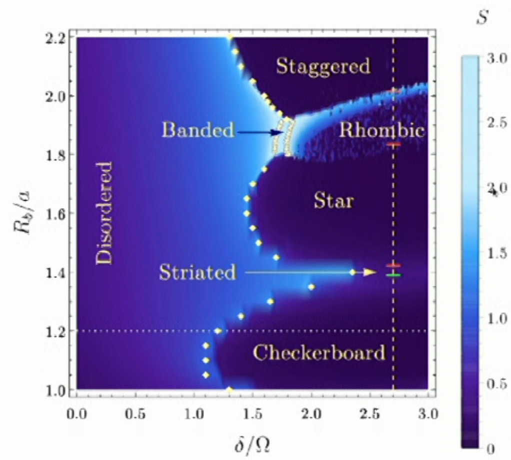
Competition between (positive) detuning, parameterized by Δ/Ω,

and blockade effect, originating from atom-atom interaction, parameterized by R_b/a.

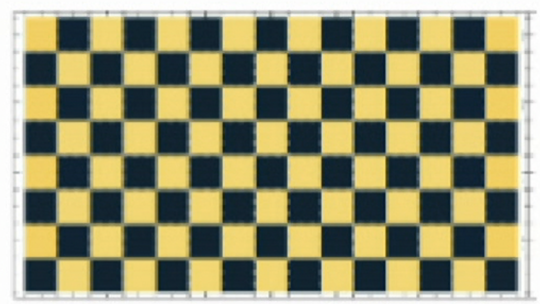

Ω
Rb

The Rydberg phase diagram: Ordered phases

Competition between (positive) detuning, parameterized by Δ/Ω, and blockade effect, originating from atom-atom interaction, parameterized by R_b/a.



(a) Full Rydberg phase diagram.

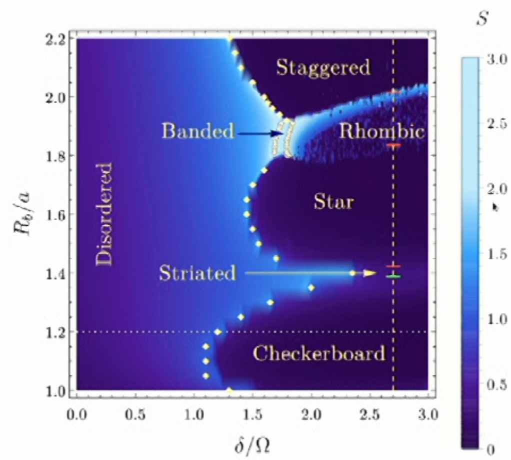


(b) Checkerboard phase, $R_b/a = 1.2$.

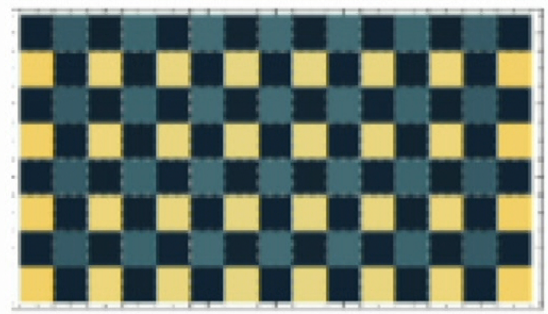
Figures reproduced from Samajdar et al. (2020) [5]. Yellow corresponds to an excited atom in a Rydberg state, dark blue to a ground state atom.

The Rydberg phase diagram: Ordered phases

Competition between (positive) detuning, parameterized by Δ/Ω, and blockade effect, originating from atom-atom interaction, parameterized by R_b/a.



(c) Full Rydberg phase diagram.



(d) Striated phase, $R_b/a = 1.4$.

Figures reproduced from Samajdar et al. (2020) [5]. Yellow corresponds to an excited atom in a Rydberg state, dark blue to a ground state atom and light blue indicates quantum fluctuations.

The Rydberg phase diagram: Not just theory!

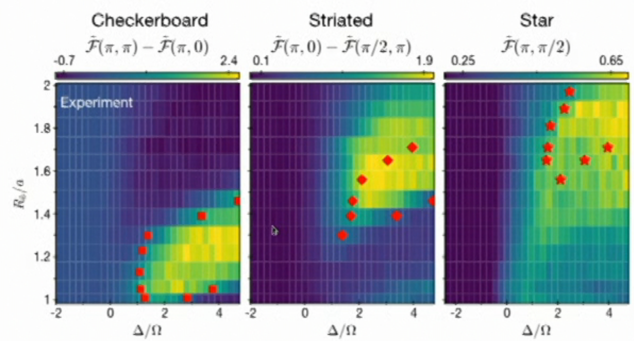


Figure: Experimental detection of ordered phases, reproduced from Ebadi et al. (2020) [2].

The Rydberg phase diagram: Not just theory!

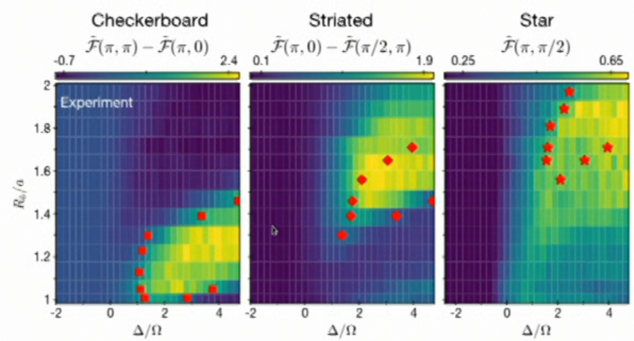


Figure: Experimental detection of ordered phases, reproduced from Ebadi et al. (2020) [2].

The Rydberg phase diagram is currently being investigated using a multitude of methods: theoretical, numerical and experimental. Numerical simulation methods include DMRG, tensor networks and Quantum Monte Carlo (QMC).

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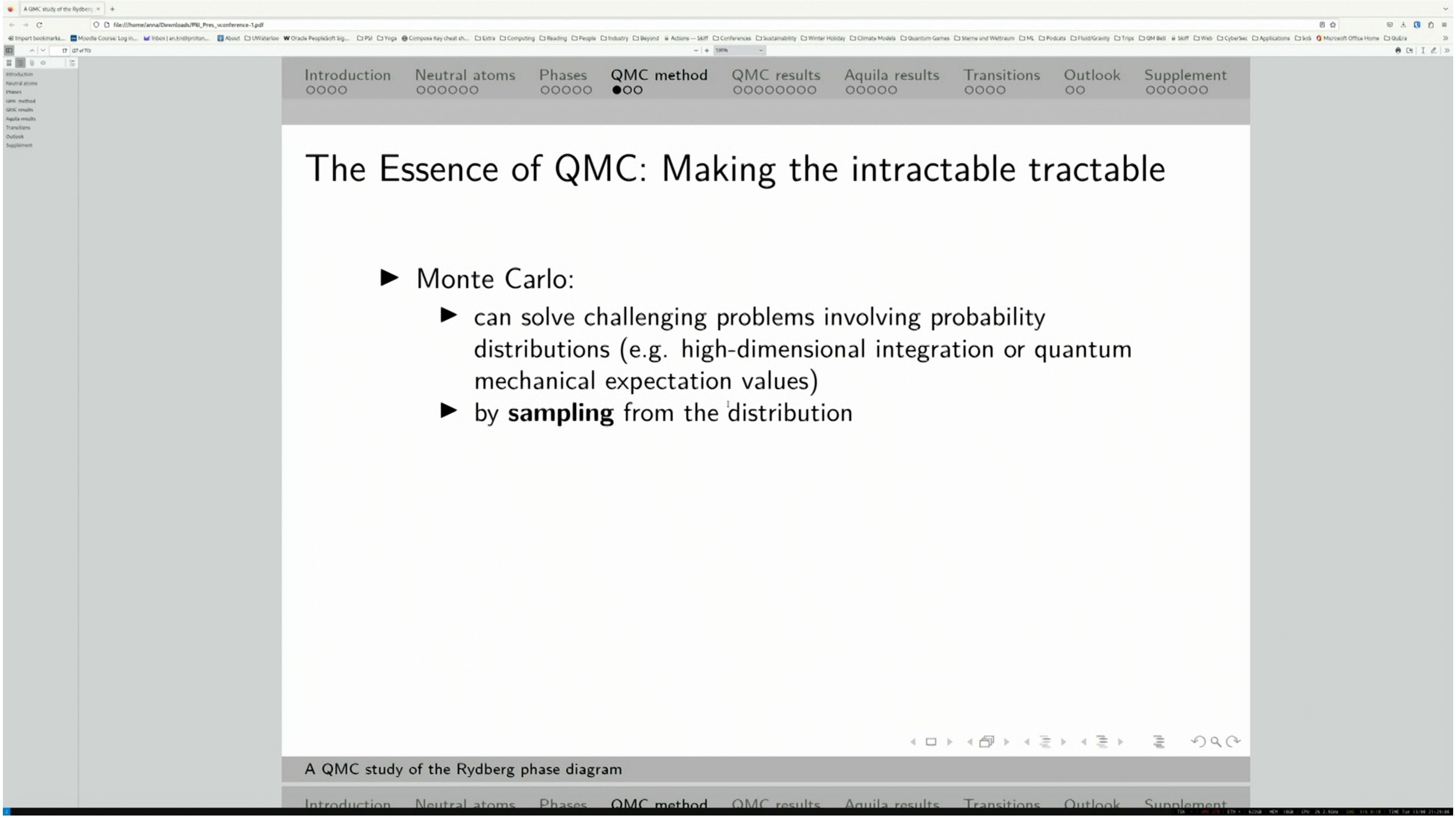
The Essence of QMC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The Essence of QMC: Making the intractable tractable
Monte Carlo:
can solve challenging problems involving probability distributions (e.g. high-dimensional integration or quantum mechanical expectation values)
by sampling from the distribution
A QMC study of the Rydberg phase diagram

The Essence of QMC: Making the intractable tractable

- Monte Carlo:
  - can solve challenging problems involving probability distributions (e.g. high-dimensional integration or quantum mechanical expectation values)
  - by **sampling** from the distribution
- Markov Chain Monte Carlo:
  - instead of drawing samples *randomly*...
  - ... generate a chain of samples to find the important parts of configuration space

The Essence of QMC: Making the intractable tractable

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😃 More efficient!

😟 Correlated samples!

The Essence of QMC: Making the intractable tractable

- Quantum Monte Carlo: classical (i.e. does *not* run on quantum hardware!) method of applying stochastic Monte Carlo approach to solve a quantum many-body problem.
    - Note: QMC is an umbrella term and subsumes many different flavors of implementation, each tailored to solve a specific type of problem as efficiently as possible.

Our QMC flavor: Stochastic Series Expansion (SSE)

Check out: *Stochastic Series Expansion Quantum Monte Carlo for Rydberg Arrays* (Merali et al. 2023, arxiv:2107.00766)

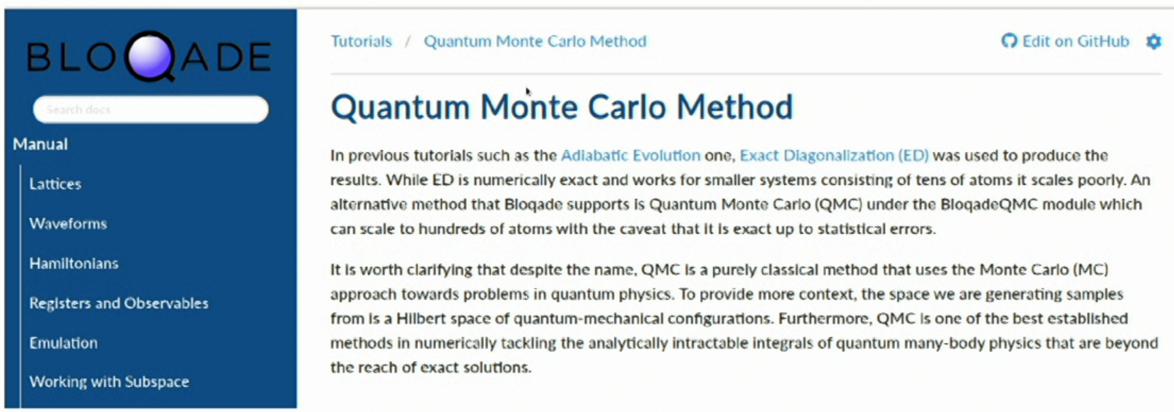
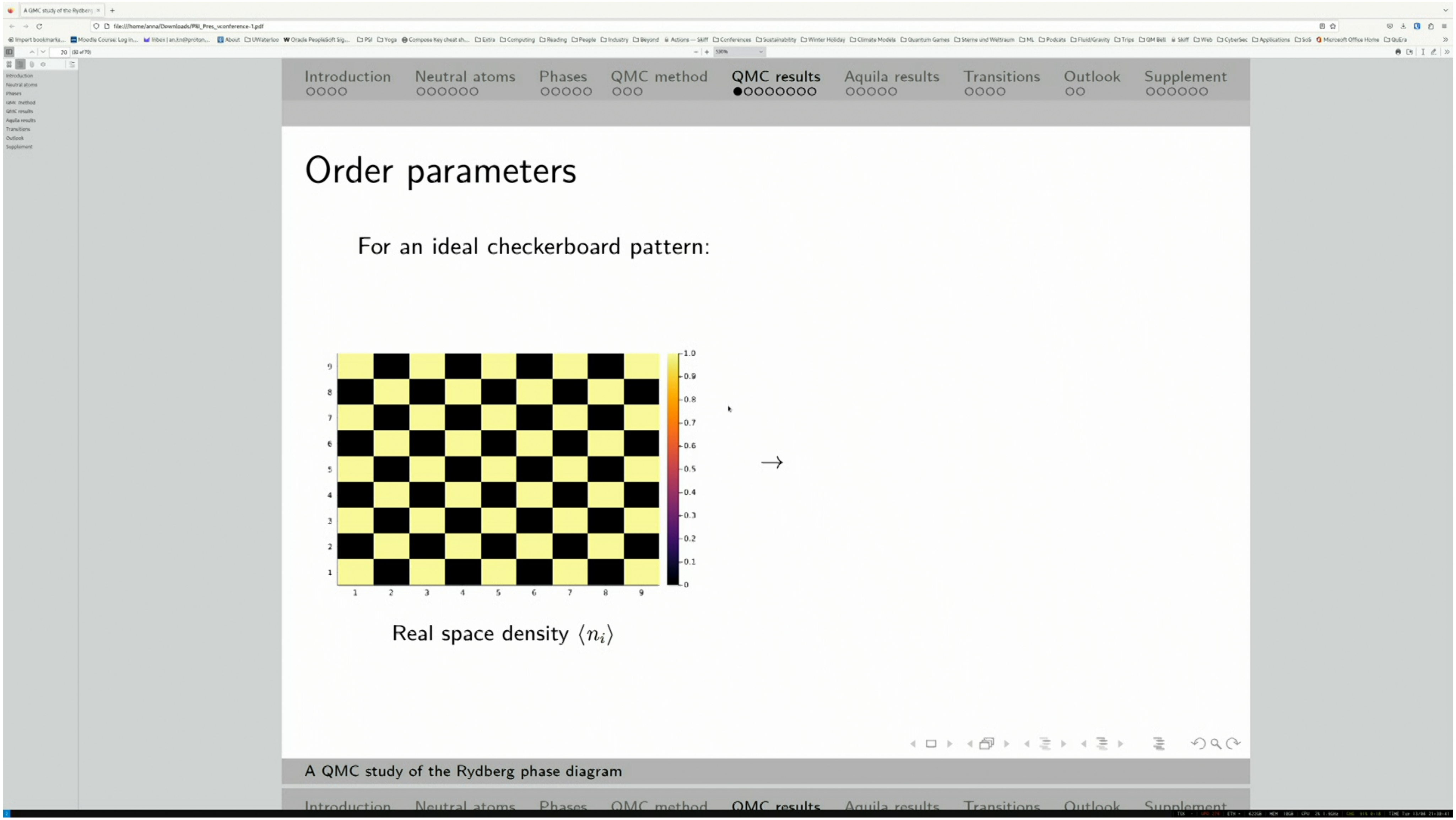


Figure: Check out the BloqadeQMC tutorial! 💪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Order parameters
For an ideal checkerboard pattern:
Real space density $\langle n_i \rangle$
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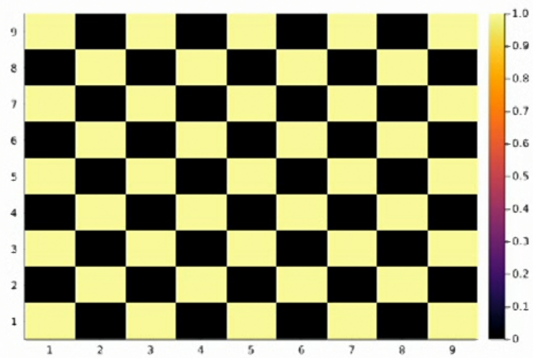
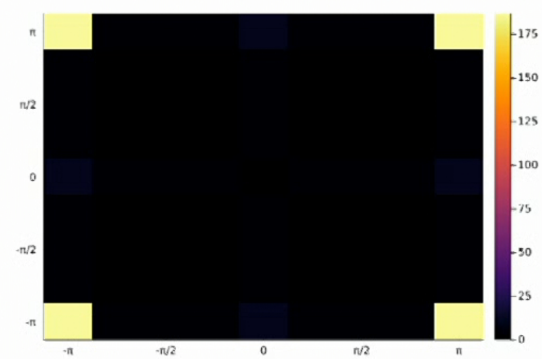
Order parameters

For an ideal checkerboard pattern:



Real space density $\langle n_i \rangle$

$\rightarrow$

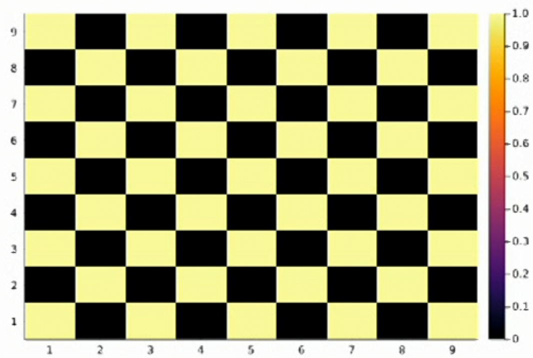


Fourier transform of $\langle n_i n_j \rangle - \langle n_i \rangle \langle n_i \rangle$

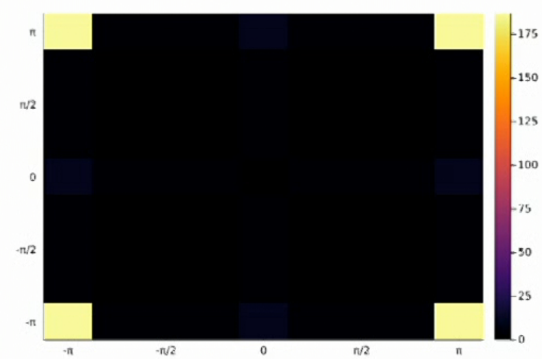
$\rightarrow$ FT is a more compact, compressed representation of the same data.

Order parameters: Peaks in Fourier spectrum

For an ideal checkerboard pattern: Peaks at (π, π) and 90°-rotated counterparts.



$\rightarrow$



Real space density $\langle n_i \rangle$

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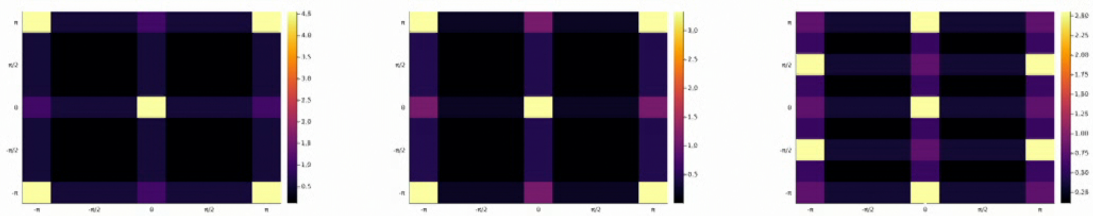
Order parameters



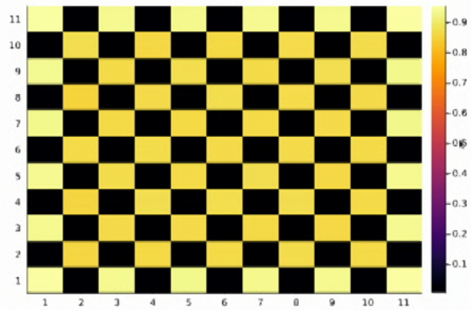
(a) Checkerboard spectrum (b) Striated spectrum (c) Star spectrum

Figure: Fourier transforms of $\langle n_i \rangle$.

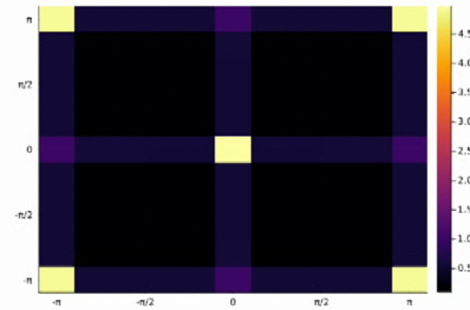
Checkerboard	(π, π)
Striated	$(0, \pi), (\pi, \pi)$
Star	$\pm(\pi/2, \pi), (\pi, 0)$

Table: Summary of expected peaks in Fourier spectrum of the one/two-point density function.

QMC Results: Checkerboard phase 👍



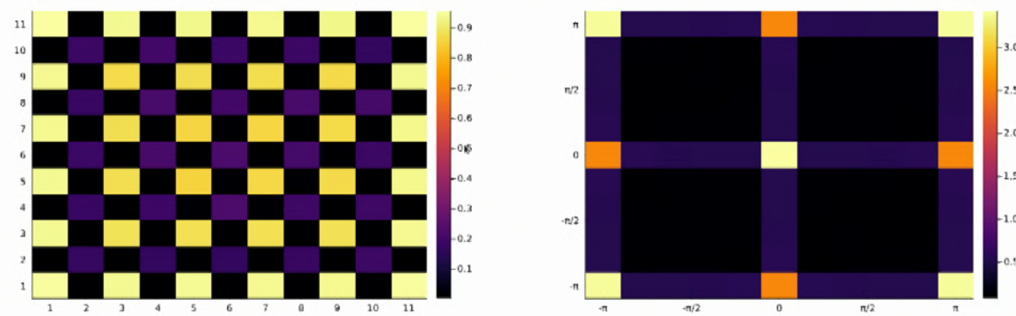
(a) Real space density



(b) FT of $\langle n_i \rangle$

Figure: Checkerboard pattern detected at $R_b/a = 1.2, \Delta/\Omega = 2.7$

QMC Results: Striated phase 👍



(a) Real space density (b) FT of $\langle n_i \rangle$

Figure: Striated pattern detected at $R_b/a = 1.4, \Delta/\Omega = 2.7$

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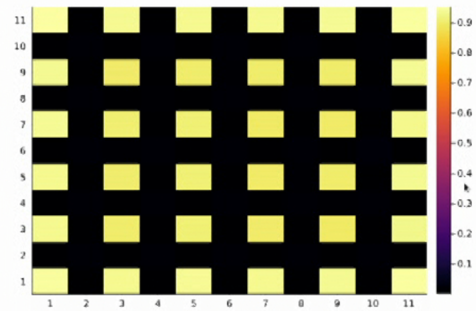
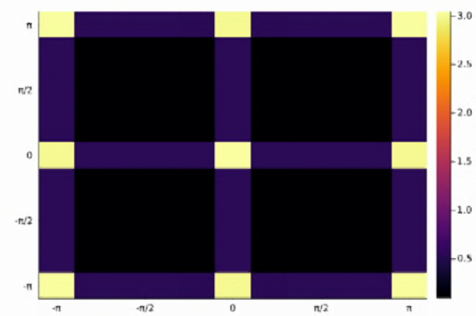
QMC search for star phase 🤔



(a) Real space density



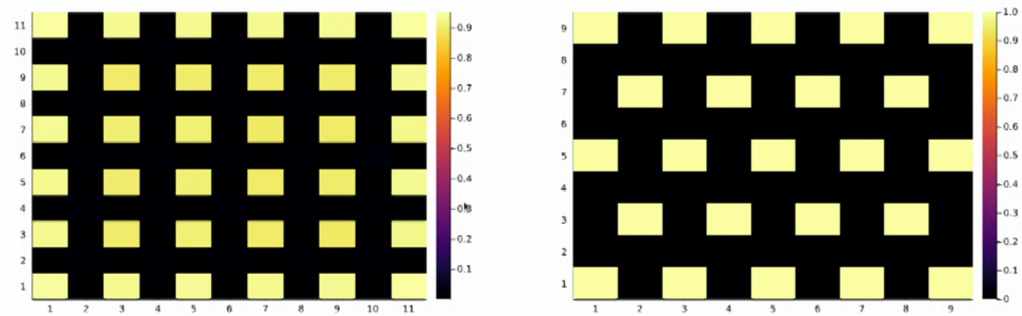
(b) FT of $\langle n_i \rangle$

Figure: Parameter values: $R_b/a = 1.6, \Delta/\Omega = 2.7$

Instead of star phase, rather striated without quantum fluctuations.

Ergodicity issues? Is the QMC stuck in a local minimum?

QMC search for star phase 🤔



(a) Simulation parameter values: $R_b/a = 1.6, \Delta/\Omega = 2.7$

(b) Ideal star pattern

Figure: Comparison of real space densities of local & global minimum configuration.

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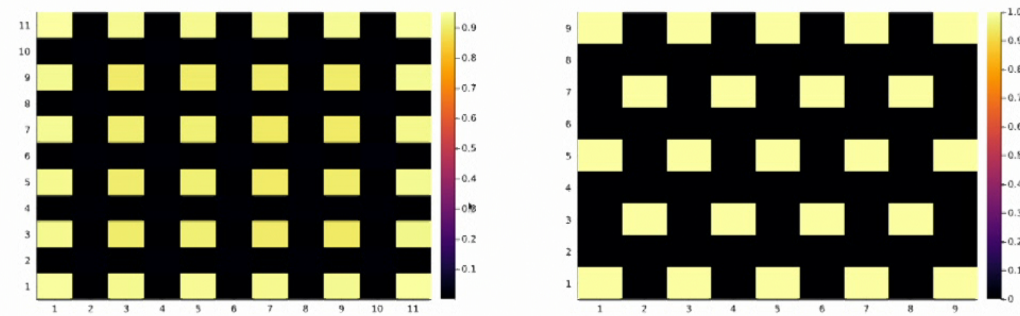
QMC search for star phase 🤔



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Meet QuEra's Aquila processor

- 256 neutral atom qubits

Figure: The real thing. Photo credits: QuEra Computing Inc.

Meet QuEra's Aquila processor

- 256 neutral atom qubits
- currently operators in the *analog mode*
  - uses *continuous* control parameters, instead of discrete gates as in digital mode
- Architecture: "field programmable qubit array" (FPQA)

Figure: The real thing. Photo credits: QuEra Computing Inc.

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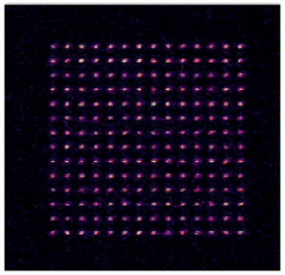
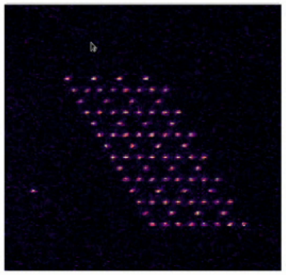
FPQAs

Atoms can be **moved** individually, using optical tweezers!

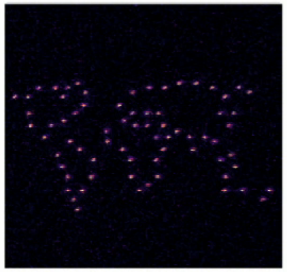
→ Field programmable qubit arrays offer **nearly arbitrary qubit configurations**.



Square lattice



Kagome lattice



World map

Figure: Nearly arbitrary qubit configurations are possible using Aquila!
Photo credits: QuEra Computing Inc.

Experimental data from Aquila

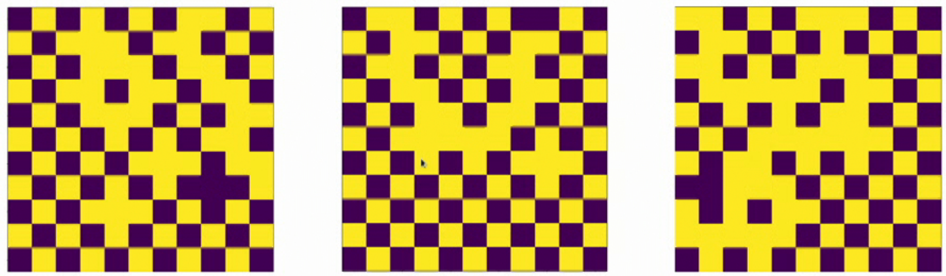
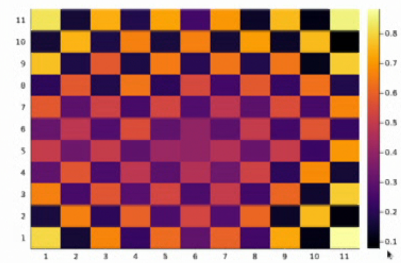


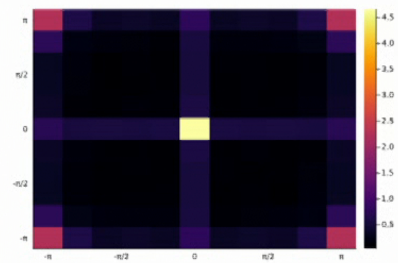
Figure: Individual shots from QuEra's Aquila processor, at $R_b/a = 1.2, \Delta/\Omega = 2.7$, showing experimental defects.

Experimental data kindly provided by Fangli Liu & Jonathan Wurtz (QuEra Computing Inc.)

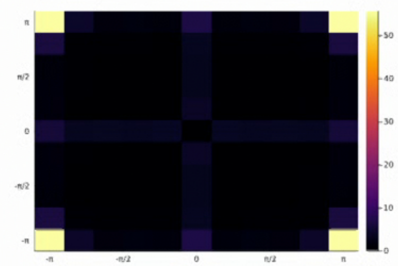
Comparison with Aquila



(a) Real space density



(b) FT of $\langle n_i \rangle$



(c) FT of $\langle n_i n_j \rangle - \langle n_i \rangle \langle n_i \rangle$

Figure: Experimental data from QuEra's Aquila processor at $R_b/a \approx 1.2, \Delta/\Omega = 2.7$.

Critical exponents

How can we describe phase transitions?

Scaling hypothesis (for infinite system)

Power-law behavior of observables near the critical point, e.g.

$$\xi \propto |t|^{-\nu}$$
$$m \propto \xi^{-\beta/\nu}$$

Critical exponents describe *how* we cross a phase transition.

Finite size scaling analysis

Scaling hypothesis... for finite system!

$$m \propto L^{-\beta/\nu}\tilde{m}(L^{1/\nu}|t|).$$

where $\tilde{m}$ is a universal function, independent of the system size.

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One can further simplify the dependence on L by introducing the Binder cumulant

$$U_4 = \frac{1}{2}\left(3 - \frac{\langle m_s^4 \rangle}{\langle m_s^2 \rangle^2}\right),$$

governed by the even simpler scaling formula

$$U_4 \propto \tilde{U}_4(L^{1/\nu}(\Delta - \Delta_c)/\Delta_c), \tag{1}$$

where we have now also explicitly replaced the reduced temperature with our actual control parameter, namely the global detuning Δ.

Finite size scaling analysis

Step 1: Locating the critical point

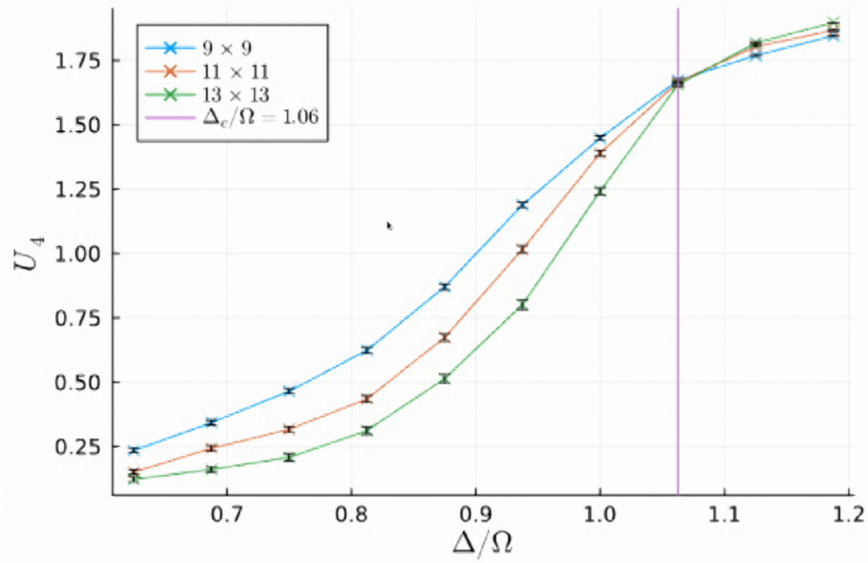

Figure: From plotting the intersection of the Binder cumulant for various system sizes, we find the critical point at $\Delta_c/\Omega \approx 1.06$.

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Introduction Neutral atoms Phases QMC method QMC results Aquila results Transitions Outlook Supplement

Finite size scaling analysis

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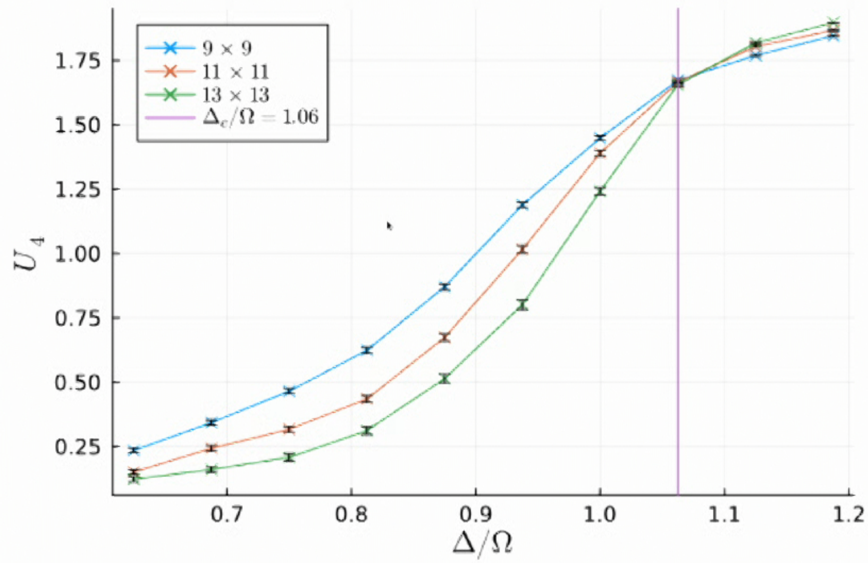
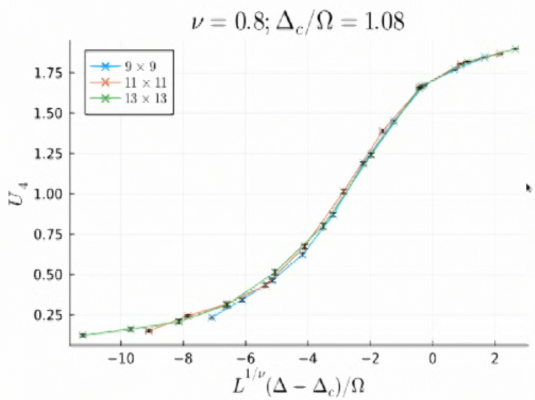


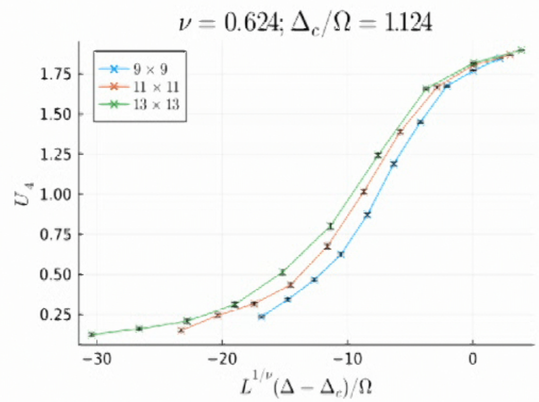
Figure: From plotting the intersection of the Binder cumulant for various system sizes, we find the critical point at $\Delta_c/\Omega \approx 1.06$.

Finite size scaling analysis

Step 2: Extracting critical exponents



(a) ... optimized parameters from our data, i.e. $\Delta_c/\Omega \approx 1.08$ and $\nu \approx 0.8$.



(b) ... using optimized parameters from Ref. [2], i.e. $\Delta_c/\Omega \approx 1.124$ and $\nu \approx 0.624$.

Figure: Scaling collapse of Binder cumulant using ...

Useful quantum advantage?

- Introducing frustration: Rydberg Hamiltonian on Shasty-Sutherland lattice
  - $\rightarrow$ QMC ergodicity stress test!

Useful quantum advantage?

- Introducing frustration: Rydberg Hamiltonian on Shasty-Sutherland lattice
  - $\rightarrow$ QMC ergodicity stress test!
- Beyond QMC: Using neutral atom quantum processor to implement the Heisenberg Hamiltonian
  - $\rightarrow$ sign problem for anti-ferromagnetic interaction on the off-diagonal
- *Analogue* avenues: using neutral atom processor to conduct "experiments by analogy"
  - $\rightarrow$ e.g. possible to study hadronization processes

Climate table

Numerical simulations	
Total Kernel Hours [h]	8260
Thermal Design Power Per Kernel [W]	5.75
Total Energy Consumption Simulations [kWh]	82
Average Emission Of CO_2 In Germany [kg/kWh]	0.56
Total CO_2-Emission For Numerical Simulations [kg]	45
Were The Emissions Offset?	**Yes**
Transport	
Total CO_2-Emission For Transport [kg]	1050
Were The Emissions Offset?	**Yes**
Total CO_2-Emission [kg]	1095

Table: Example of a CO_2-table that can be included towards the end of a scientific publication. Please also consider referencing scientific-conduct.github.io to enhance visibility in your community. To be adapted to our project!