Stochastic Series Expansion Quantum Monte Carlo for Rydberg Arrays

SSE – an efficient quantum Monte Carlo (QMC) method for many quantum systems

SciPost Physics Submission

Stochastic Series Expansion Quantum Monte Carlo for Rydberg Arrays

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Overview

1. rydberg atoms system
2. Quantum simulation algorithm
3. Quantum monte carlo SSE
4. Result and prospect

Why we concern Rydberg atoms systems

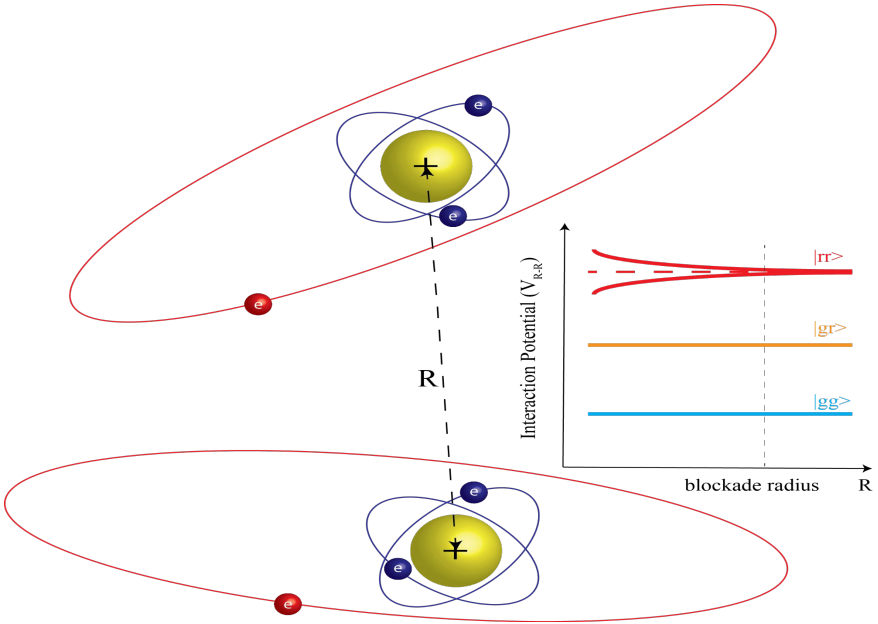
Arrays of neutral atoms provide one of the most coherent and well-controlled experimental quantum many-body platforms available today

Rydberg atom

Rydberg states – highly excited atomic states

Atoms excited to Rydberg states have orders of magnitude larger interactions than atoms in the ground states.

By finely tuned laser coupling from the ground to the Rydberg states



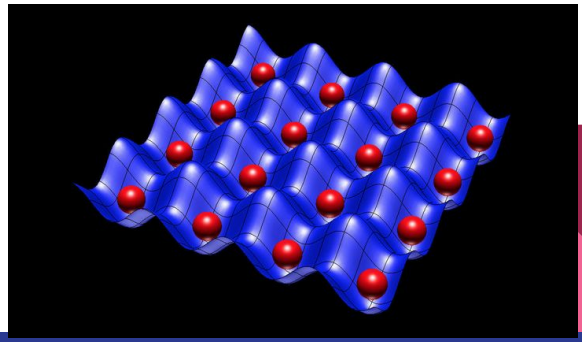
Rydberg atom arrays

– Neutral atoms (Rb, Sr, Yb) are loaded into a lattice formed by an array of optical tweezers

– Atoms can be in their ground state, or excited with lasers with a large principle quantum number (a Rydberg state）

– They form a strongly-interacting system due to the electric dipole moment

– can achieve long achievable coherence times

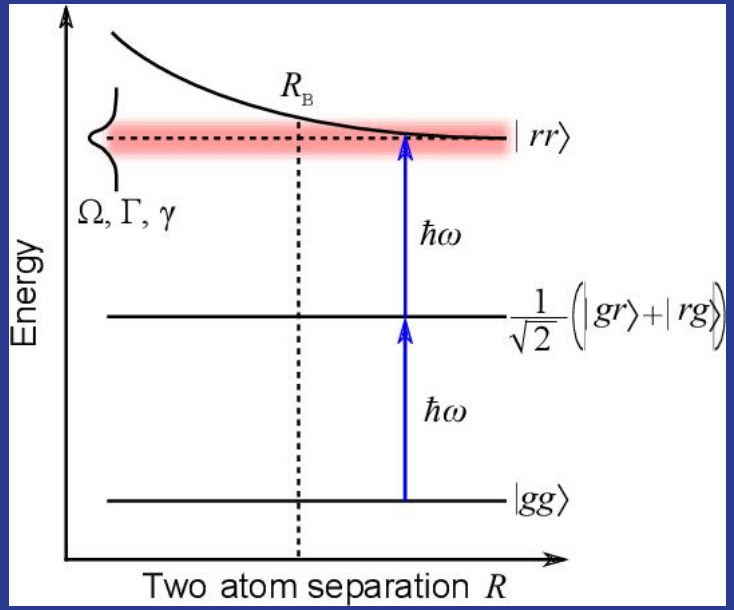


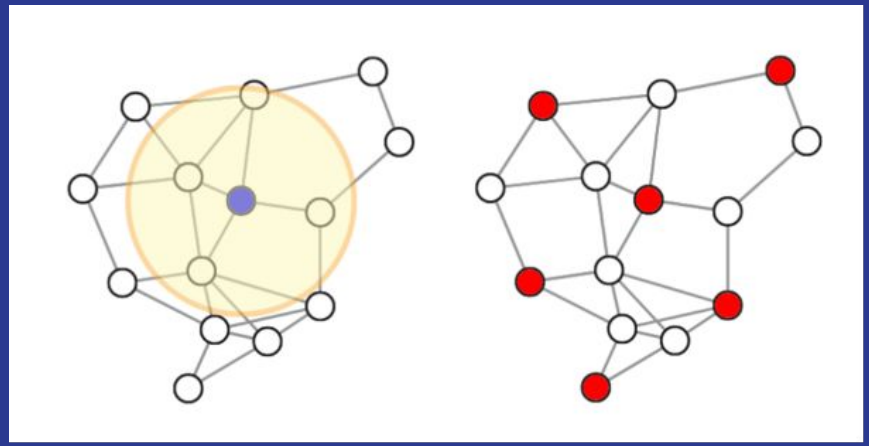
Rydberg blockade

van der Waals (VDW) interaction interactions penalize the simultaneous excitation of two atoms in close proximity to each other

$$V_{ij} = \Omega \left(\frac{R_b}{r_{ij}} \right)^6$$

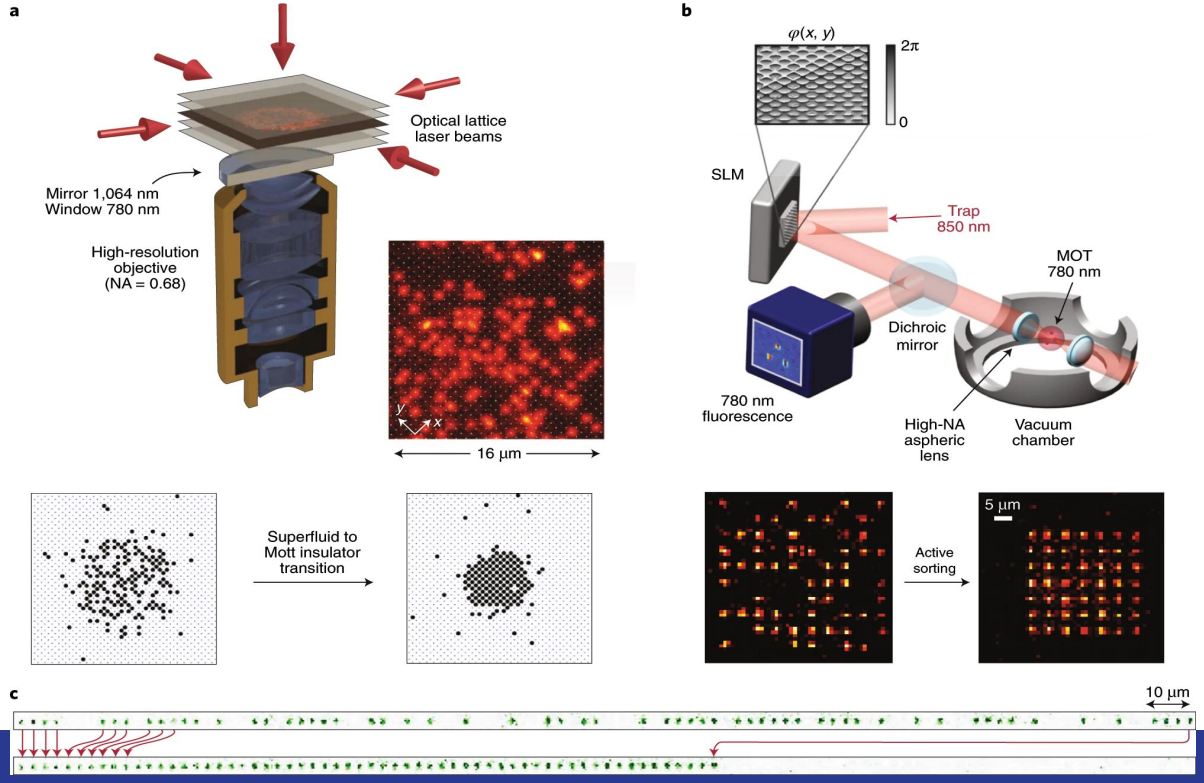
r_ij is the distance between the atoms,Rb is called the blockade radius





Application for many body physics

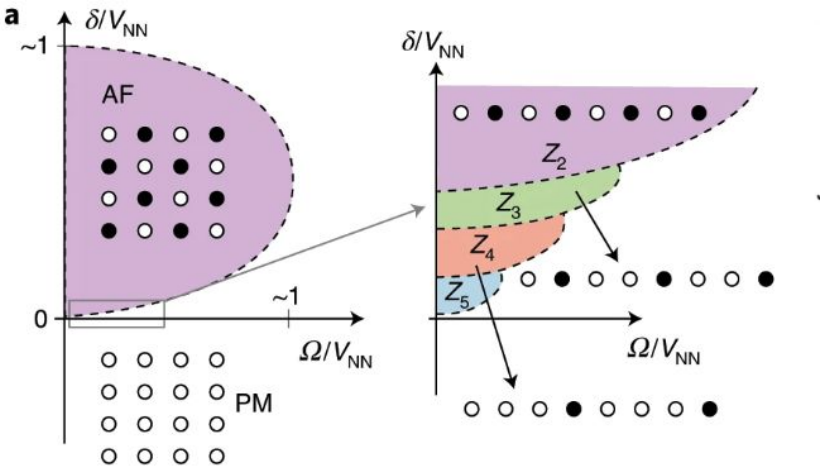
Experimental platforms for realizing arrays of individually controlled neutral atoms



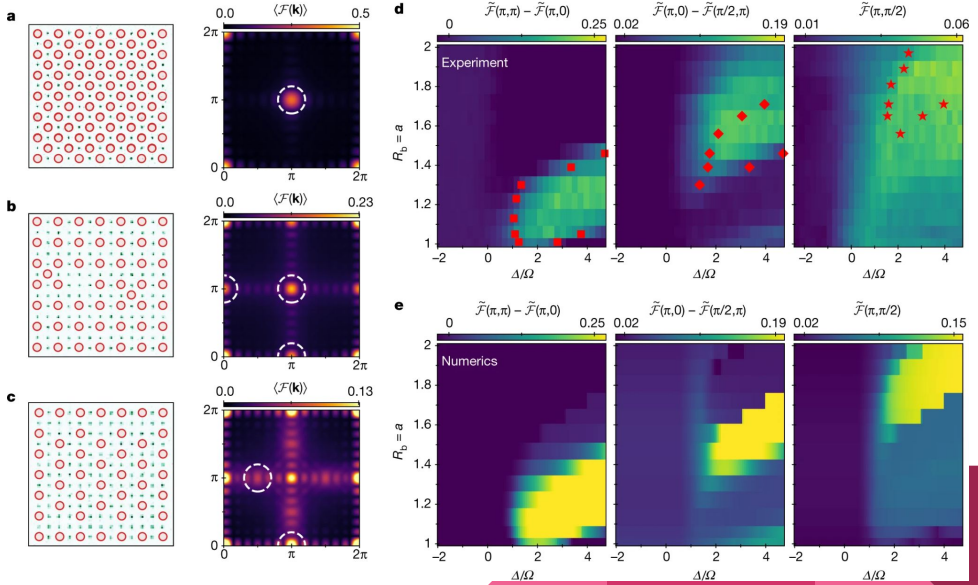
Browaeys, A., Lahaye, T. Many-body physics with individually controlled Rydberg atoms. *Nat. Phys.* 16, 132–142 (2020)

Rydberg atoms for quantum simulation

Quantum quench experiments for the Ising model

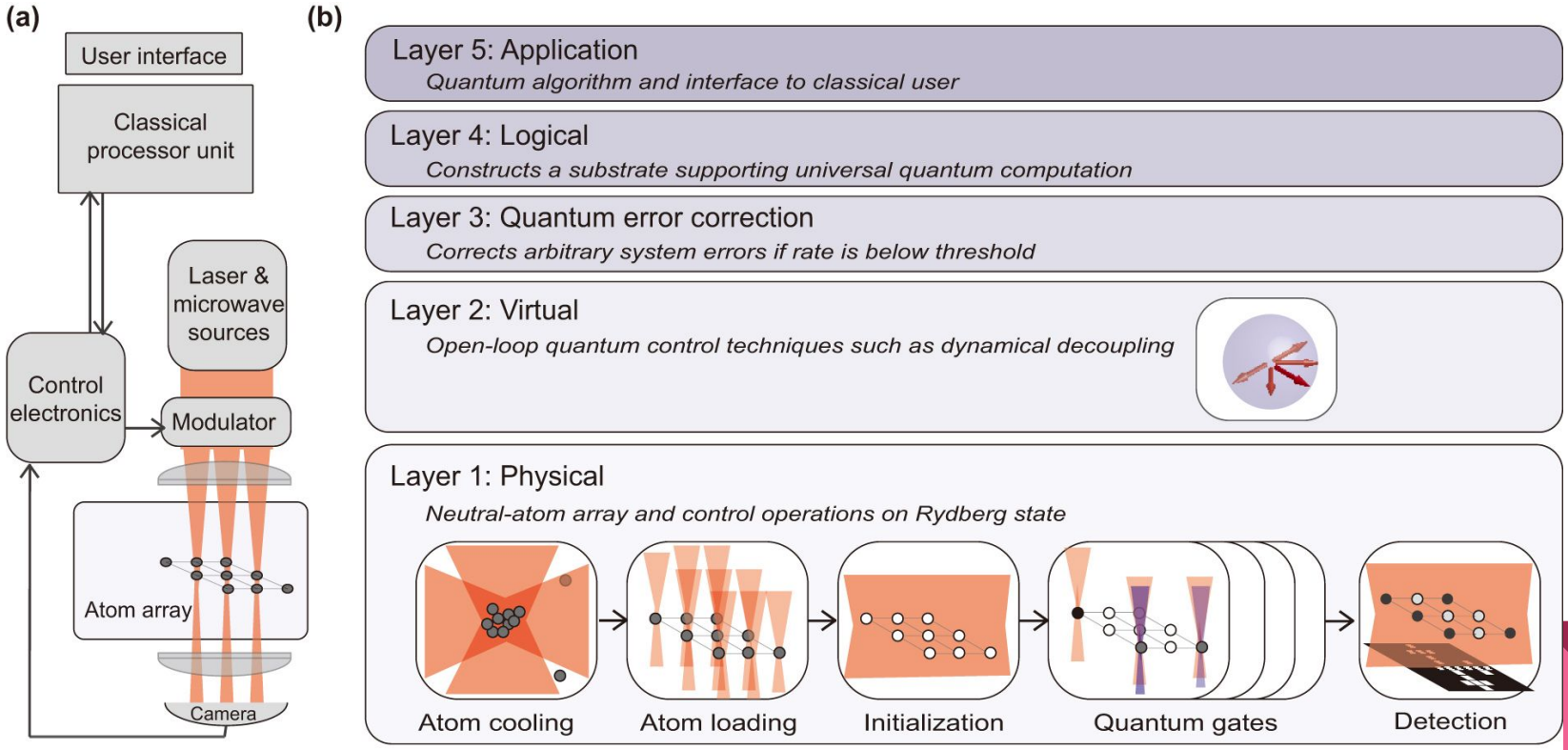


Phase diagram of the two-dimensional square lattice.

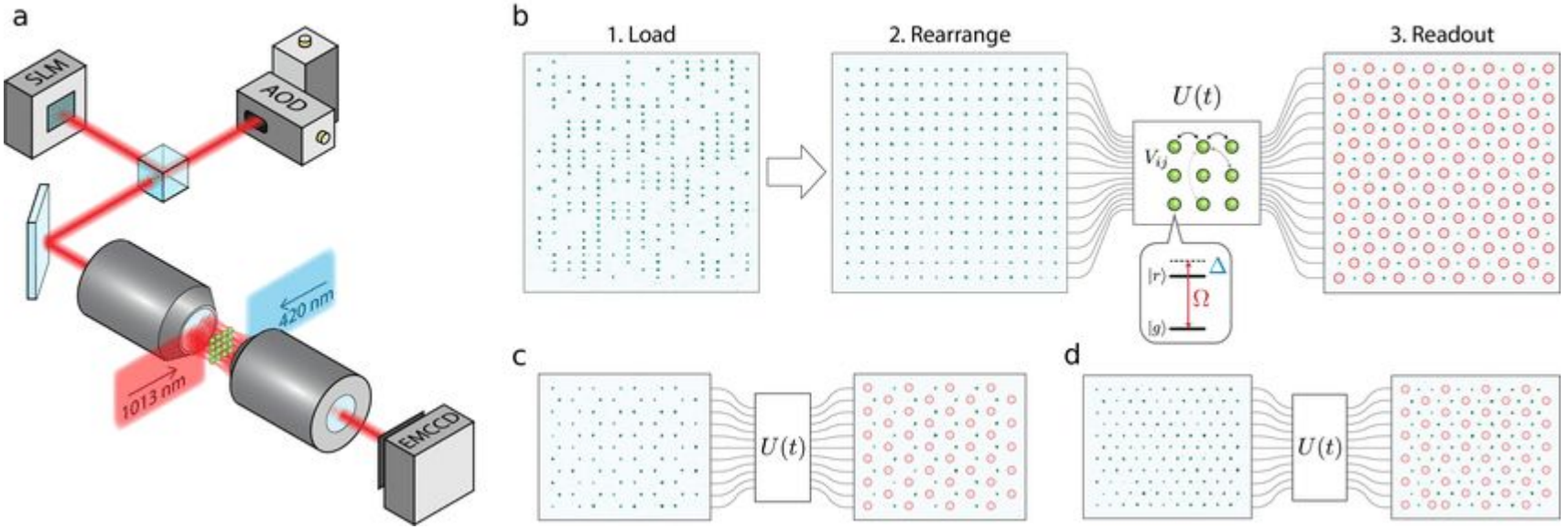


Ebadi, S., Wang, T.T., Levine, H. *et al.* Quantum phases of matter on a 256-atom programmable quantum simulator. *Nature* 595, 227–232 (2021).

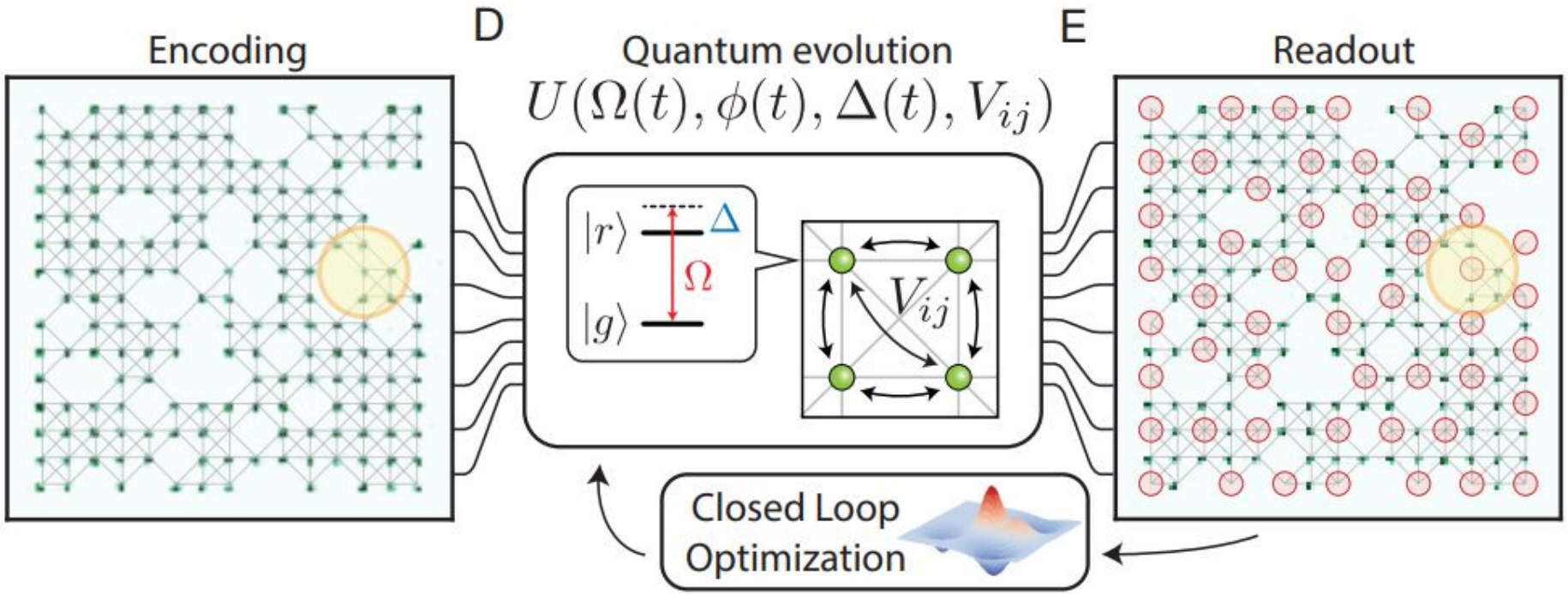
Quantum computation with Rydberg atoms



Programmable two-dimensional arrays



Ebadi, S., Wang, T.T., Levine, H. *et al.* Quantum phases of matter on a 256-atom programmable quantum simulator. *Nature* 595, 227–232 (2021)



quantum many-body evolution under a programmable laser drive U(Ω(t), φ(t), Δ(t)) & long-range Rydberg interactions Vij

update the parameters of the quantum evolution (Ω(t), φ(t), Δ(t)) to finding the MIS

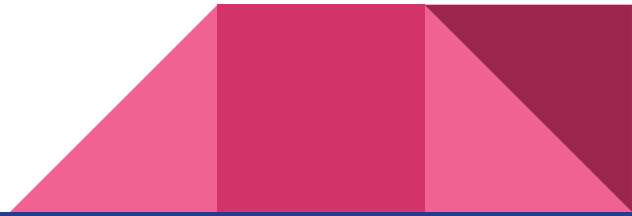
S. Ebadi *et al*,Quantum optimization of maximum independent set using Rydberg atom arrays.*Science***376**,1209-1215(2022)

Experimentally benchmark the quantum algorithm

Typically, a relevant cost function is encoded in a quantum Hamiltonian

To get low energy state – a generic initial state either through an adiabatic evolution or a variational approach via closed optimization loops

The computational performance of such algorithms has been investigated theoretically and experimentally in small quantum systems with shallow quantum circuits



Limited for Exact Diagonal & DMRG

Exact diagonal

- **PXP model**

  study the dynamical behavior of quantum systems such as Rydberg atom arrays.

  P and X represent the projection operator and the exchange operator, respectively.

  The Hamiltonian $H = \sum_i (P_i X_{i+1} P_{i+2} + h.c.)$

- **scales poorly**

  numerically exact and works for smaller systems consisting of tens of atoms[50]

Density Matrix Renormalization Group

- **scales more large up to 100 atoms**
- **Can not simulate quantum dynamics**
- **Complex for 2D system**

Apply more efficient algorithm on Rydberg atom system is important!

Why we need Quantum Monte Carlo Algorithm

– efficient for simulation

– What is monte carlo

– What is quantum monte carlo Stochastic Series Expansion

Efficient for simulation

Advantage of Quantum monte carlo

scale to hundreds of atoms

one of the best established methods in numerically tackling the analytically intractable integrals of quantum many-body physics

Have sign problem【but if the systems' hamiltonian is stoquastic-MA, sign problem will be avoided】

Which systems can simulate which others?

Hamiltonian complexity

Rydberg atom system hamitonian is stoquastic-MA

【Hamiltonians where all the off-diagonal elements in the standard basis are real and non-positive are called "stoquastic】

a Julia Language package for quantum computation and quantum dynamics based on neutral-atom architecture

– the easy design and fast execution of quantum dynamics

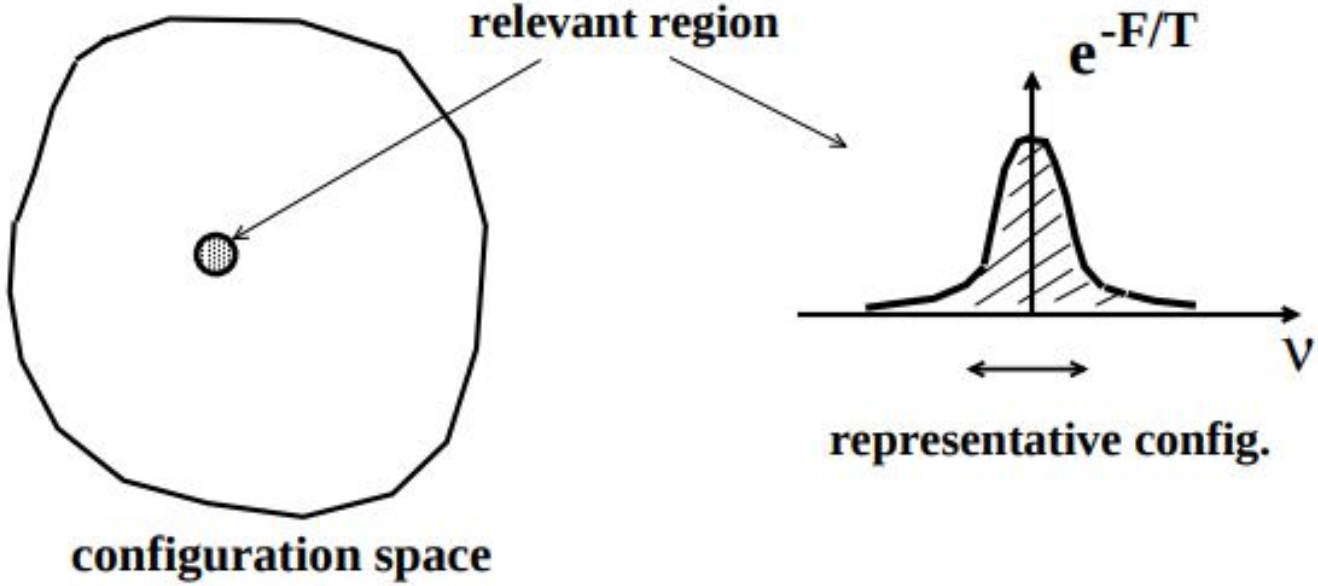
– fast full Hilbert-space simulation on CPUs

– multithreaded CPU (CPU Acceleration) and GPU-accelerated simulation (GPU Acceleration), and more

– recently Quantum Monte Carlo (QMC) under the BloqadeQMC module

classical monte carlo

Importance sampling
Markov chain
Detailed balance
Metropolis algorithm



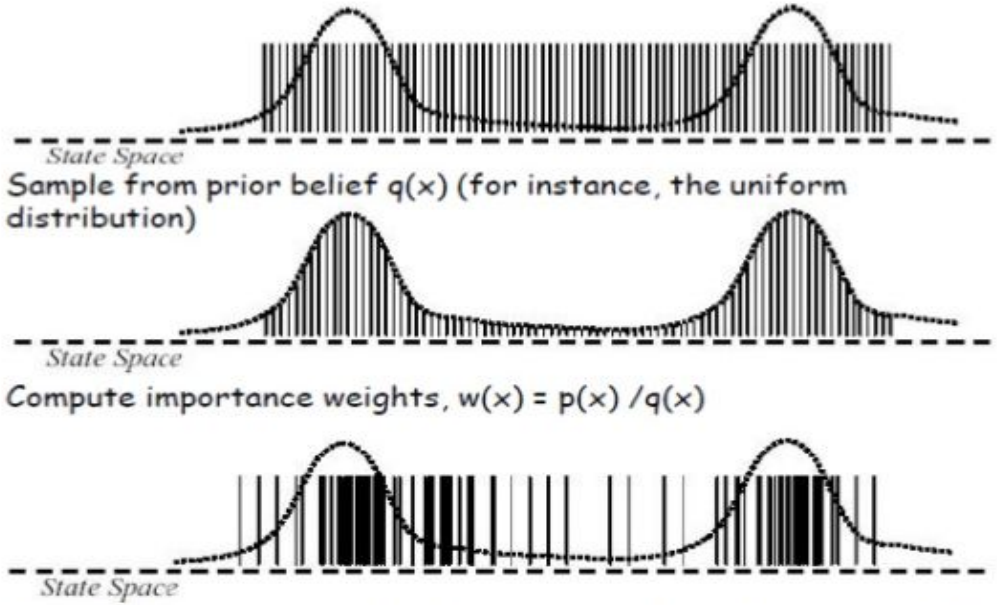
discard most of configurations and deal with a much smaller number of terms

if we can select configurations with probabilities proportional to their weight, since then configurations with large weights are most likely to be selected.

Importance sampling

$$E[f(x)] = \int f(x)p(x)dx = \int f(x)\frac{p(x)}{q(x)}q(x)dx \approx \frac{1}{n}\sum_i f(x_i)\frac{p(x_i)}{q(x_i)}$$

SIS : Sequential Importance Sampling



Markov chain

Let X1, X2, ... describe some states in our system, these states constitute a Markov chain.

$$P(X_{i+1}|X_i, X_{i-1}, ..., X_0) = P(X_{i+1}|X_i)$$

the probability of making a transition to Xi+1 depends only on its immediate past Xi and not on its history.

$$N_1(X_i) = N_0(X_i) + \sum_{j \neq i} [N_0(X_i)P(X_j \to X_i) - N_0(X_i)P(X_i \to X_j)]$$

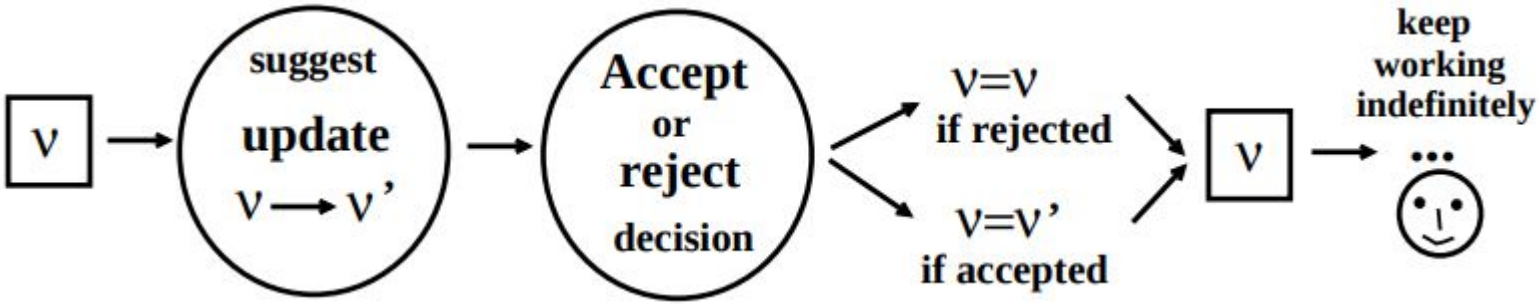
$$P(X_j)P(X_j \to X_i) = P(X_i)P(X_i \to X_j).$$

Detailed balance

$$\frac{P(X_i \to X_j)}{P(X_j \to X_i)} = \frac{W(C_j)}{W(C_i)}$$

probability distribution W(x)

Metropolis algorithm



quantum monte carlo - SSE

Partition function

Rydberg atom system hamiltonian

$$\hat{H} = \frac{\Omega}{2}\sum_{i=1}^{N}\hat{\sigma}_i^x - \delta\sum_{i=1}^{N}\hat{n}_i + \sum_{i<j}V_{ij}\hat{n}_i\hat{n}_j, \qquad V_{ij} = \Omega\left(\frac{R_b}{r_{ij}}\right)^6.$$

$$Z = \mathrm{Tr}\left\{e^{-\beta\hat{H}}\right\}$$

Finite T $$Z = \sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}\sum_{\{\alpha\}_n}\langle\alpha_0|H|\alpha_{n-1}\rangle\cdots\langle\alpha_2|H|\alpha_1\rangle\langle\alpha_1|H|\alpha_0\rangle$$

Divide the hamiltonian

$$\hat{U}^\dagger \hat{H} \hat{U} = -\frac{\Omega}{2} \sum_{i=1}^{N} \hat{\sigma}_i^x - \delta \sum_{i=1}^{N} \hat{n}_i + \sum_{i<j} V_{ij} \hat{n}_i \hat{n}_j$$

$$\hat{H}_{0,0} = \mathbb{I},$$

$$\hat{H}_{-1,a} = \frac{\Omega}{2} \hat{\sigma}_i^x,$$

$$\hat{H}_{1,a} = \frac{\Omega}{2} \mathbb{I},$$

$$\langle 1|\hat{H}_{-1,a}|0\rangle = \langle 0|\hat{H}_{-1,a}|1\rangle = \frac{\Omega}{2},$$

$$\langle 1|\hat{H}_{1,a}|1\rangle = \langle 0|\hat{H}_{1,a}|0\rangle = \frac{\Omega}{2},$$

$$W_{ij}^{(1)} \equiv \langle 00|\hat{H}_{1,b}|00\rangle = C_{ij},$$

$$W_{ij}^{(2)} \equiv \langle 01|\hat{H}_{1,b}|01\rangle = \delta_b + C_{ij},$$

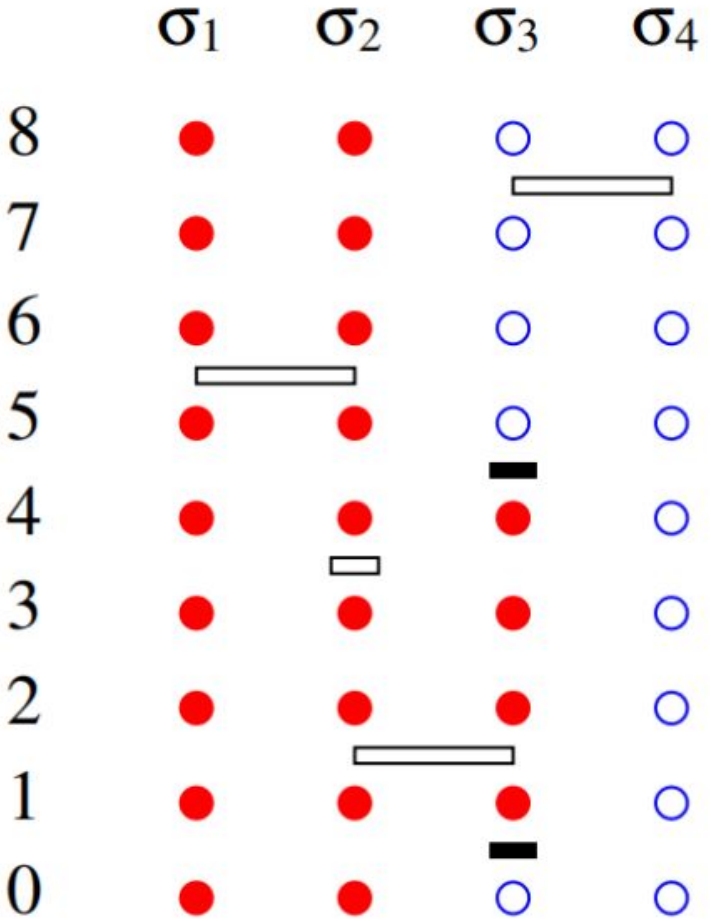
$$W_{ij}^{(3)} \equiv \langle 10|\hat{H}_{1,b}|10\rangle = \delta_b + C_{ij},$$

$$\hat{H}_{1,b} = -V_{ij} \hat{n}_i \hat{n}_j + \delta_b (\hat{n}_i + \hat{n}_j) + C_{ij}.$$

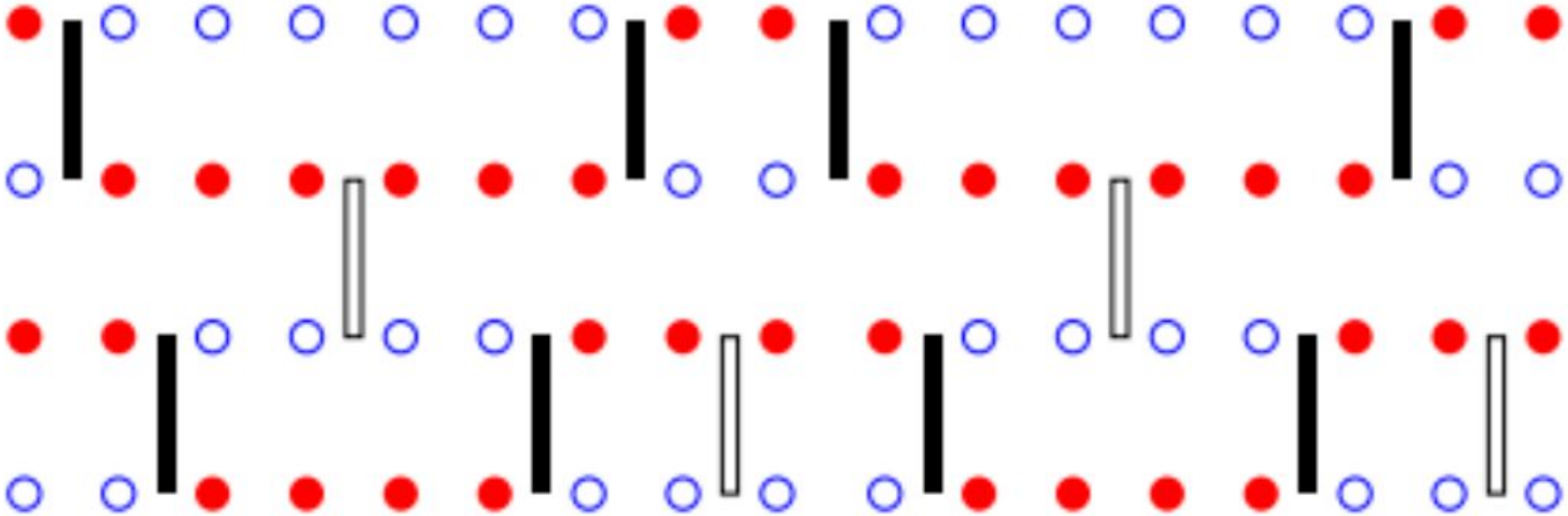
$$W_{ij}^{(4)} \equiv \langle 11|\hat{H}_{1,b}|11\rangle = -V_{ij} + 2\delta_b + C_{ij},$$

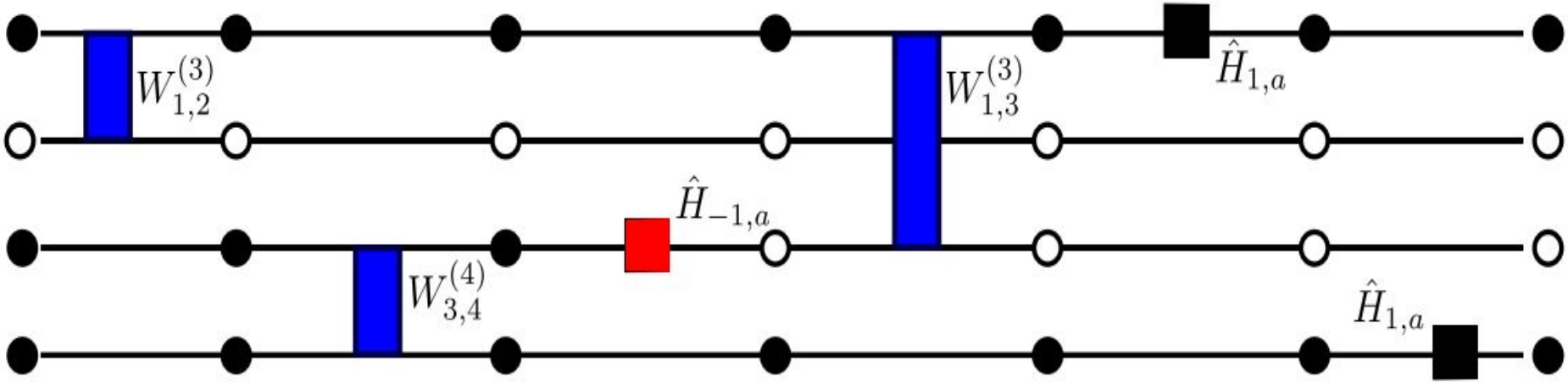
Sign the imaginary time on every piece!

Note: get random numbers from 0 to beta with equal probability!



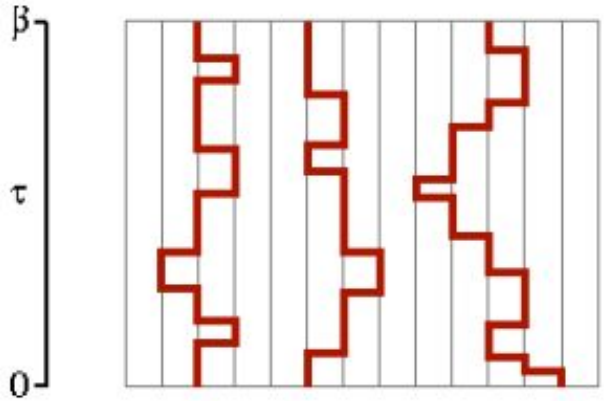
$$Z_{\mathrm{SSE}} = \sum_{\{\alpha\}} \sum_{S_M} \frac{\beta^n (M-n)!}{M!} \langle \alpha_0 | H_{b_M} | \alpha_{M-1} \rangle \cdots \langle \alpha_2 | H_{b_2} | \alpha_1 \rangle \langle \alpha_1 | H_{b_1} | \alpha_0 \rangle,$$

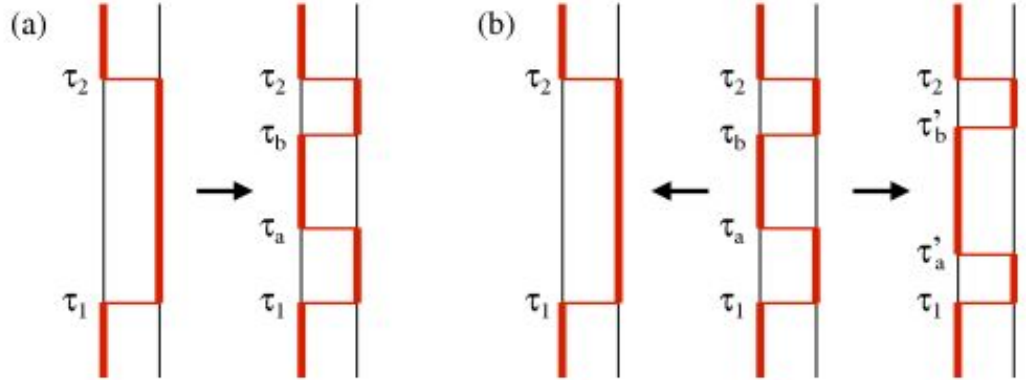



$W^{(3)}_{1,2}$
$W^{(3)}_{1,3}$
$\hat{H}_{1,a}$
$\hat{H}_{-1,a}$
$W^{(4)}_{3,4}$
$\hat{H}_{1,a}$

The continuous time limit

Limit $\Delta_\tau \to 0$: number of kinetic jumps remains finite, store events only





Special methods (**loop and worm updates**) developed for efficient sampling of the paths in the continuum

local updates

consider probability of inserting/removing events within a time window

⇐ Evertz, Lana, Marcu (1993), Prokofev et al (1996)
Beard & Wiese (1996)

Diagonal update for finite T

1. If H_1,a or H_1,b is encountered, remove it (n → n − 1) with probability

$$A([1,a]_p \text{ or } [1,b]_p \to [0,0]_p) = \min\left(\frac{M-n+1}{\beta\mathcal{N}}, 1\right)$$

2. If H_0,0 is encountered, decide whether or not to attempt inserting Hˆ 1,a or Hˆ 1,b (n → n + 1) with the probability

$$A([0,0]_p \to [1,a]_p \text{ or } [1,b]_p) = \min\left(\frac{\beta\mathcal{N}}{M-n}, 1\right)$$

Diagonal update for finite T

3. insert H_1,a or H_1,b in the previous step – choose H_1,a at site i or H_1,b at bond (i, j) by sampling the (unnormalized) probability distribution

$$P_{ij} = \begin{cases} \frac{\Omega}{2} & i = j \\ \max\left(W_{ij}^{(1)}, W_{ij}^{(2)}, W_{ij}^{(3)}, W_{ij}^{(4)}\right) & i \neq j \end{cases}.$$

the normalizing constant of this distribution N = /sum_ij Pij

If H_1,a is chosen, its insertion at site i is accepted.

If H_1,b is chosen, $|n_{1,p}, n_{2,p}, \cdots, n_{N,p}\rangle$ means the configuration at the current imaginary time slice p

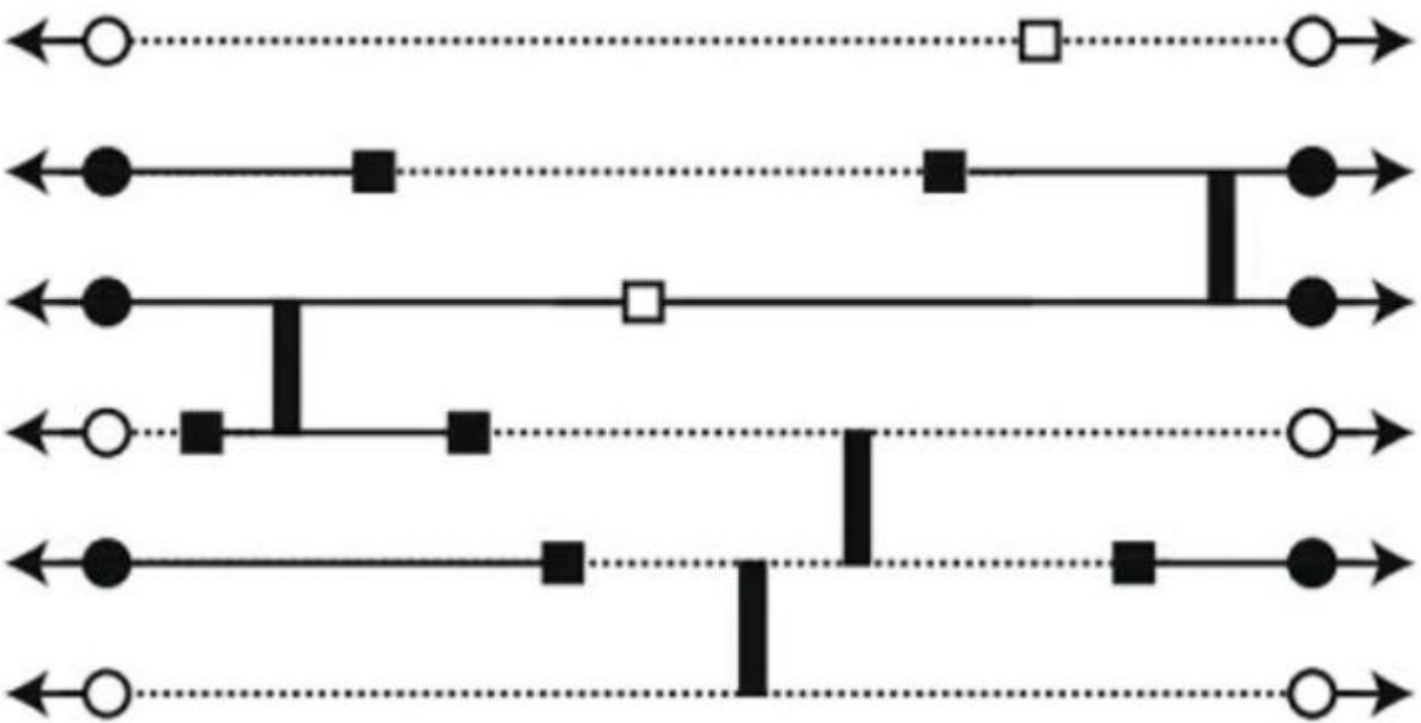
If $|n_{i,p}, n_{j,p}\rangle$ matches the sampled matrix element of H_1,b (one of W (1)_ij , W(2)_ij , W (3)_ij , or W (4)_ij), the insertion is accepted

Otherwise, the insertion of H_1,b at location (i, j) is accepted with probability $\frac{W_{ij}^{(\text{actual})}}{W_{ij}^{(\text{sampled})}}$

$$W_{ij}^{(\text{actual})} = \langle n_{i,p}, n_{j,p} | \hat{H}_{1,b} | n_{i,p}, n_{j,p} \rangle$$

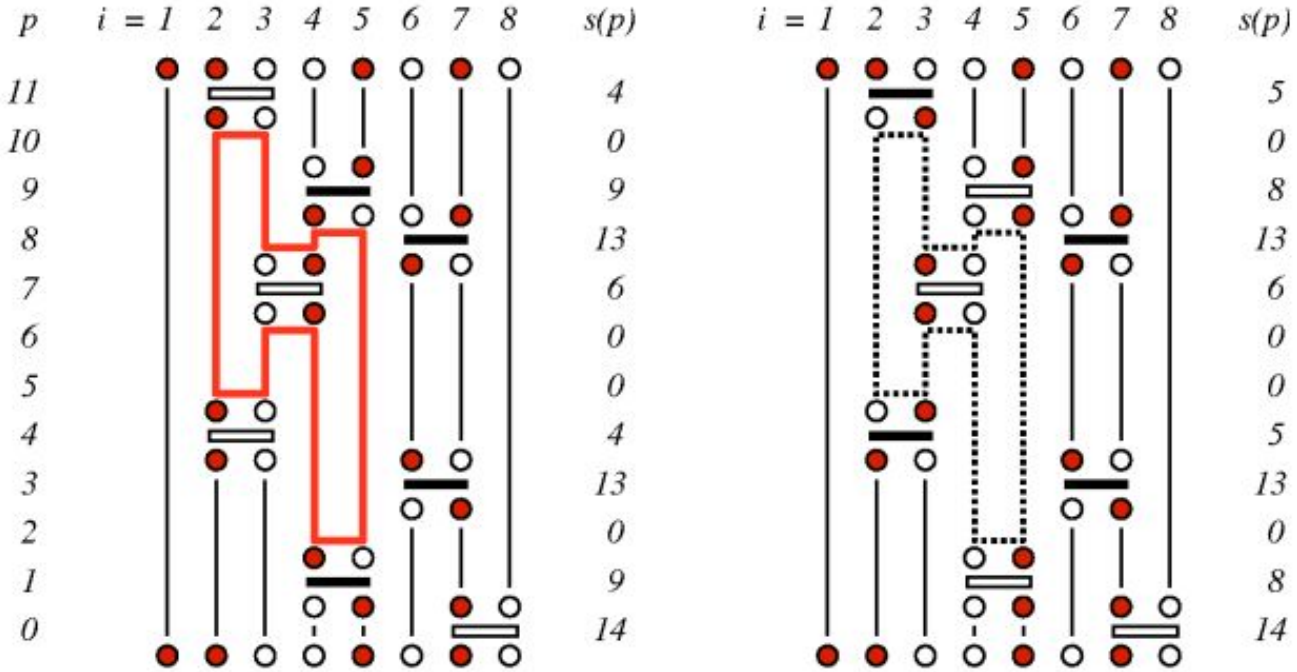
Repeat step 1 at the next imaginary time slice.

Loop update



Operator-loop update

Many spins and operators can be changed simultaneously



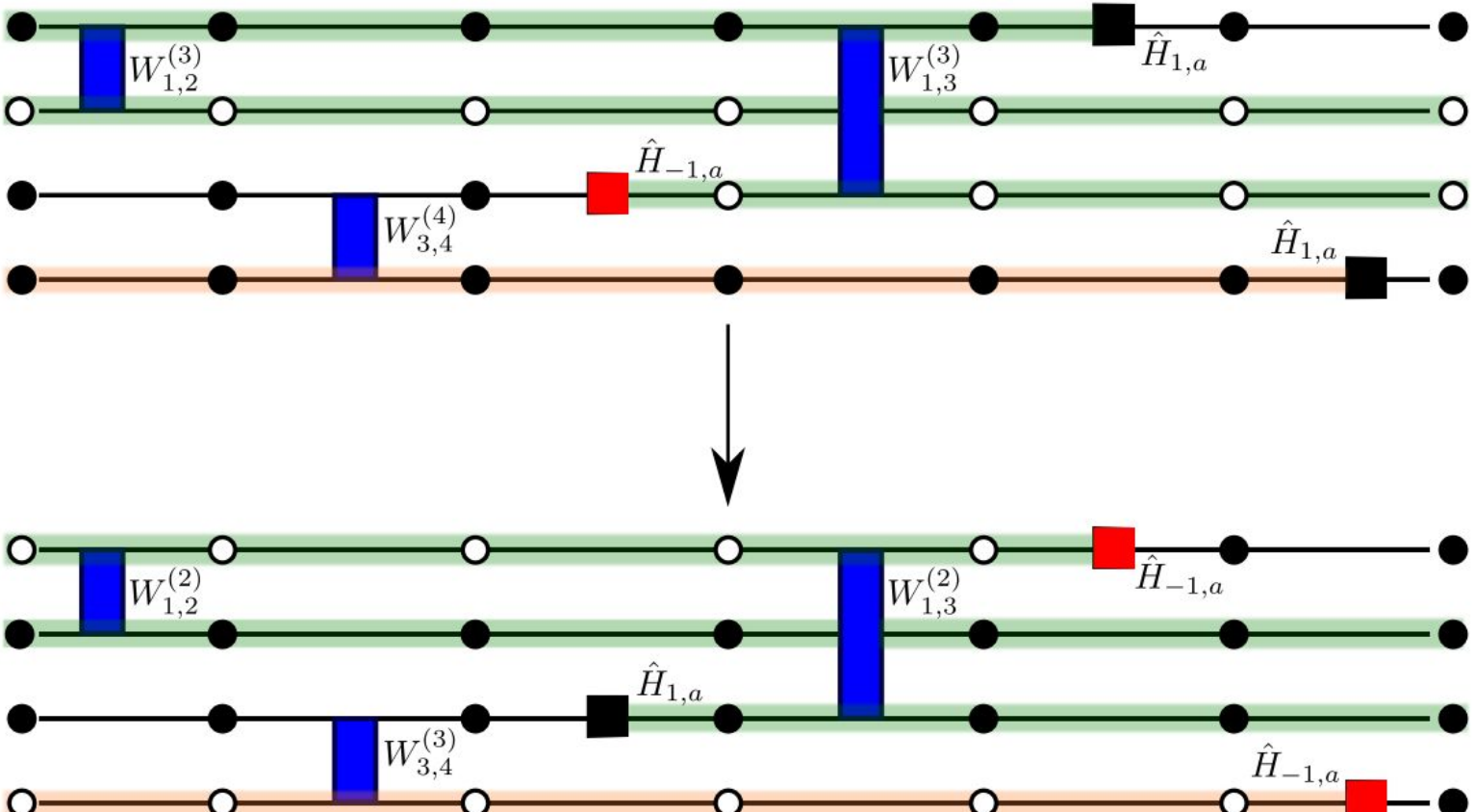
Pseudocode

moving horizontally
in the list corresponds
to changing v even↔odd

- **flipbit**(*v,0*) flips bit 0 of v

- a given loop is only constructed once
- vertices can be erased
- *X(v) < 0* = erased
- *X(v) = -1* not flipped loop
- *X(v) = -2* flipped loop

Cluster update



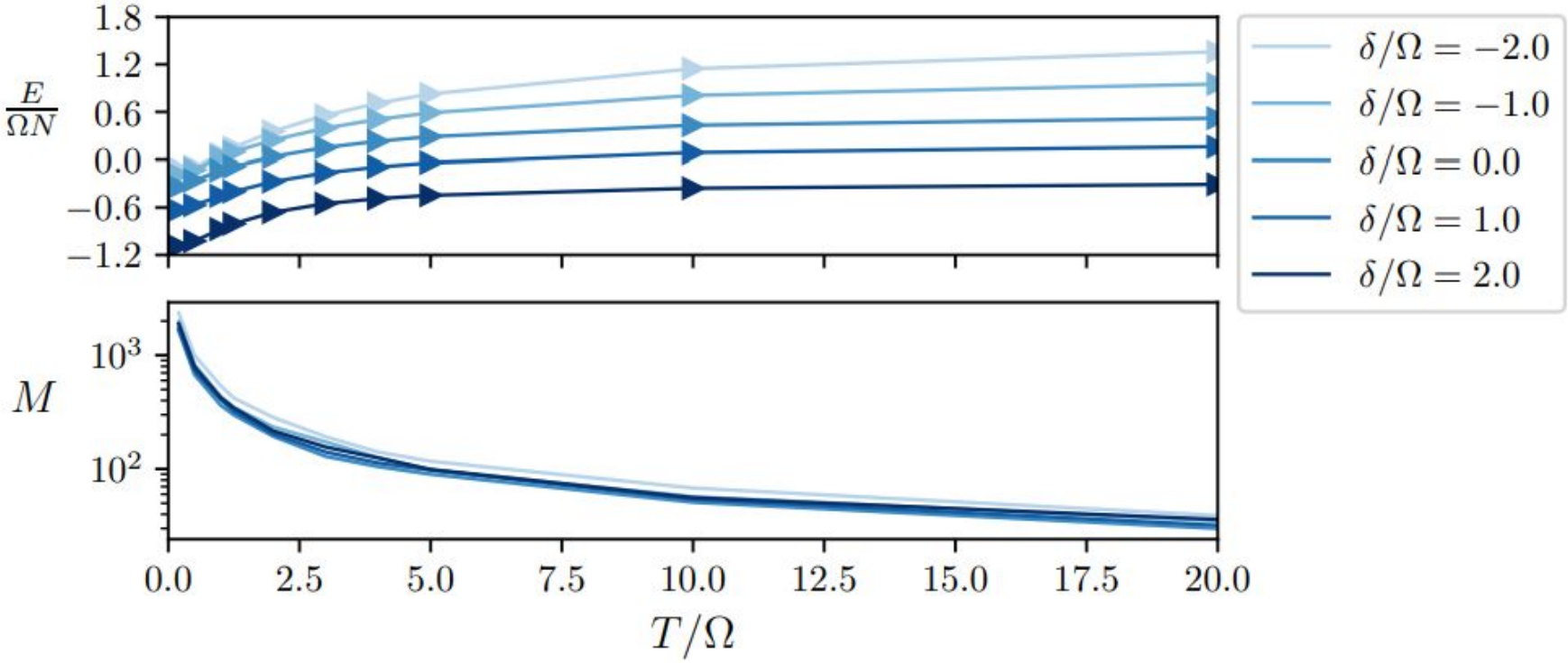
results

SSE QMC algorithm for a 51 atom one-dimensional (1D) chain and a 16 ×16 square array of Rydberg atoms

its efficiency and convergence properties

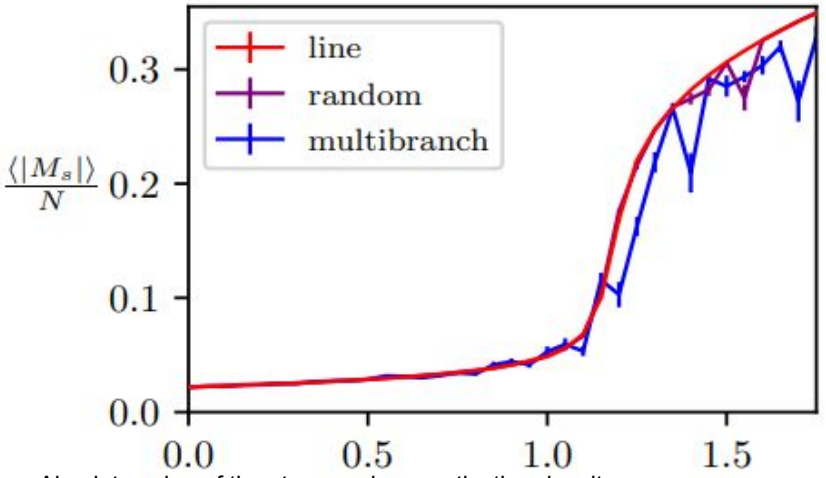
Monte Carlo autocorrelation times for estimators of physical observables – a **function of the detuning parameter** (in the vicinity of quantum phase transitions)

compare in particular **the original multibranch cluster update** to **a modified line update**, for some detunings near criticality, this new line update shows improvements

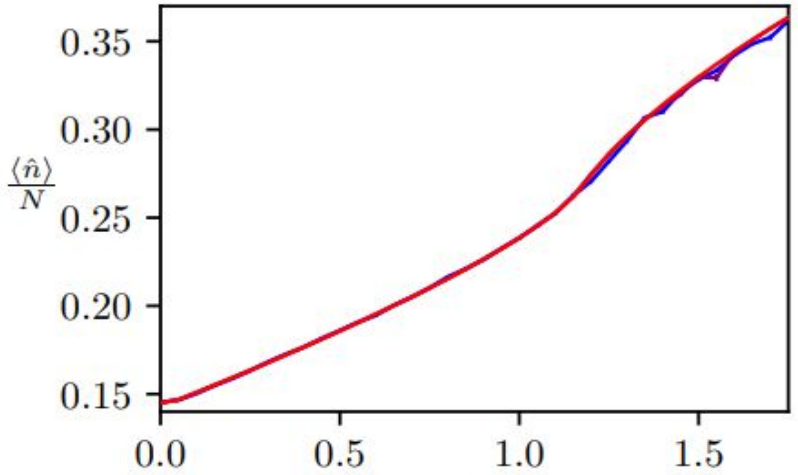


which cluster update is best to employ will undoubtedly depend on Rb, δ/Ω, and system size

Each data point represents an independent SSE QMC simulation of a 16×16 Rydberg array Rb = 1.2 in 10^6 successive measurements



Absolute value of the staggered magnetization density



The Rydberg excitation density δ/Ω

Research prospects

offer more numerical insights into exotic physics contained in Rydberg atom arrays through detailed finite size scaling analyses, such as replica measurements of the Renyi entanglement entropies [1]

QMC simulations will be crucial for providing data for pre-training generative machine learning models, which are poised to become important tools in state reconstruction and tomography [2]

[1]Measuring Renyi Entanglement Entropy in Quantum Monte Carlo Simulations, Phys. Rev. Lett. 104(15), 157201 (2010)

[2]Integrating neural networks with a quantum simulator for state reconstruction, Phys. Rev. Lett. 123, 230504 (2019)

Thanks!

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