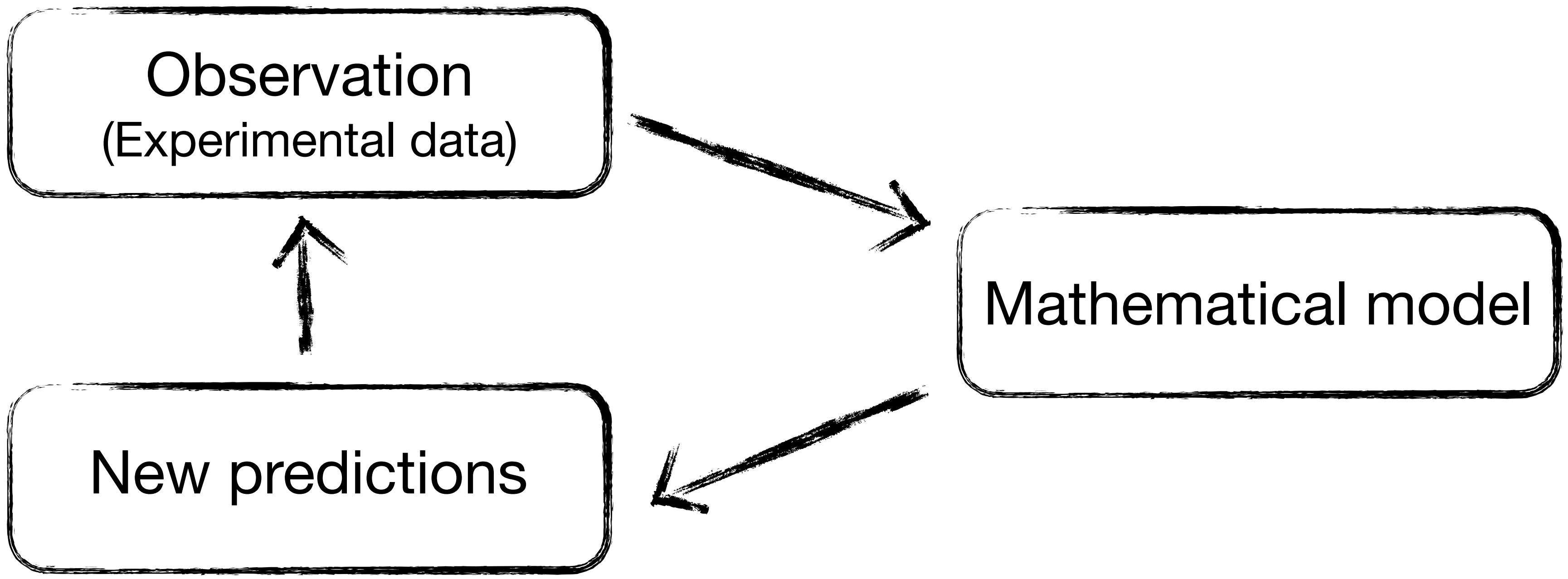
9th March, 2024 - Morning of Theoretical Physics, Oxford

Simulating Physics Beyond Computer Power

Alessio Lerose

UNIVERSITY OF OXFORD

The Theory Game: From Models to Predictions



Simplest predictions given by solvable limits

Harder predictions involve:

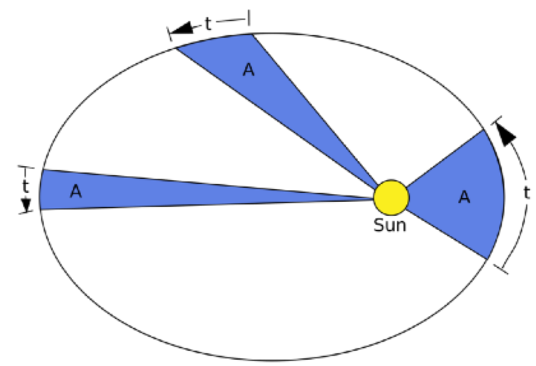
- Brute-force simulations
- Approximation schemes
- Phenomenological approaches (i.e. higher-level theory)

Predicting Classical Mechanical Motion

Newton's equation for Planet-Sun:

$$m\ddot{\vec{r}} = -GMm\frac{\vec{r}}{|\vec{r}|^3}$$

Exact solution: Kepler laws



Many-body problem:

$$m_i\ddot{\vec{r}}_i = -G\sum_{j(\neq i)}^{N} m_i m_j \frac{\vec{r}_i - \vec{r}_j}{|\vec{r}_i - \vec{r}_j|^3} \qquad i = 1,\ldots,N$$

Famously non-solvable for $N \geq 3$

Numerical simulation: System of $3N$ *2nd-order differential equations*

$$\begin{cases} \Delta\vec{r}_i = \vec{v}_i\,\Delta t \\ \Delta\vec{v}_i = \dfrac{1}{m_i}\overrightarrow{F}_i(\vec{r}_1,\ldots,\vec{r}_N)\,\Delta t \end{cases} \qquad i = 1,2,\ldots,N$$

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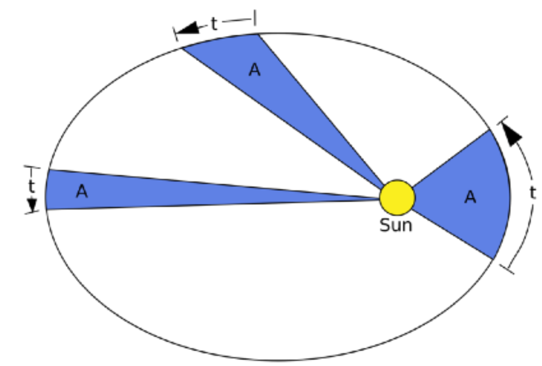

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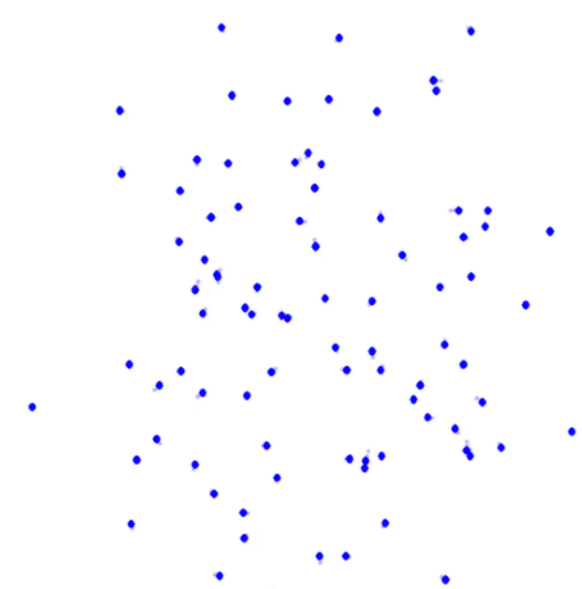
Brute-force simulation at reach for computers ✓



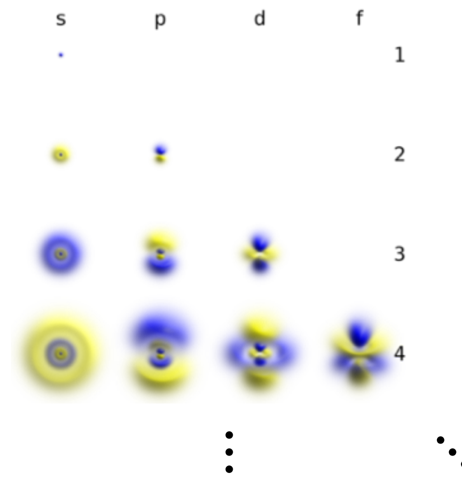
Very large systems (gases, plasma, galaxies) → Boltzmann equation, Hydrodynamics, …

Predicting Quantum Mechanical Motion

Schrödinger's equation for Electron-Proton:

$$i\hbar\partial_t\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) - \frac{e^2}{|\vec{r}|}\psi(\vec{r},t)$$

Exact solution: Hydrogen spectrum



Many-body problem:

$$i\hbar\partial_t\Psi(\vec{r}_1,\ldots,\vec{r}_N,t) = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2\Psi(\vec{r}_1,\ldots,\vec{r}_N,t) + \sum_{i<j}\frac{e_ie_j}{|\vec{r}_i-\vec{r}_j|}\Psi(\vec{r}_1,\ldots,\vec{r}_N,t)$$

Famously non-solvable for $N \geq 3$

Numerical simulation: 2nd-order partial differential equation for a function of $3N$ variables

from Walter Kohn's Nobel lecture (1999)

I begin with a provocative statement. *In general the many-electron wavefunction $\Psi(r_1,\ldots,r_N)$ for a system of N electrons is not a legitimate scientific concept, when $N \geq N_0$, where $N_0 \approx 10^3$.*

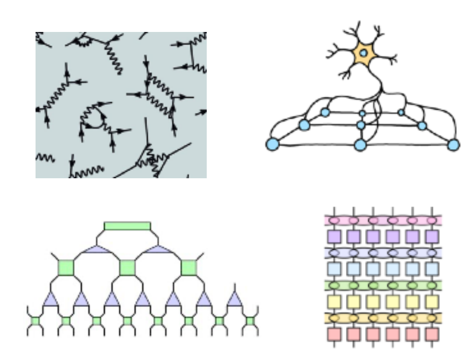
Let us now assume that somehow we have obtained an accurate approximation to $\tilde{\Psi}$, in the sense of Eq (2.16), and wish to record it so it can be reproduced at a later time. How many bits are needed? Let us take q bits per variable. Then the total number of bits is

$$B = q^{3N} \qquad (2.18)$$

For $q = 3$, a very rough fit, and $N = 10^3$, $B = 10^{1500}$, a quite unrealistic number. (The total number of baryons in the accessible universe is estimated as $10^{80\pm}$).

Brute-force simulation out of reach for any foreseeable supercomputer ✗

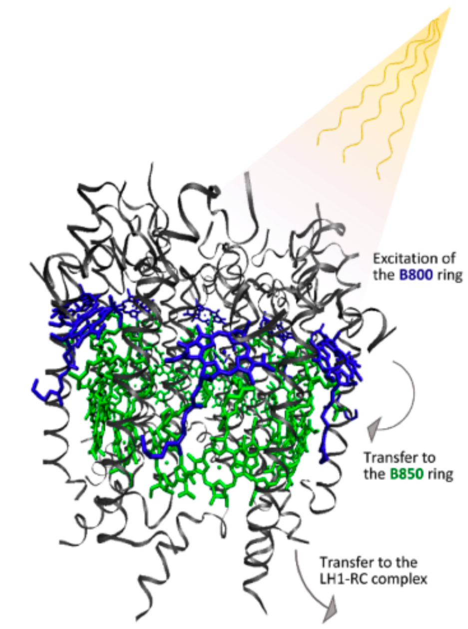
Google search:



Approximation schemes: Perturbation Theory, Mean-Field Theory, Density-Functional Theory … + *Phenomenological schemes*

Why bothering about Quantum Many-Body Physics (QMBP)?

Many important phenomena are intrinsically **QUANTUM** & **MANY-BODY**



Chemistry

- *First-principle computation of molecular structure, reaction rates*
- *Prediction of new molecules*
- *Applications: Drug design, …*

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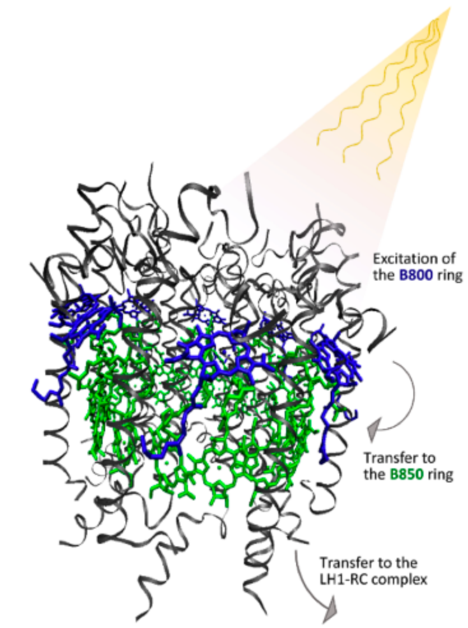
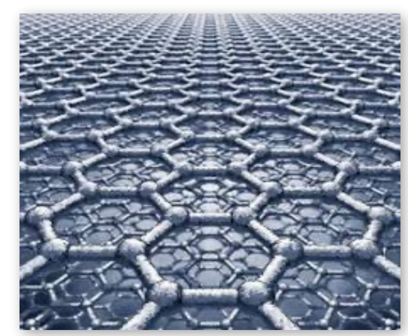


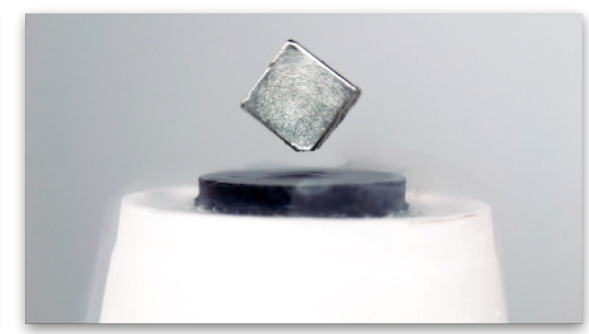
Chemistry

- *First-principle computation of molecular structure, reaction rates*
- *Prediction of new molecules*
- *Applications: Drug design, …*

Condensed Matter Physics

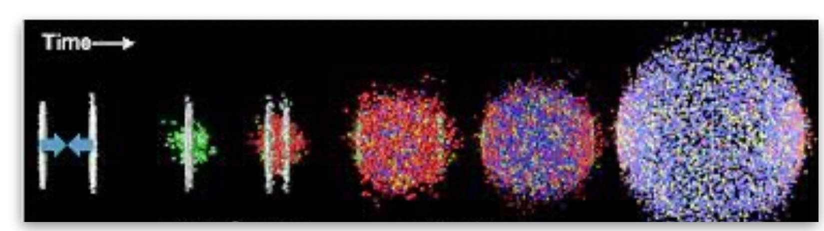
- *First-principle computation of material structure, non-equilibrium response*
- *Prediction of new materials and new phases of ordinary matter*
- *Applications: Material functionality design, …*





High-Energy Physics

- *First-principle computation of hadron & nuclei structure, nuclear reaction rates*
- *Prediction of behavior in extreme conditions and new phases of extreme matter*
- *Applications: Beyond Standard Model phenomena (?), Nuclear reactions (?), …*



Dr Brewer’s talk

…Beyond Physics

- *Cryptography (e.g. Shor’s factoring algorithm)* *Dr Placke’s talk*

Feynman’s vision of Quantum Simulation

- Solving QMBP → huge progress in several branches of Science
- However
    - *Brute-force simulation impossible*
    - *Controlled approximation schemes suffer*
    - *Phenomenology unavailable or unreliable*

…Is there a way out?

Richard Feynman’s vision (1982):

Simulating quantum system using classical machine is hard → Use a quantum machine!

Hardware encoding and control

How do we simulate a quantum system with a quantum machine?

Need **HARDWARE** :

a reference **highly controllable quantum many-body system** encoding degrees of freedom of the system of interest

1) Mapping between states: $\mathscr{H}_{\text{system}} \longleftrightarrow \mathscr{H}_{\text{hardware}}$ $[\longleftarrow]$

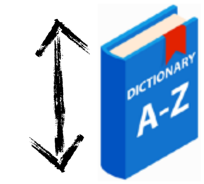
2) Prepare initial state of interest: $|\psi(0)\rangle_{\text{system}} \longleftrightarrow |\psi(0)\rangle_{\text{hardware}}$

3) Design forces of interest: $\hat{H}_{\text{system}} \longleftrightarrow \hat{H}_{\text{hardware}}$

4) Measure observable of interest: $\hat{O}_{\text{system}} \longleftrightarrow \hat{O}_{\text{hardware}}$

System of interest

- *Macromolecule*
- *Material*
- *Heavy nucleus*



Hardware

- *Controllable atoms*
- *Controllable photons*
- *Controllable electrons*

$$_{\text{system}}\langle\psi_0|\, e^{it\hat{H}_{\text{system}}}\hat{O}_{\text{system}}e^{-it\hat{H}_{\text{system}}}\,|\psi_0\rangle_{\text{system}} = {}_{\text{hardware}}\langle\psi_0|\, e^{it\hat{H}_{\text{hardware}}}\hat{O}_{\text{hardware}}e^{-it\hat{H}_{\text{hardware}}}\,|\psi_0\rangle_{\text{hardware}}$$

Analog vs Digital Quantum Simulation

Quantum hardware has “native” physical Hamiltonian

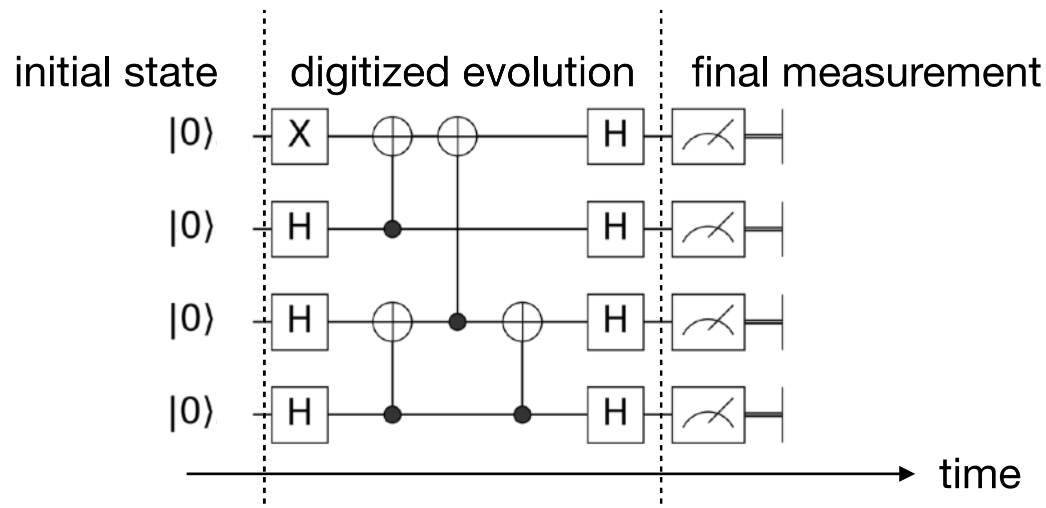
Analog quantum simulation:

- *Extend reach of native Hamiltonian by additional engineering*
- *Extend reach of native Hamiltonian by devising clever encoding mappings*

Digital quantum simulation:

- *Use native interactions to perform elementary building-block operations on single units or pairs of units (**unitary gates**)*
- *Choose a **universal gate set**, such that an arbitrary global operation on many units can be decomposed into a sequence of gates*
- ***Compile** the target evolution as an optimal sequence of gates:* **SOFTWARE**

Quantum circuit:



⟹ **Universal quantum processor**

Dr Placke’s talk

David Deutsch, Artur Ekert, Andrew Steane, Vlatko Vedral,…

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Hardware implementation: Where do we stand?

Several competing experimental platforms in the race

Atomic-Molecular-Optical (AMO) systems

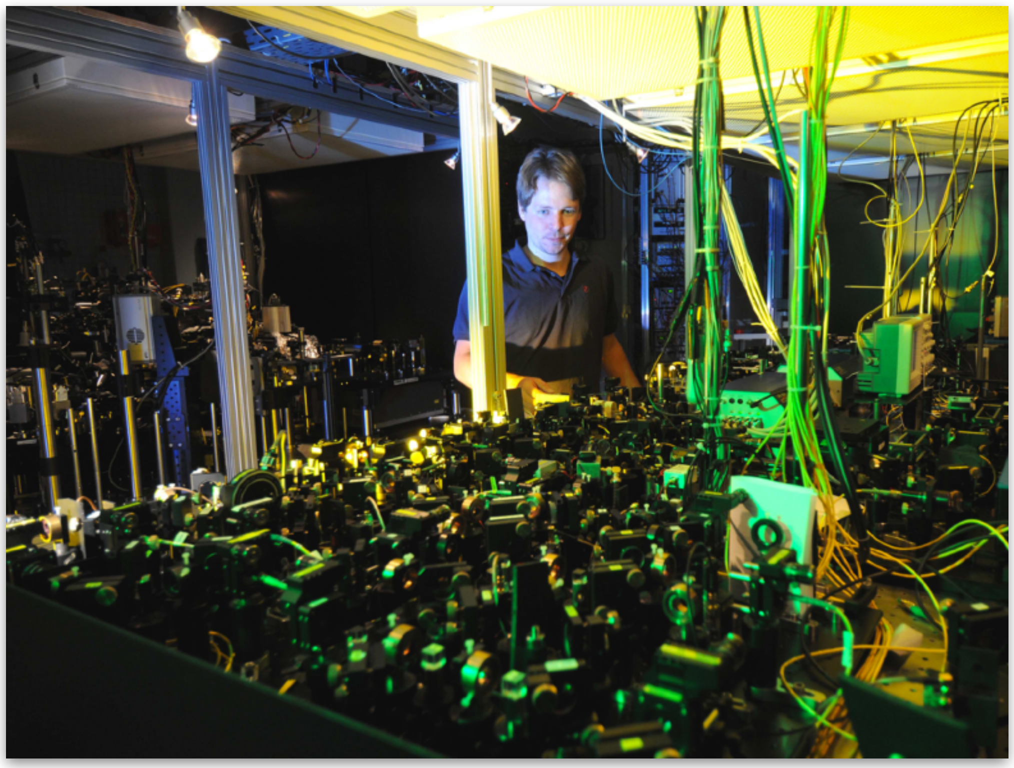


image: Bloch lab @ Munich

Solid-state systems

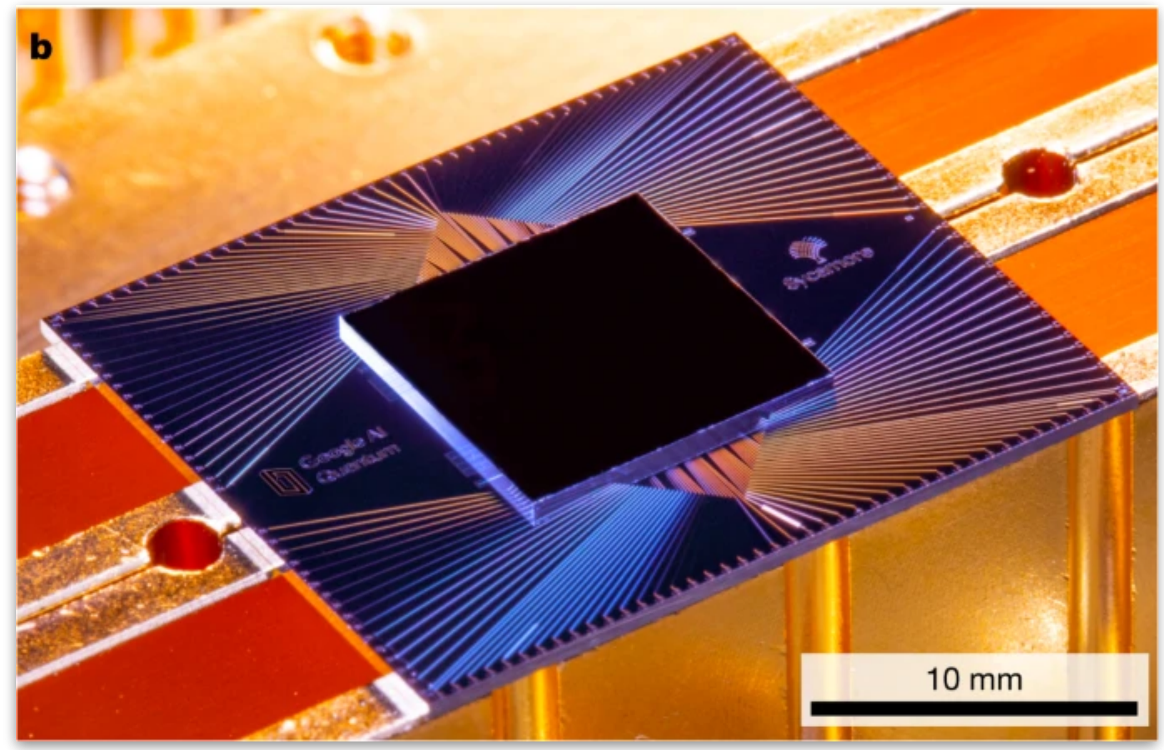


image: Google Quantum AI

Currently: *Noisy Intermediate-Scale Quantum (NISQ)* devices: **Limited size and coherence time**

Holy Graal: *Scalable Fault-Tolerant Quantum* devices: **Unlimited size and coherence time** *Dr Placke's talk*

…NEED YEARS AND £££

Crash course on Cold-Atom Quantum Simulators

Gas of atoms (ions, molecules)

Electromagnetically trapped & cooled to very low temperature

- magneto-optical trap
- laser cooling
- evaporative cooling
- sympathetic cooling
- ...

N reduced: $10^{23} \longrightarrow 10^3$ to 10^6

De Broglie wavelength > trap $\rightarrow$ Deep quantum regime!

Bose-Einstein Condensate (BEC) of bosonic atoms

Cornell-Wieman 1994 *(≈ 2000 ^{87}Ru atoms below $170\,nK$)*
Ketterle 1994 *(^{23}Na atoms)*
$\Longrightarrow$ *Nobel prize 2001*

Controllable interactions
- *1d & 2d confinement*
- *Feshbach resonance*
- *Rydberg dressing*
- *...*

BCS-BEC crossover of fermionic atoms
Analog "Superconductivity" with neutral particles

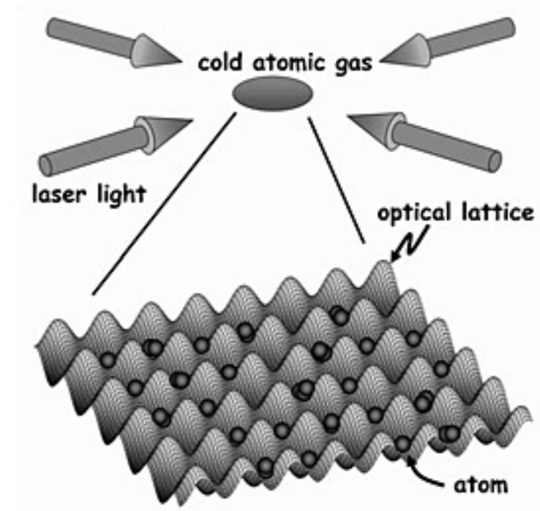
Imaging techniques
- *Time-of-flight*
- *Quantum gas microscope*
- *Ramsey interferometry*
- *State-dependent fluorescence*
- *...*

Far-from-equilibrium dynamics
Single-site and real-time resolution
Measurement of quantum entanglement

Optical Lattices

Periodic potential by counterpropagating lasers (standing wave)

$$\hat{H}_{\text{opt.latt.}} = +J\sum_{\langle i,j\rangle}\hat{c}_i^\dagger\hat{c}_j + U\sum_i \hat{n}_i(\hat{n}_i+1)$$



Bloch, Dalibard, Zwerger RMP (2002)

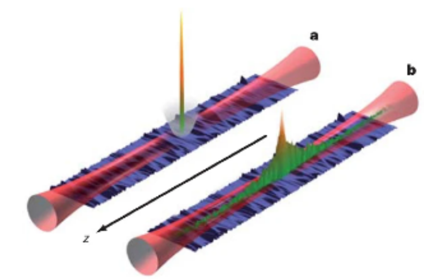
Arbitrary lattice geometry

Bloch lab @ Munich

Speckle pattern → Quasirandom potential

Anderson localization

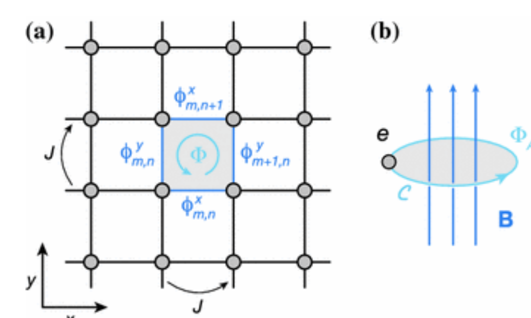
Aspect lab, Nature (2008)



Shaking → Control of hopping, Artificial magnetic field

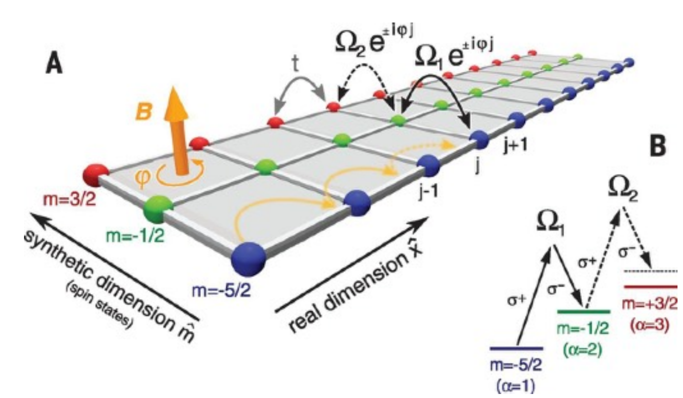
Dynamical localization, Quantum Hall Effect, Chiral edge states

Bloch lab, PRL (2011)



Internal spin states → Synthetic dimension

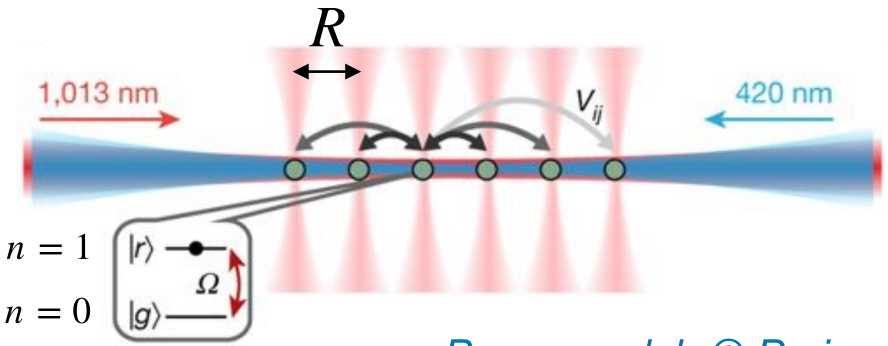
Fallani lab, Science (2015)



…Understanding high-T_c superconductivity?

Rydberg Atom Arrays

Alkali (hydrogen-like) atoms trapped in optical tweezers



Browaeys lab @ Paris
Lukin lab @ Harvard

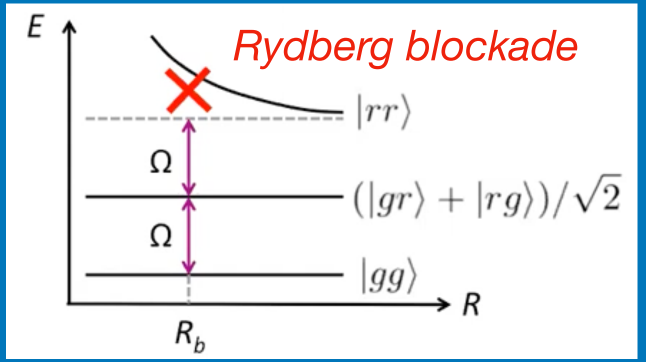
Two lasers drive transition to highly-excited Rydberg state

$$\hat{H}_{\text{Rydberg}} = \Omega \sum_{i=1}^{L} \hat{\sigma}_i^z + \delta \sum_{i=1}^{L} \hat{n}_i + \sum_{i,j}^{L} V_{i,j} \hat{n}_i \hat{n}_j$$

Strong Van der Waals interactions, controlled by distance

$$V_{i,i+1} \sim \frac{C}{R^6}$$

$|g\rangle$ $|r\rangle$



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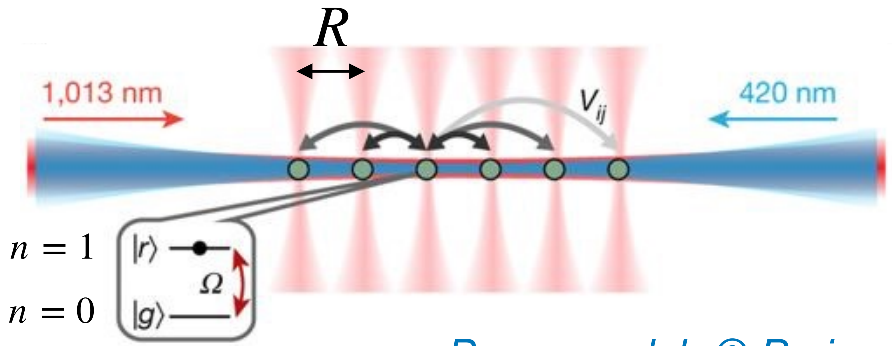

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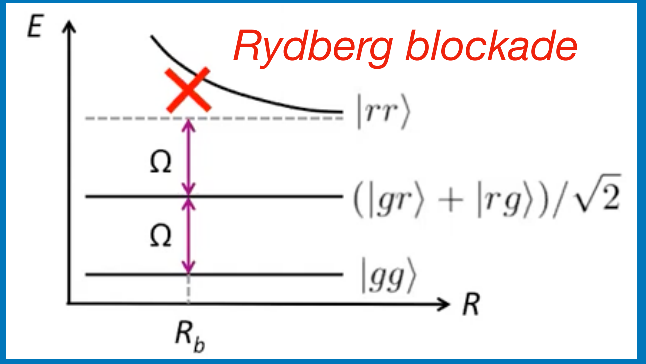
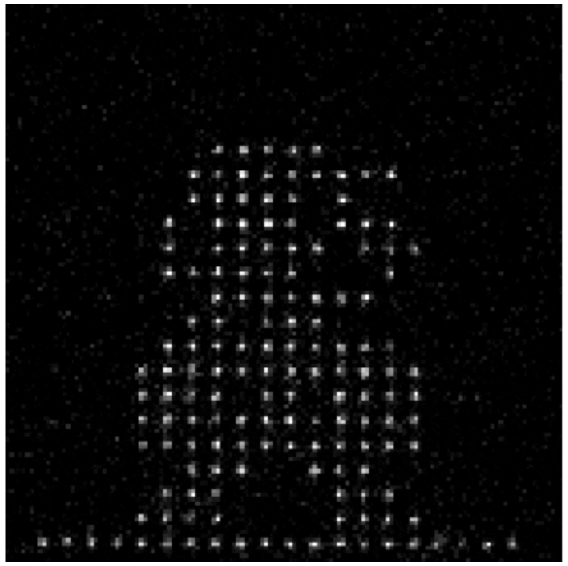


Fully reconfigurable geometry



Ion Crystals

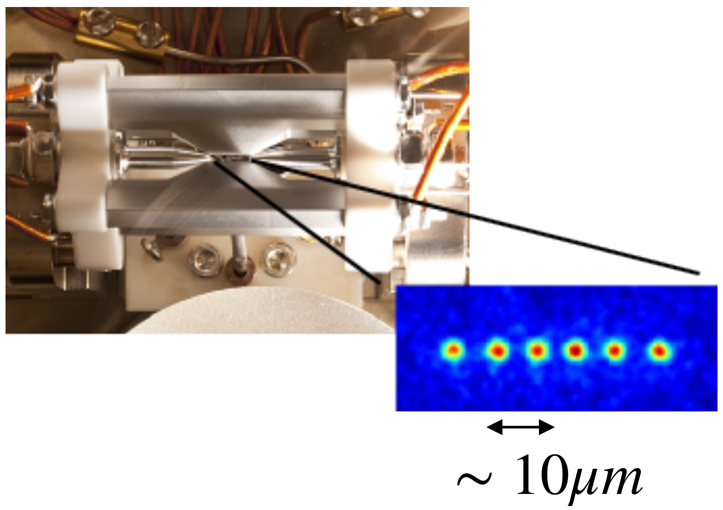
Trapped charged atoms (ions) via electromagnetic fields

Primary role played by Oxford

Artur Ekert, Andrew Steane (inspiration)

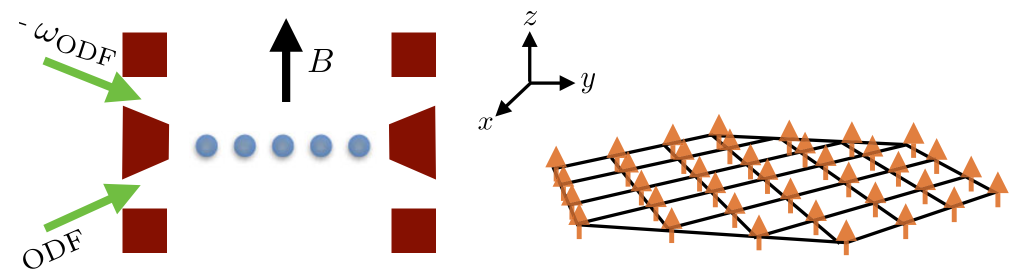
David Lucas, Chris Ballance, Andrew Steane,… (Ion Trap Quantum Computing)

Paul (rf) trap



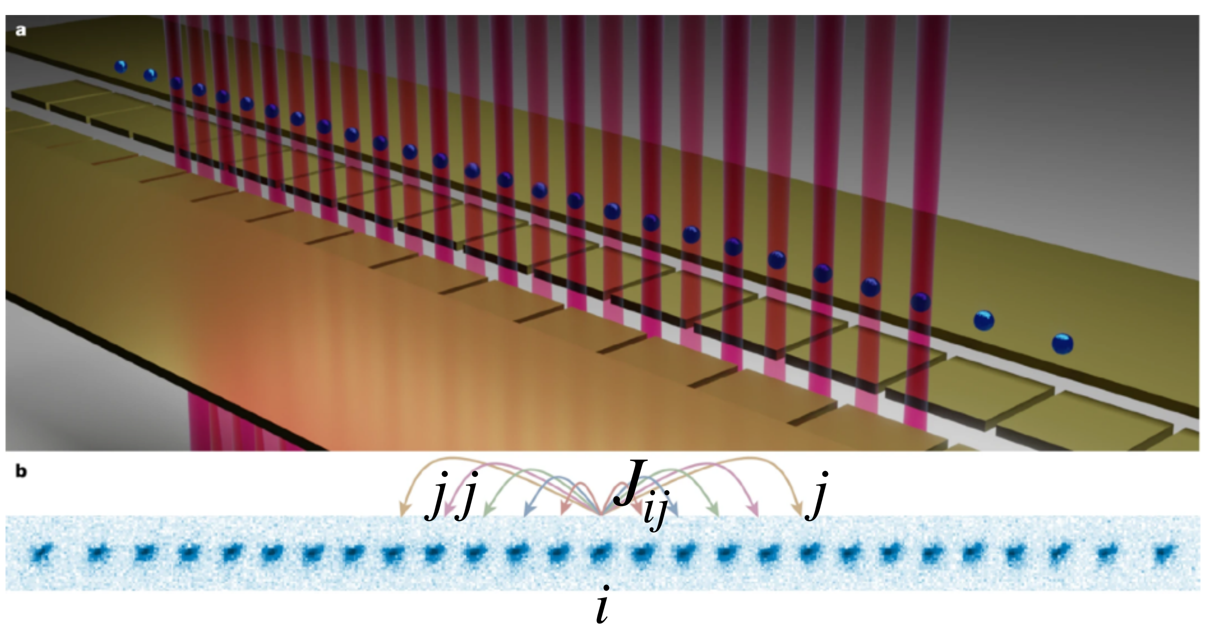
Oxford
Innsbruck
Duke
…

Penning trap



Colorado
…

Largely programmable 1d spin chain



from Feng et al., Nature (2023)

$$\hat{H}_{\text{spin-phonon}} = \frac{1}{2}\sum_{i,m} \eta_{i,m}\Omega_i \hat{\sigma}_i^x \left(\hat{a}_m^\dagger e^{i\delta_{im}t+\psi_i} + \hat{a}_m e^{-i\delta_{im}t-\psi_i} \right)$$

$$\hat{H}_{\text{spin-spin}} = \sum_{i<j} J_{ij}\hat{\sigma}_i^x\hat{\sigma}_j^x + \sum_i (g_i\hat{\sigma}_i^x + h_i\hat{\sigma}_i^z)$$

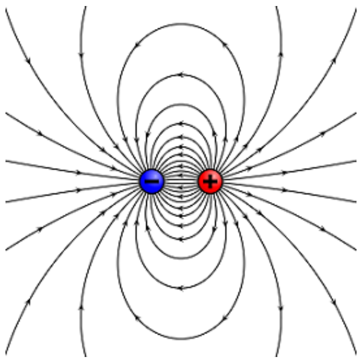
Simulating Quantum Field Theory with Cold Atoms

Simulating theories of fundamental interactions?

- *Matter and gauge fields: interacting fermions and bosons together*
- *Multiple species (charge, spin, color, flavor)*
- *Hard local constraints by gauge symmetry*

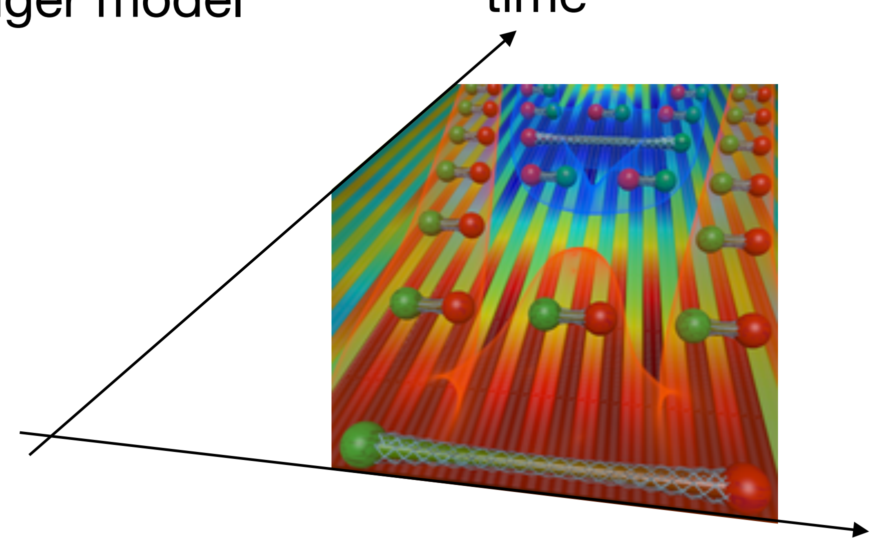
$\Longrightarrow$ Very challenging task for analog & digital quantum simulators

Recent progress in Electro-Dynamics



(1+1)-dimensional Quantum Electro-Dynamics: Schwinger model

Superficial similarity with Quantum Chromo-Dynamics:
Particle confinement, String breaking, Hadron collisions, …

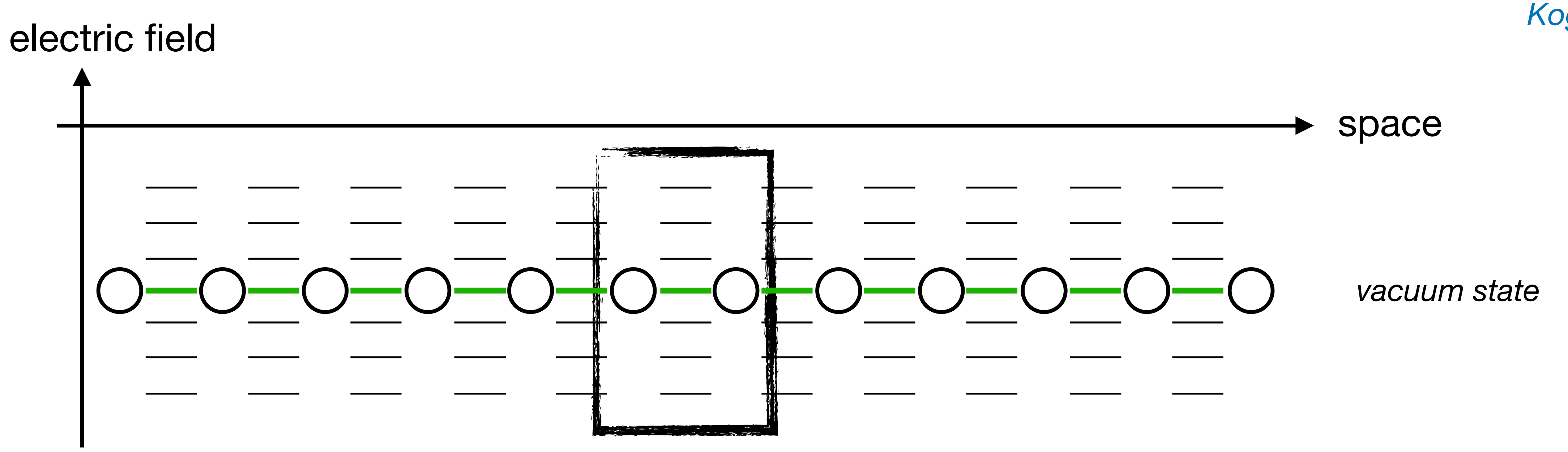


Martinez et al., Nature (2016)
Bernien et al., Nature (2017)
Yang et al., Nature (2020)

Hamiltonian formulation of Quantum Electro-Dynamics

$$\hat{H}_{\mathrm{QED}} = +m\sum_i (-)^i \hat{c}_i^\dagger \hat{c}_i \; -w\sum_i \hat{c}_i^\dagger \hat{U}_{i,i+1}\hat{c}_{i+1} + \hat{c}_i \hat{U}_{i,i+1}^\dagger \hat{c}_{i+1}^\dagger \; +J\sum_i \left(\hat{E}_{i,i+1} - \frac{\theta}{2\pi}\right)^2$$

Schwinger PR (1962)
Wilson PRD (1974)
Kogut, Susskind PRD (1975)



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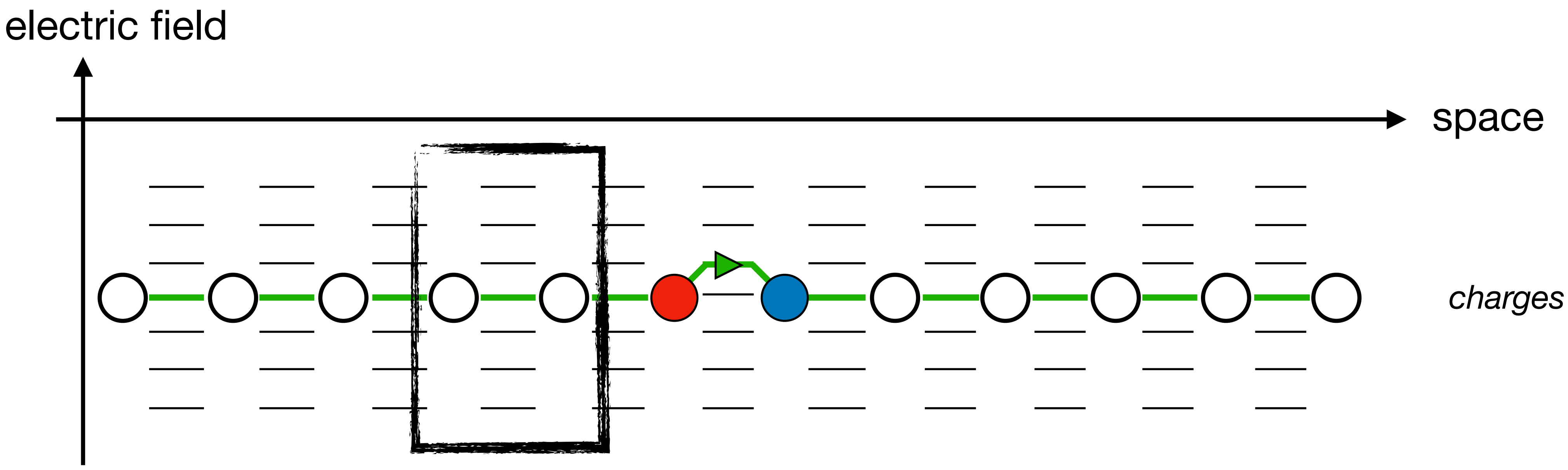

charges and electric field excitations

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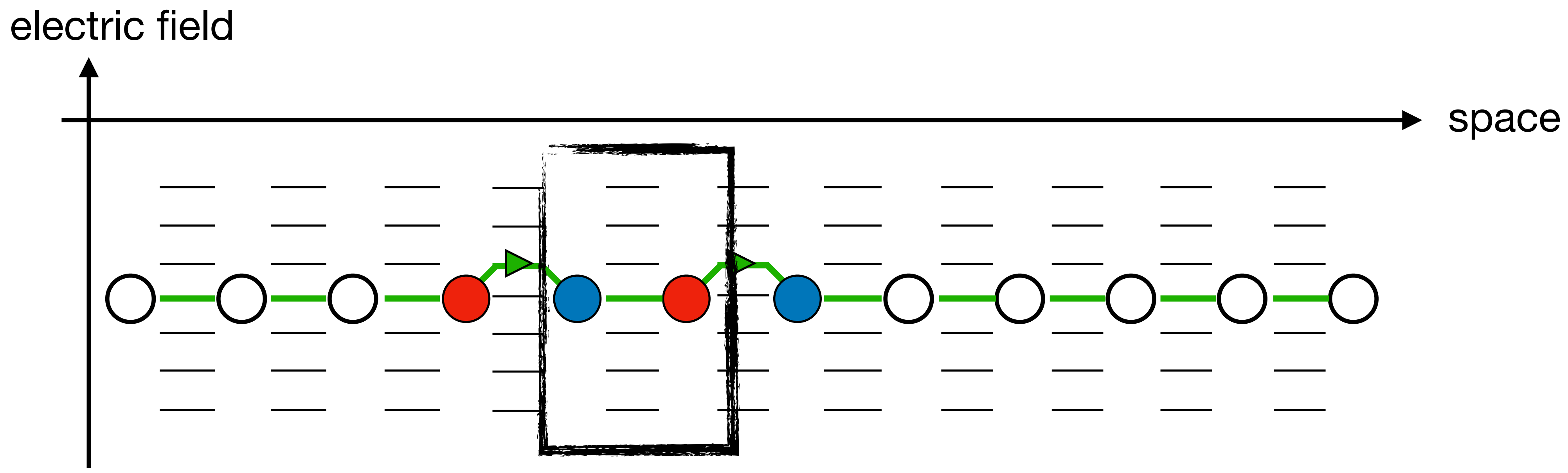

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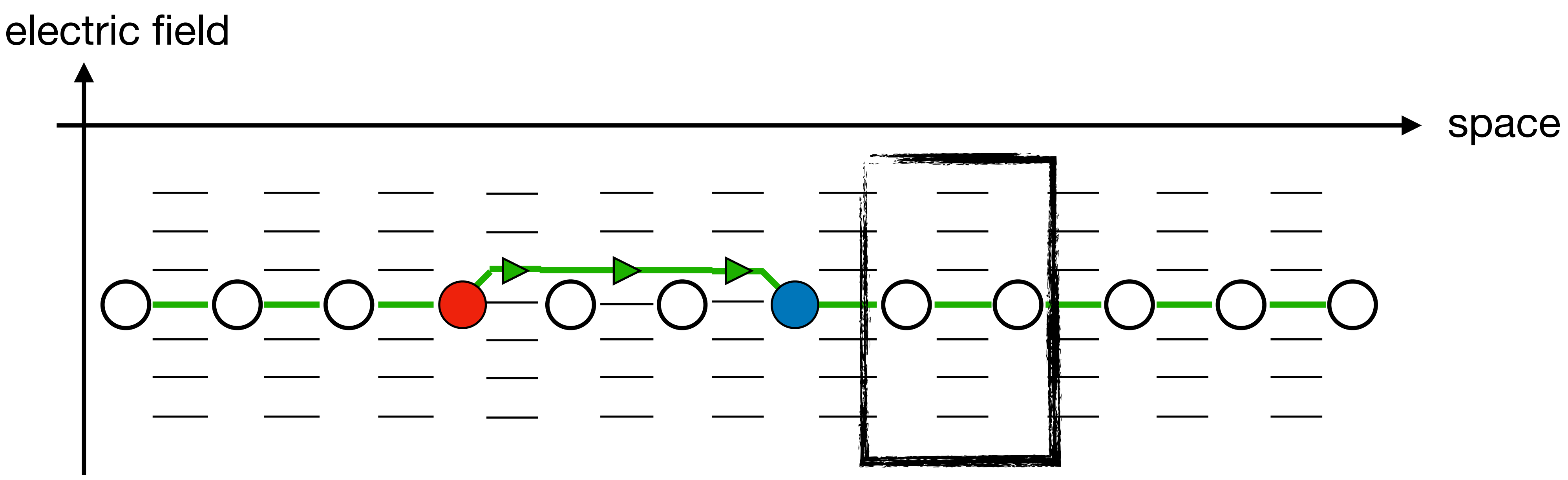

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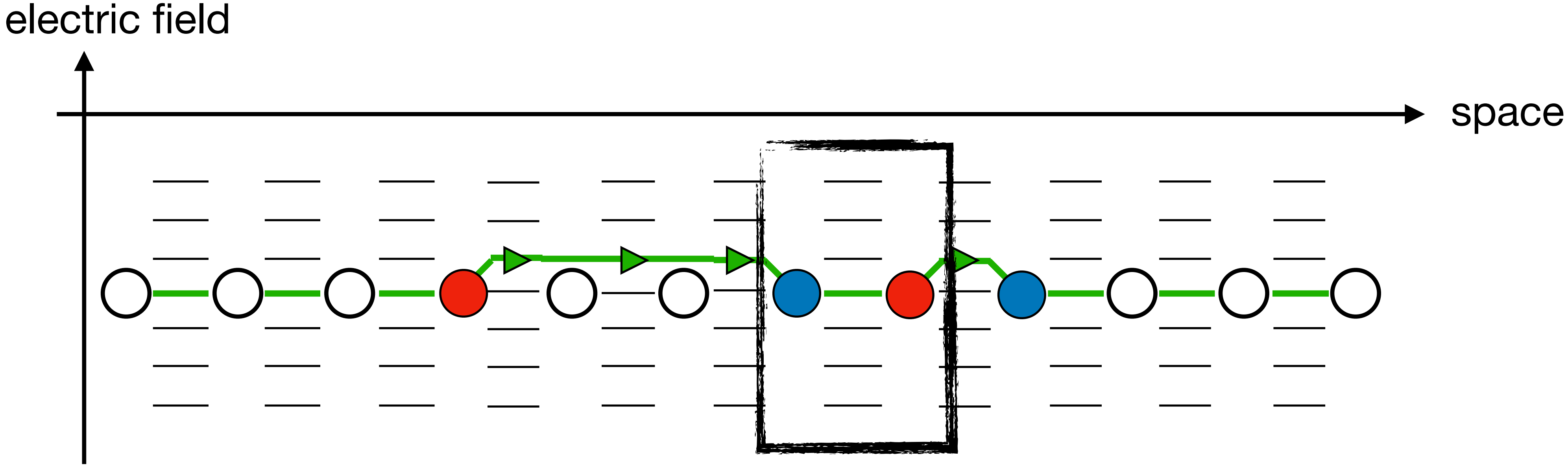
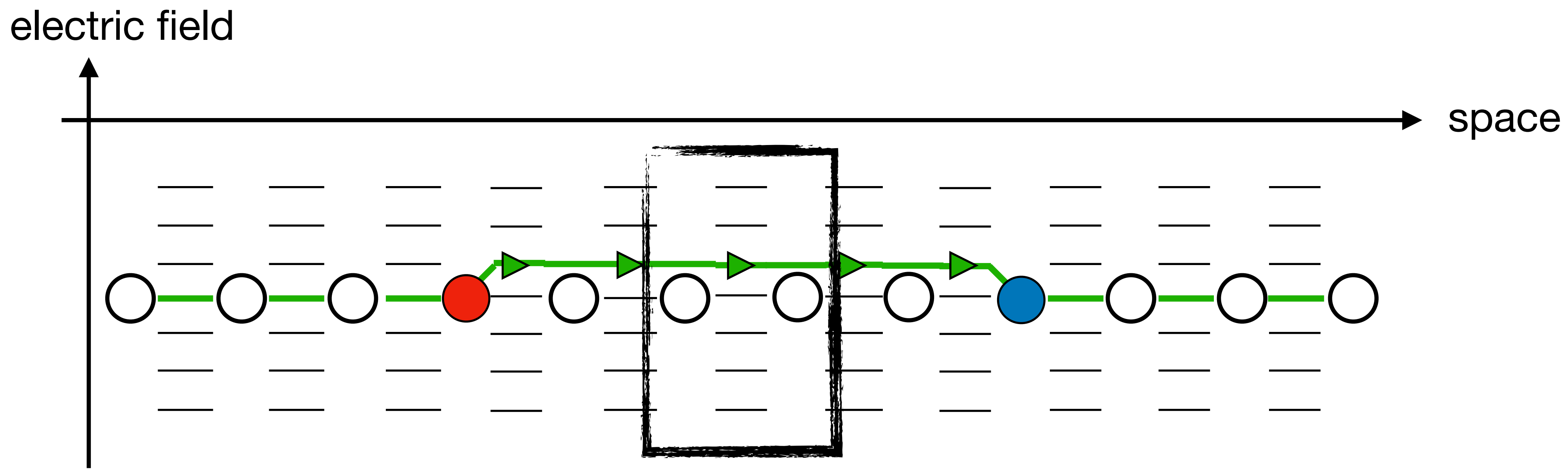


Hamiltonian formulation of Quantum Electro-Dynamics

$$\hat{H}_{\mathrm{QED}} = +m\sum_i (-)^i \hat{c}_i^\dagger \hat{c}_i \; - w\sum_i \hat{c}_i^\dagger \hat{U}_{i,i+1}\hat{c}_{i+1} + \hat{c}_i \hat{U}_{i,i+1}^\dagger \hat{c}_{i+1}^\dagger \; + J\sum_i \left(\hat{E}_{i,i+1} - \frac{\theta}{2\pi}\right)^2$$

Schwinger PR (1962)
Wilson PRD (1974)
Kogut, Susskind PRD (1975)



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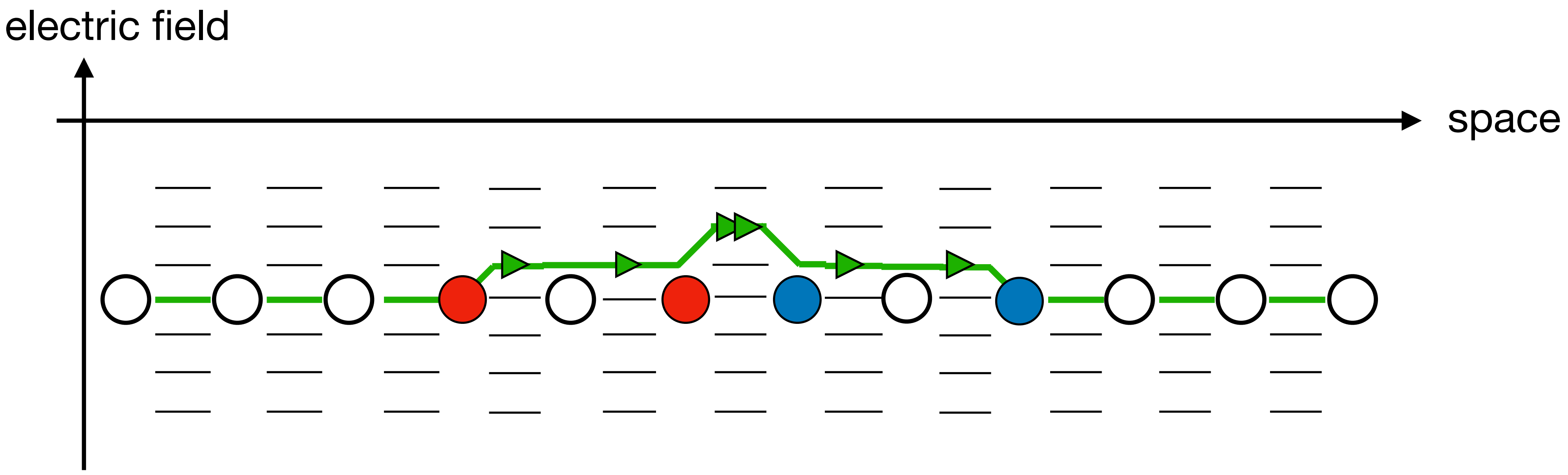
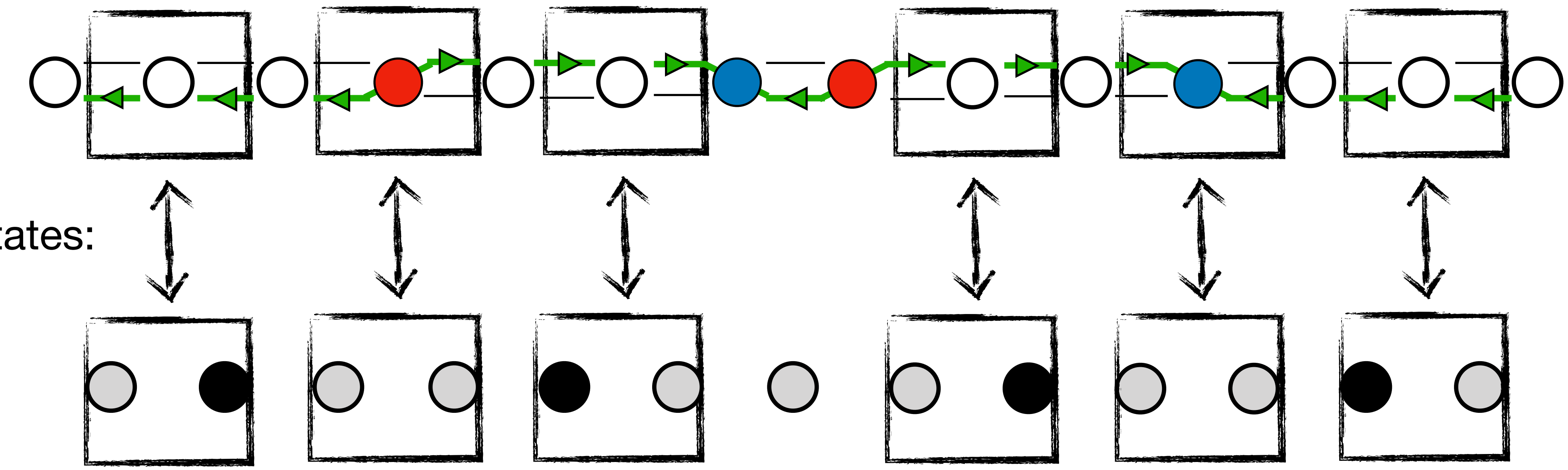


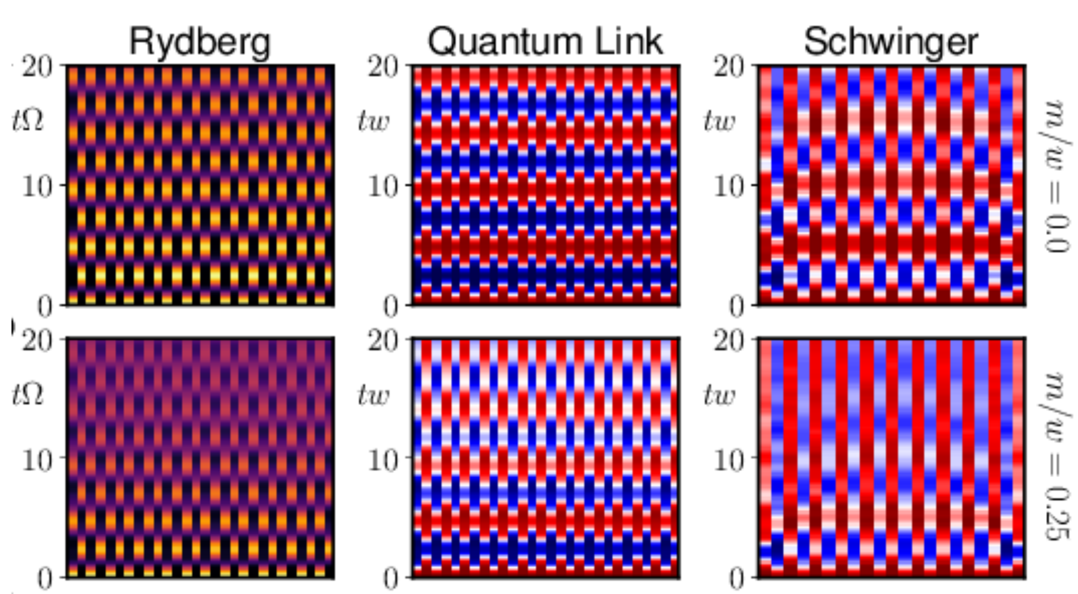
Encoding QED in Rydberg Atom Arrays

States:



Hamiltonian: $w \longleftrightarrow -\Omega \qquad m \longleftrightarrow -\delta \qquad J(\theta - \pi) \longleftrightarrow \Delta$

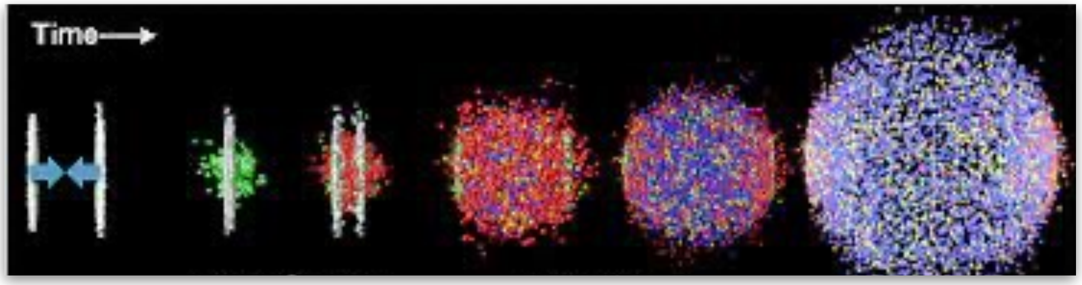
Observables:



Surace, AL, et al.
Physical Review X (2020)

Collisions in ~~Particle Accelerators~~ Tabletop Quantum Simulators - I

Outstanding goal of quantum simulation: Hadronic/Nuclear matter



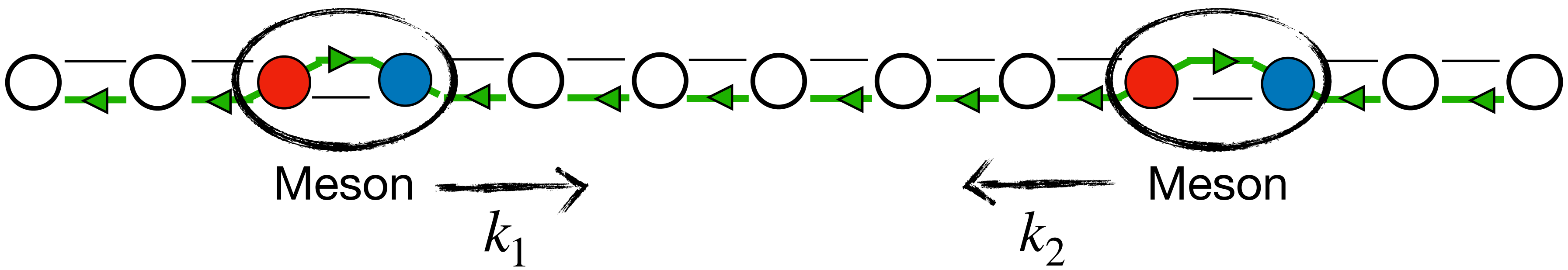
High-energy collisions of heavy nuclei:

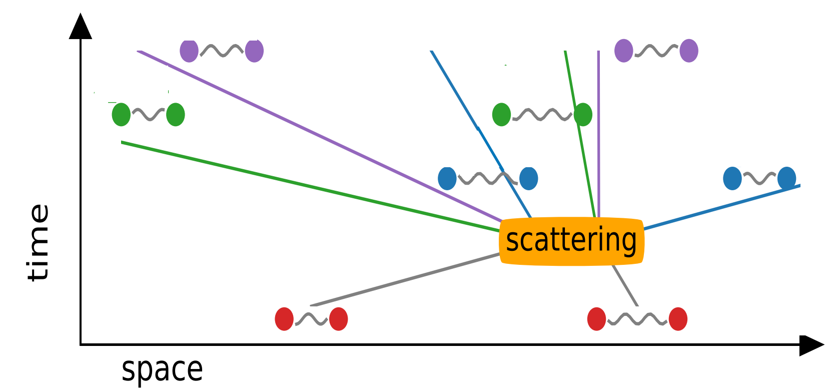
- *CERN Geneva (Pb-Pb)*
- *RHIC Brookhaven National Lab (Au-Au)*

Dr Brewer's talk

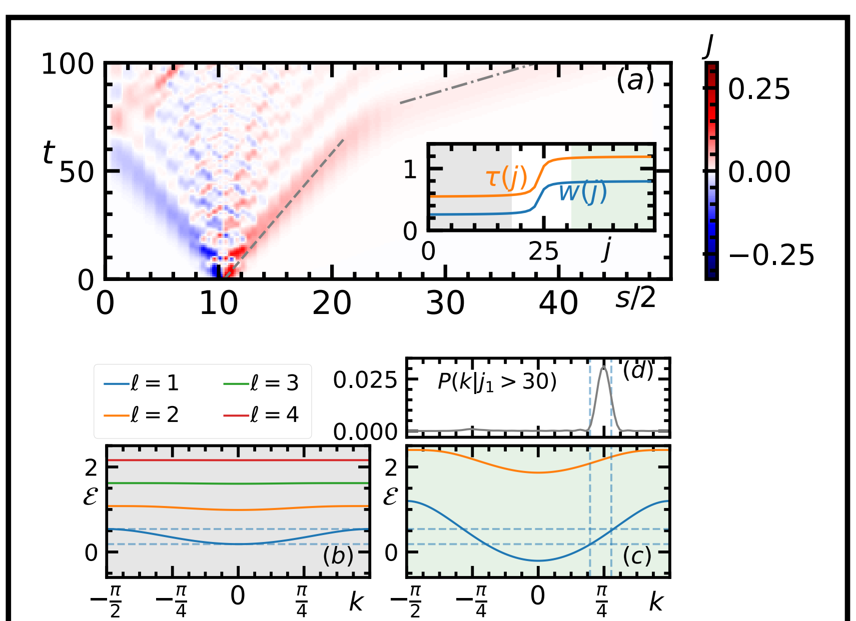
Meson-Meson Collisions in Rydberg atom arrays:

Surace & AL, New Journal of Physics (2021)

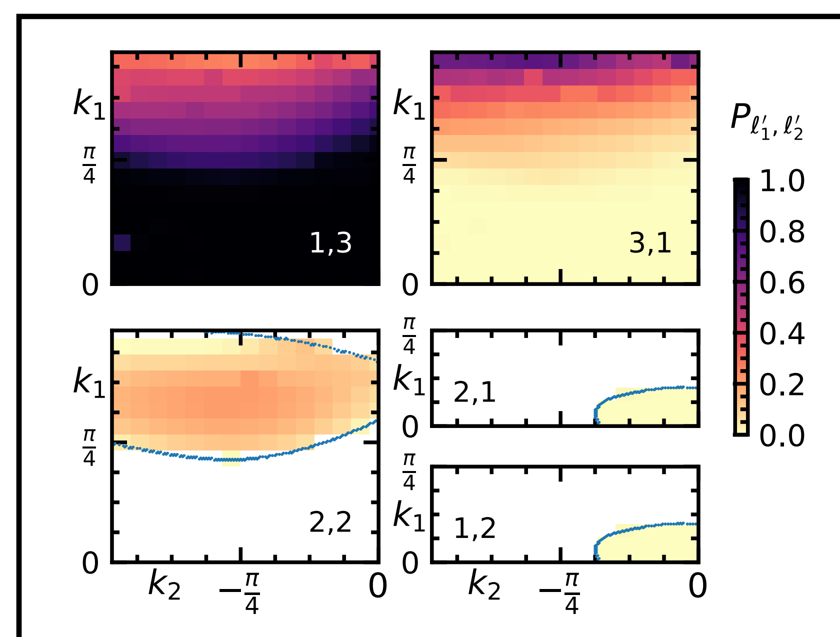




Preparation of incoming meson wavepackets



Detection of outgoing mesons (S-matrix)

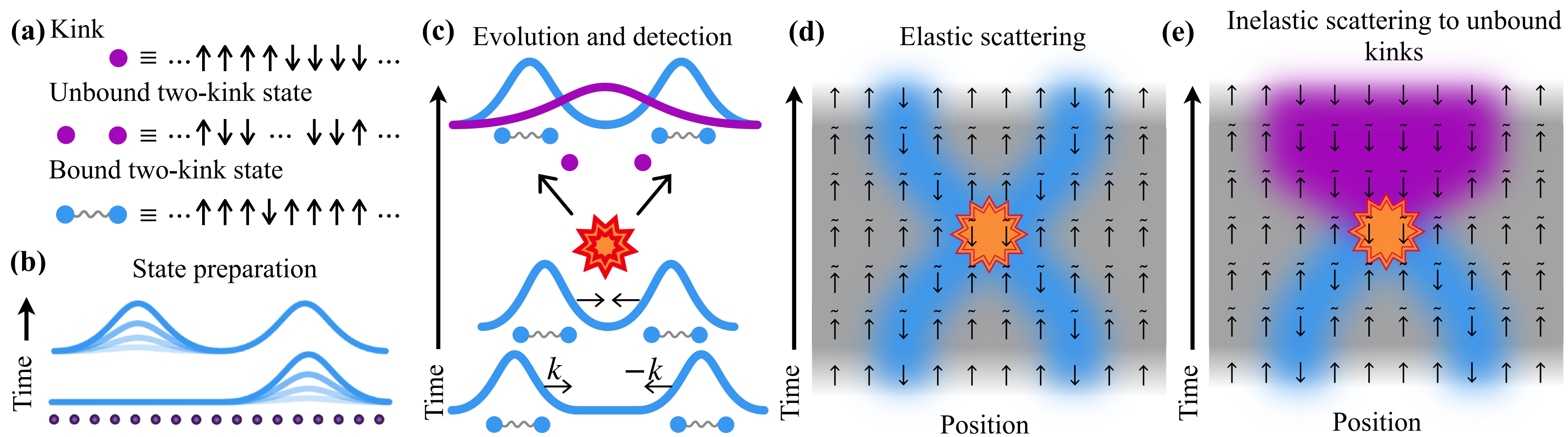


Collisions in ~~Particle Accelerators~~ Tabletop Quantum Simulators - II

Collisions of kink-antikink bound states in trapped-ions quantum simulators:

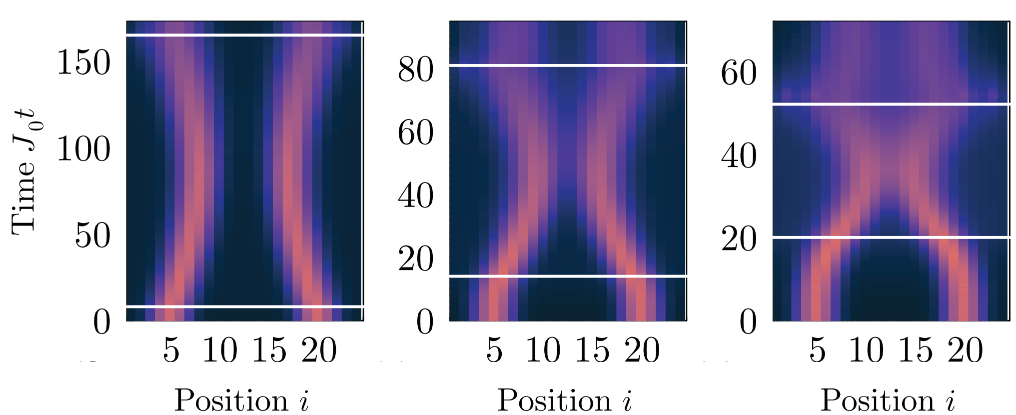
Bennewitz, …, AL, et al. in preparation (2024)

Native $\hat{H}_{\mathrm{spin-phonon}}$

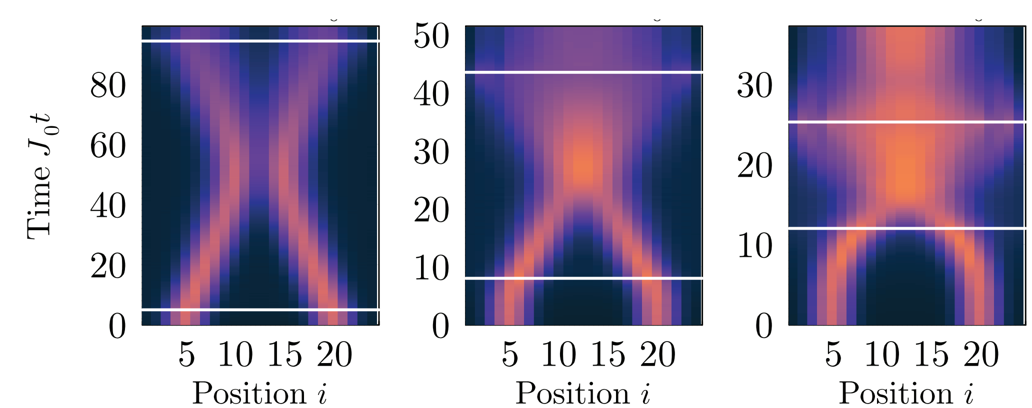


Numerical simulation of experimental collision:

Kink confinement regime



Kink deconfinement regime



…What's next?

THANK YOU