Title: Unconstrained tree tensor simulations for high-dimensional quantum many-body simulations

Speakers: Simone Montangero

Collection: Tensor Networks: from Simulations to Holography III

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Abstract: We present some recent results on the development of efficient unconstrained tree tensor networks algorithms and their application to high-dimensional many-body quantum systems. In particular, we present our results on topological two-dimensional systems, two-dimensional Rydberg atom systems, and two- and three-dimensional lattice gauge theories in presence of fermonic matter. Finally, we present their application to the study of open many-body quantum systems and in particular to the computation of the entanglement of formation in critical many-body quantum systems, resulting in the generalization of the Calabrese-Cardy formula to open systems.

UNCONSTRAINED TREE TENSOR NETWORKS SIMULATIONS

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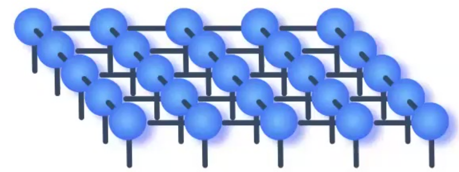
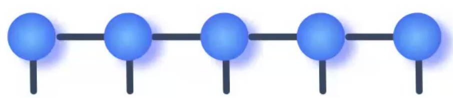
TENSOR NETWORKS STATES

$\psi_{\alpha_1,\alpha_2,\ldots\alpha_N}$ $\mathcal{O}(d^N)$

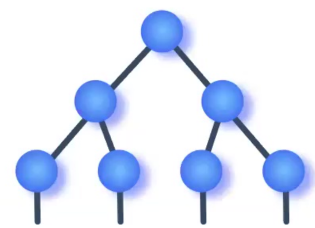


PEPS

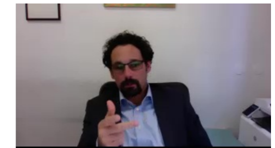


$\mathcal{O}(Ndm^2)$

$A^{\beta_1}_{\alpha_1} A^{\beta_1 \beta_2}_{\alpha_2} \ldots A^{\beta_{N-1}}_{\alpha_N}$

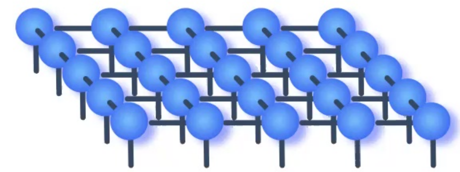


Tree Tensor Network

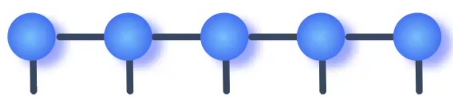


TENSOR NETWORKS STATES

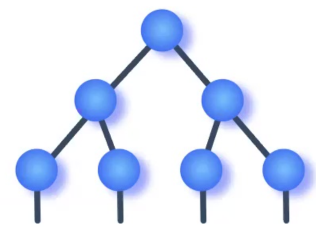
$\psi_{\alpha_1,\alpha_2,\dots\alpha_N}$ $\mathcal{O}(d^N)$



PEPS



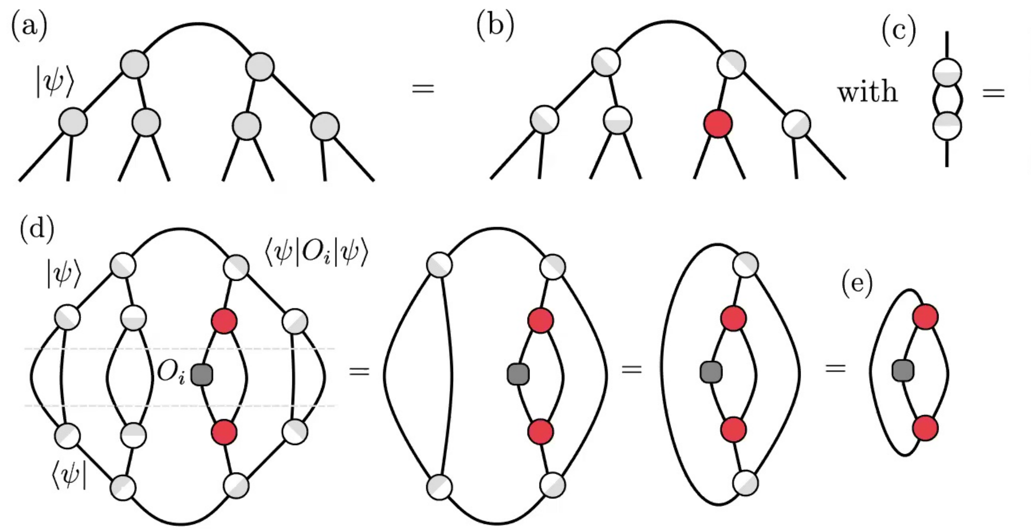
$A^{\beta_1}_{\alpha_1} A^{\beta_1\beta_2}_{\alpha_2} \dots A^{\beta_{N-1}}_{\alpha_N}$ $\mathcal{O}(Ndm^2)$

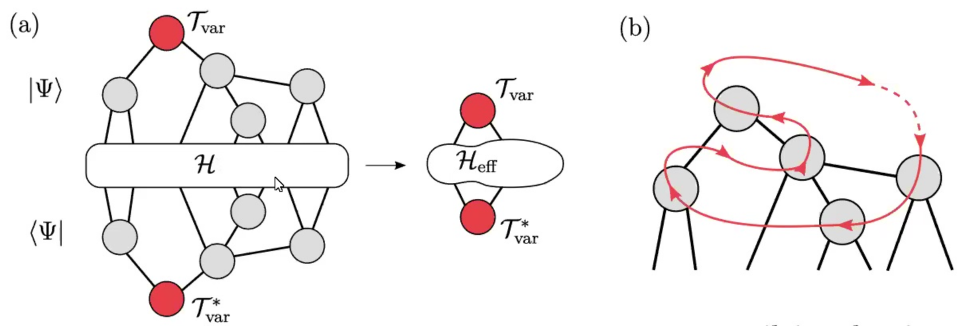


Tree Tensor Network

Tensor networks states are a compressed description of the system tunable between mean field and exact

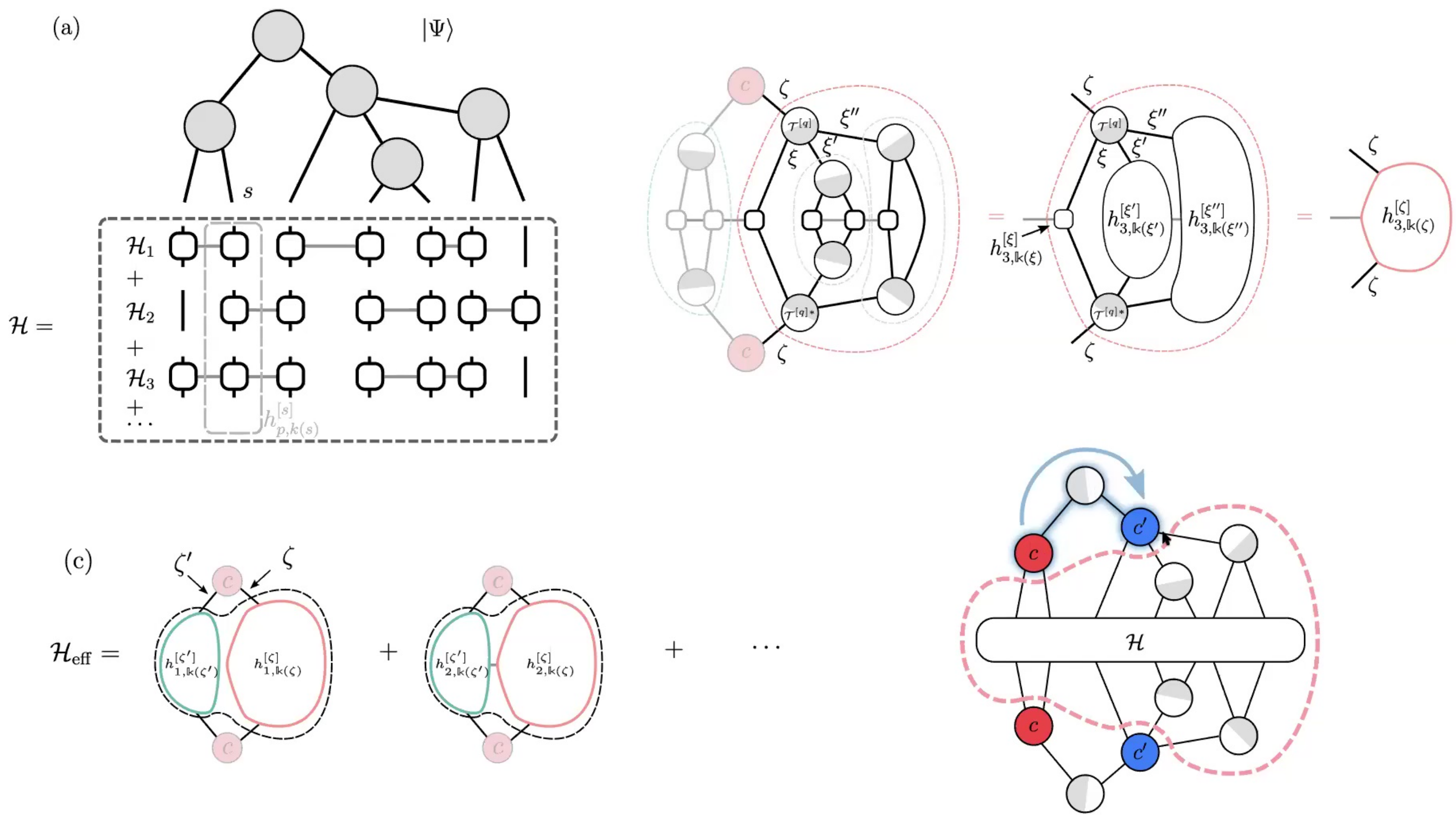
UNCONSTRAINED TREE TENSOR NETWORKS





P. Silvi et al. SciPost Phys. Lect. Notes 8 (2019)

VARIATIONAL MINIMIZATION



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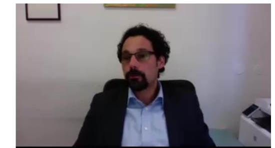
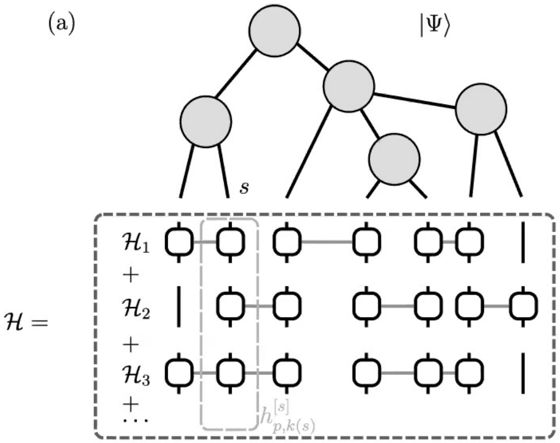
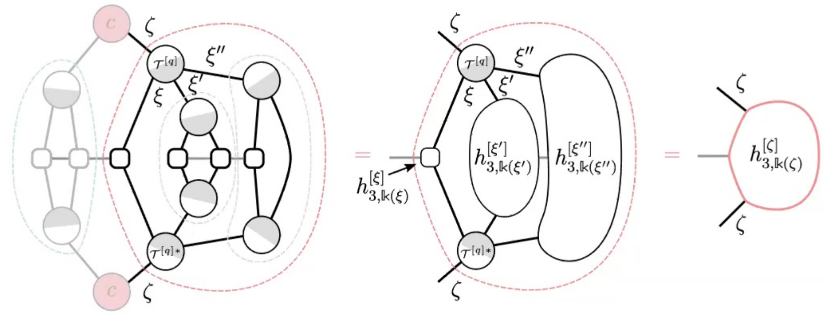


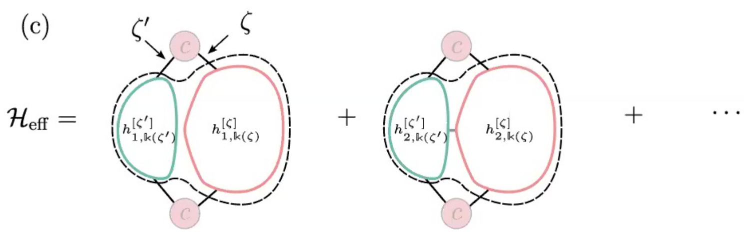
VARIATIONAL MINIMIZATION

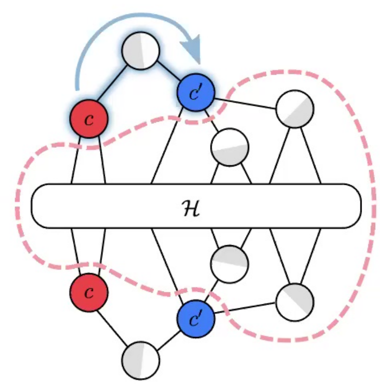
(a)

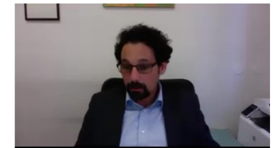




(c)







$\mathcal{O}(m^4)$

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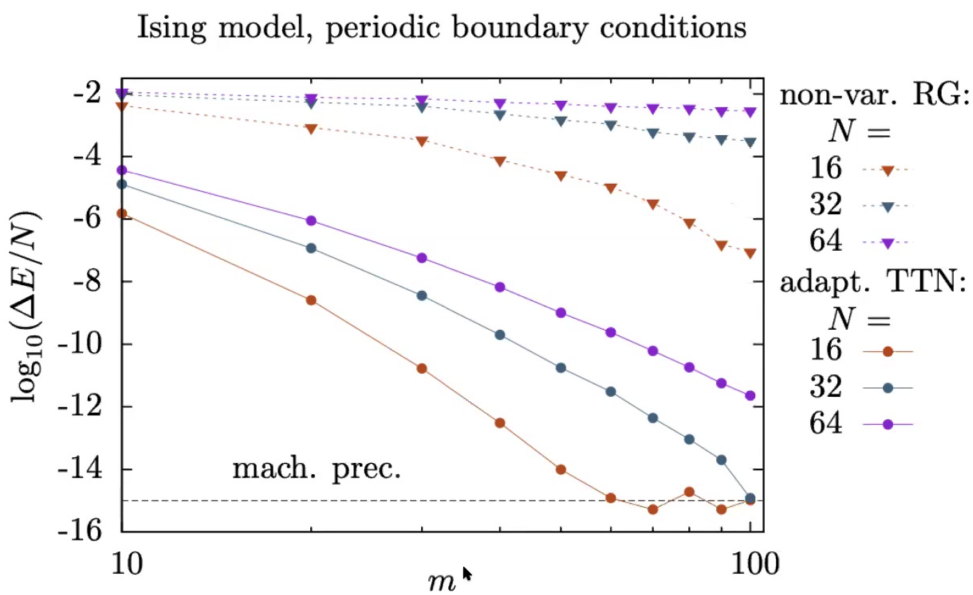
VARIATIONAL MINIMIZATION



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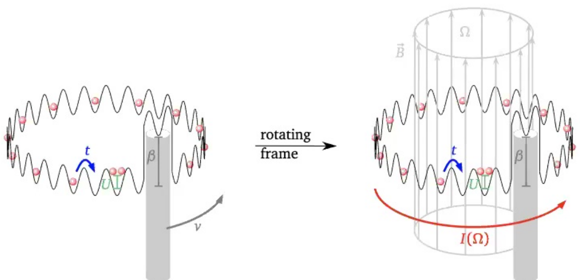
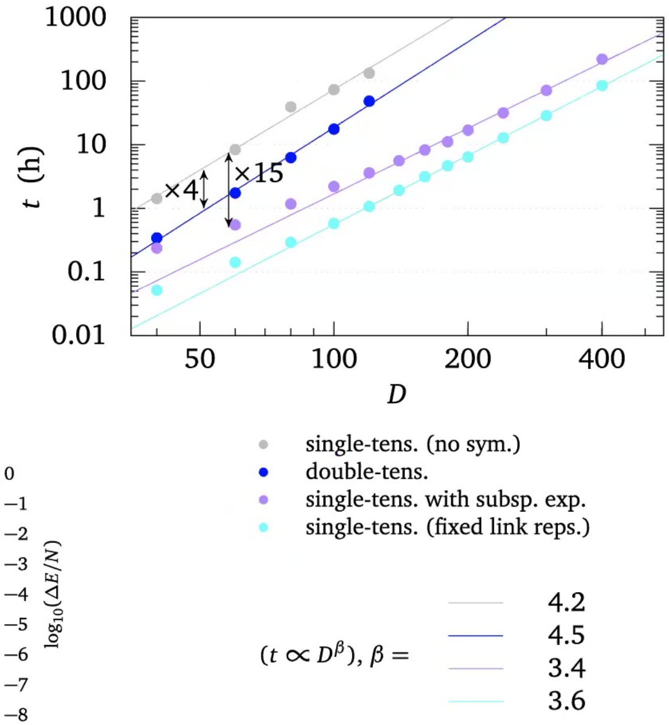
$$\mathcal{O}(m^4)$$

PERFORMANCE

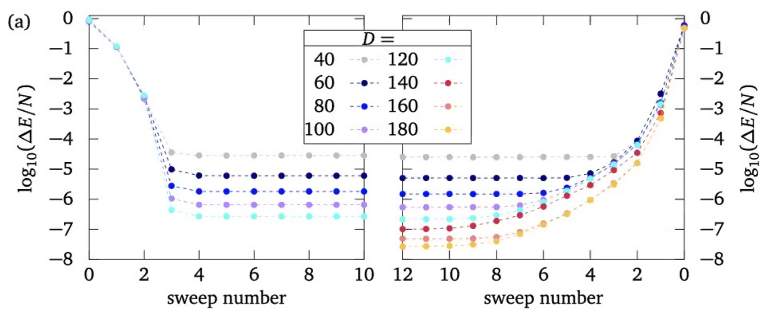


$$\mathcal{H} = -t\sum_{s=1}^{N}\left(e^{-2\pi i\Omega/N}\, b^{\dagger[s]}\, b^{[s+1]} + \text{h.c.}\right) + \frac{U}{2}\sum_{s=1}^{N} n^{[s]}\left(n^{[s]}-1\right) + \beta\, n^{[s_b]}$$

Bose Hubbard Ring



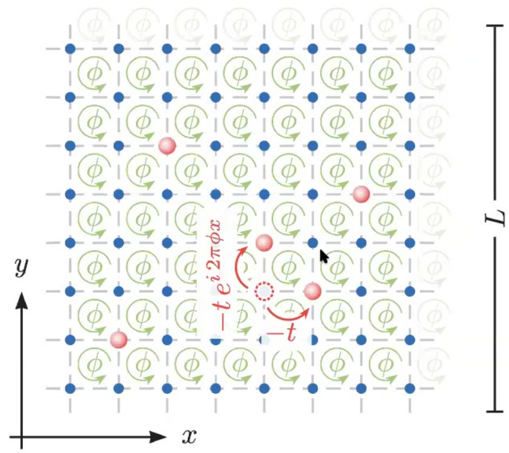
Double tensor update vs single with subspace exp.



$N = 128$, $N_b = 19$, $\beta/t = 1$, $U/t = 10$, $\Omega = 0$

S. White PRB (2005), C. Hubig et al. PRB (2015)

INTERACTING HOFSTADTER MODEL

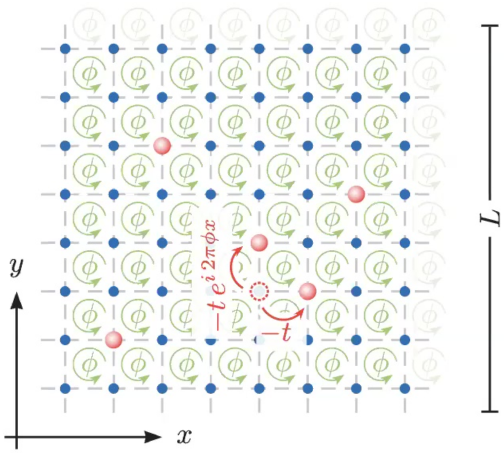


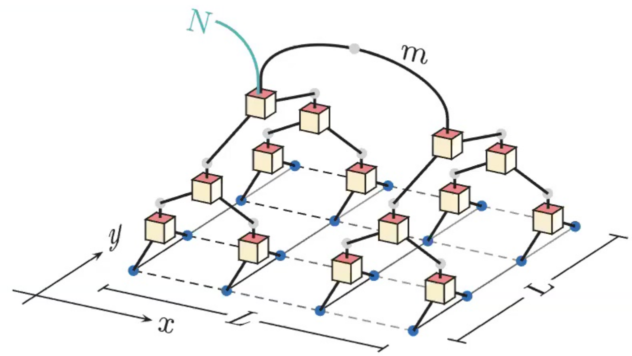
$$H = U\sum_{x,y} n_{x,y}(n_{x,y}-1) - t\sum_{x,y}\{a^\dagger_{x+1,y}a_{x,y}\,e^{-i\,2\pi\delta_{xL}\theta_x} + a^\dagger_{x,y+1}a_{x,y}\,e^{i\,2\pi(\phi x-\delta_{yL}\theta_y)} + \text{H.c.}\}$$

Spinless bosons

with magnetic field

INTERACTING HOFSTADTER MODEL



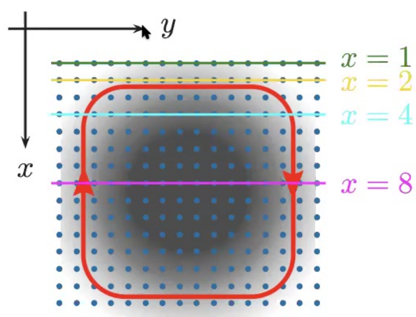


$$H = U \sum_{x,y} n_{x,y}(n_{x,y}-1) - t \sum_{x,y} \{a^\dagger_{x+1,y} a_{x,y}\, e^{-i\,2\pi \delta_{xL}\theta_x} + a^\dagger_{x,y+1} a_{x,y}\, e^{i\,2\pi(\phi x - \delta_{yL}\theta_y)} + \text{H.c.}\}$$

Filling factor

$$\nu = N/(\phi L^2) = 1/q$$

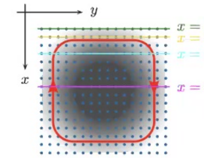
Laughlin wave function?



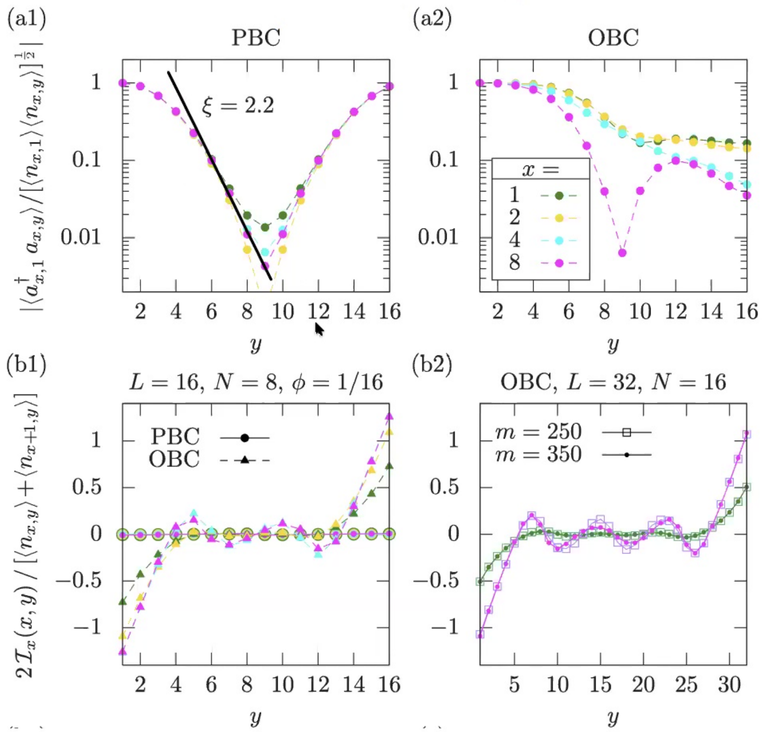
Spinless bosons

with magnetic field

RESULTS

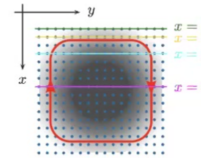


Correlations and Edge Currents

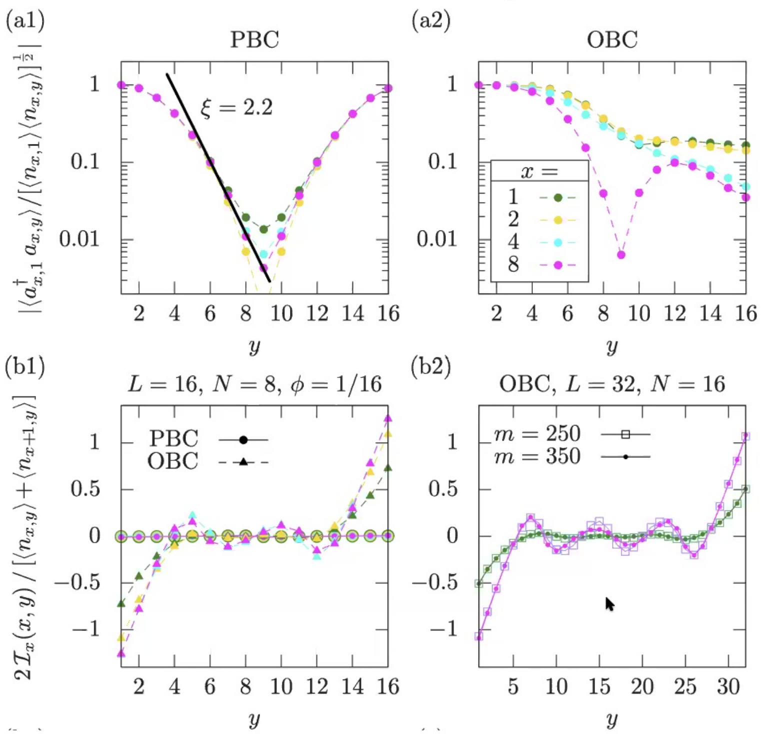


M. Gerster et al. Phys. Rev. B (2017)

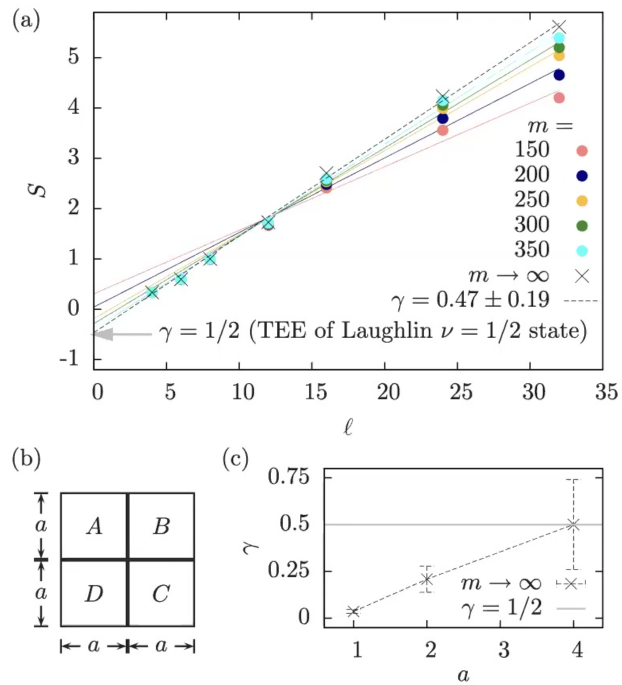
RESULTS



Correlations and Edge Currents



Topological entanglement entropy



Many-body Cern number

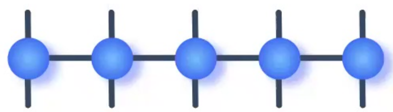
Compatible with ν=1/2 fractional QH

M. Gerster et al. Phys. Rev. B (2017)

TN REPRESENTATION OF MIXED QUANTUM STATES

$$\rho = \sum p_j |\psi_j\rangle\langle\psi_j|$$

$$\rho = XX^\dagger$$



MPDO

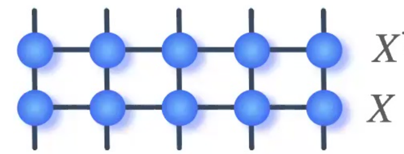
Loopless *Positive?*

F. Verstraete et al. (2004)

G. de las Cuevas et al. (2013)

Quantum jumps,

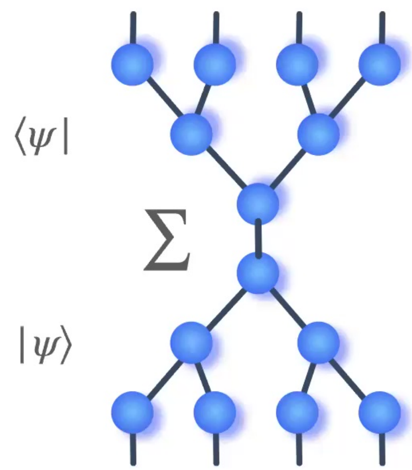
Purification…



LPTN

Positive *Looped*

A. Werner et al (2016)



TTO

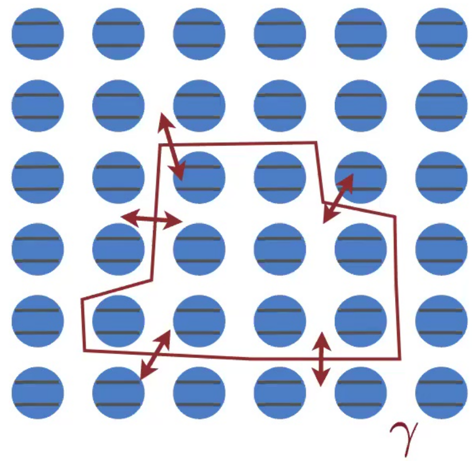
Loopless and positive!

ENTANGLEMENT OF MIXED QUANTUM SYSTEMS

For pure states:

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

Von Neumann Entropy



Area law

$$\mathcal{S} \propto \gamma$$

$$\mathcal{S} \propto N^{(D-1)}$$

1D critical systems:

$$\mathcal{S} = \frac{c}{3} \log N$$

For mixed states:

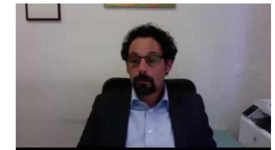
$$E_F(\rho) = \inf_{\{p_j, \psi_j\}} \left\{ \sum_j p_j \mathcal{S}(|\psi_j\rangle) : \rho = \sum_j p_j |\psi_j\rangle\langle\psi_j| \right\}$$

$$E_F(\rho, T) \overset{?}{\propto} \log N^{c/3}$$

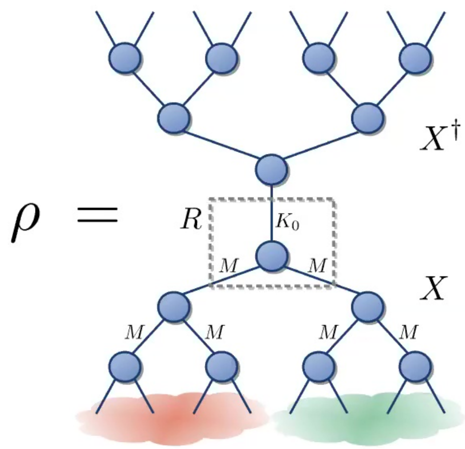
Entanglement of formation

C.H. Bennet et al. PRA 1996

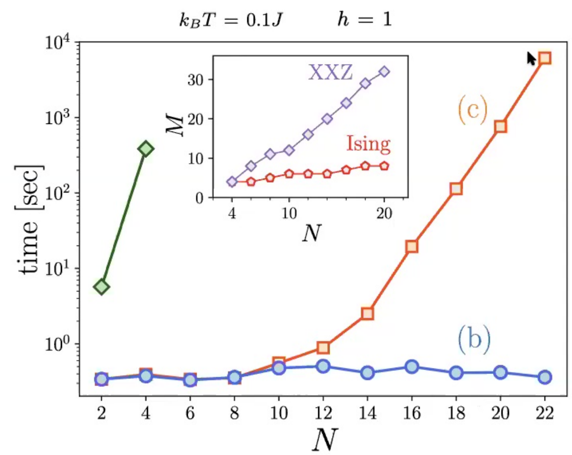
J. Eisert et al. Rev. Mod. Phys. 2009

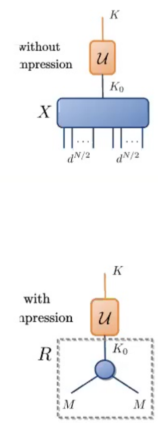


TREE TENSOR OPERATORS



$$E_F(\rho) = \min_{K \geq K_0} \inf_{\mathcal{U}} \left\{ \sum_{j=1}^{K} p_j \mathcal{S}(|\psi'_j\rangle) : X' = X\mathcal{U} \right\}$$





$$\hat{H}_{Ising} = J \sum_{i=1}^{N} \left(\hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + h \hat{\sigma}_j^z \right)$$

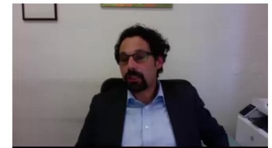
$$\hat{H}_{XXZ} = J \sum_{j=1}^{N} \left(\hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y + \xi \, \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z \right)$$

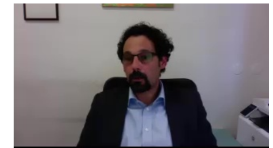
Thermal equilibrium state

(Mixture of K_0 Boltzmann factors)

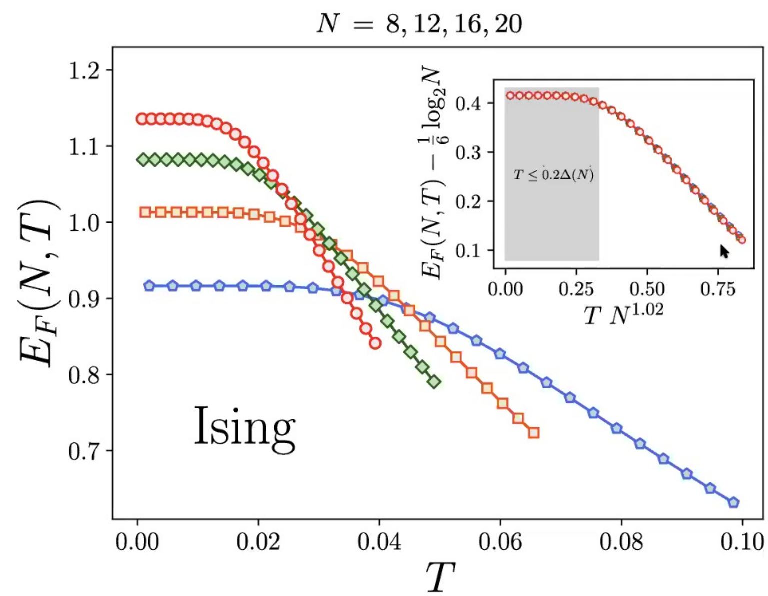
$$X = \frac{1}{\sqrt{Z}} \sum_j^{K_0} e^{-E_j/2T} |\psi_j\rangle\langle j|$$

L. Arceci, P. Silvi, and S. Montangero arXiv:2011.01247





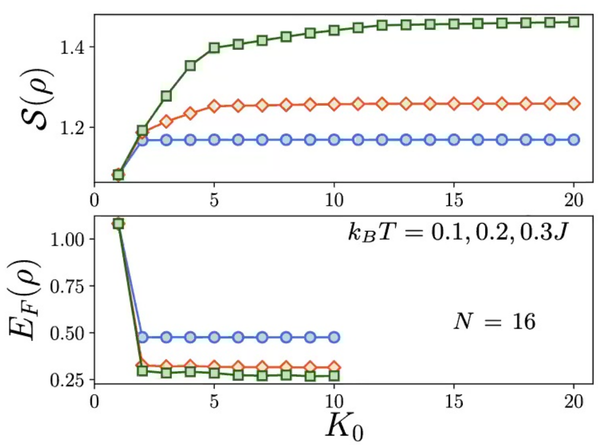
CONFORMAL SCALING OF ENTANGLEMENT OF FORMATION

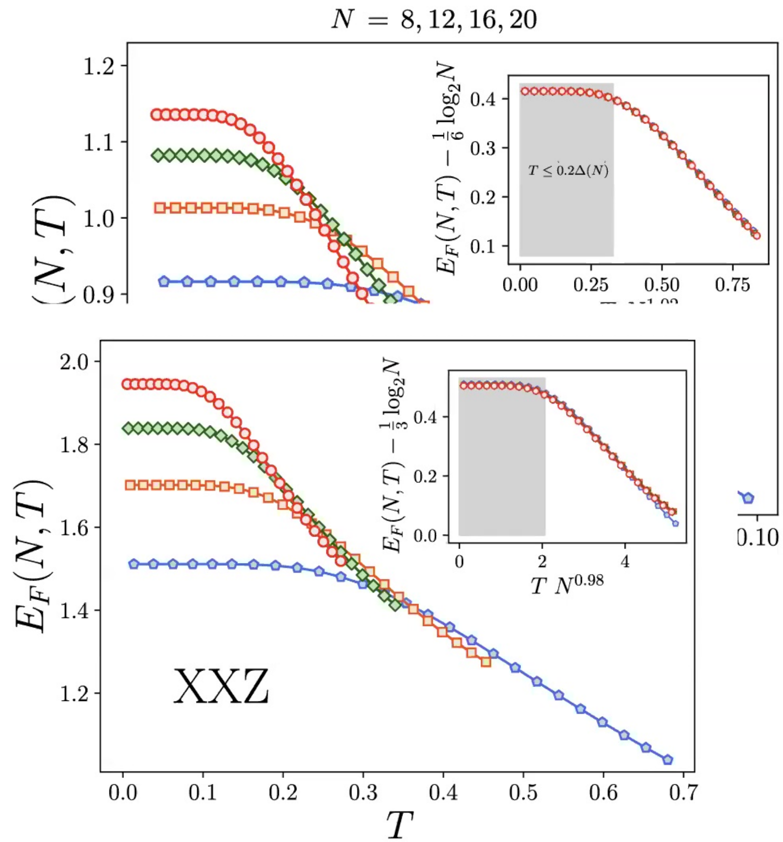


L. Arceci, P. Silvi, and S. Montangero arXiv:2011.01247

CONFORMAL SCALING OF ENTANGLEMENT OF FORMATION

$$E_F = \log(N^{c/3} f(TN^z))$$

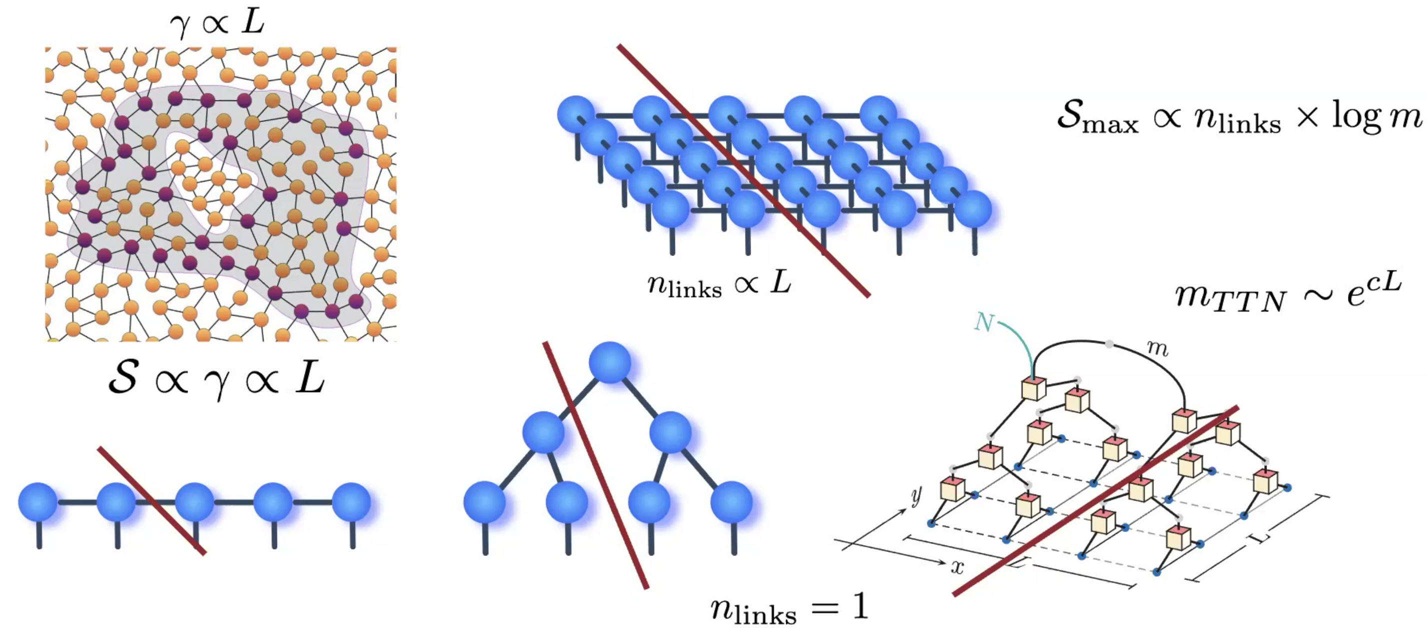




Numerical complexity depends on entropy, not entanglement!

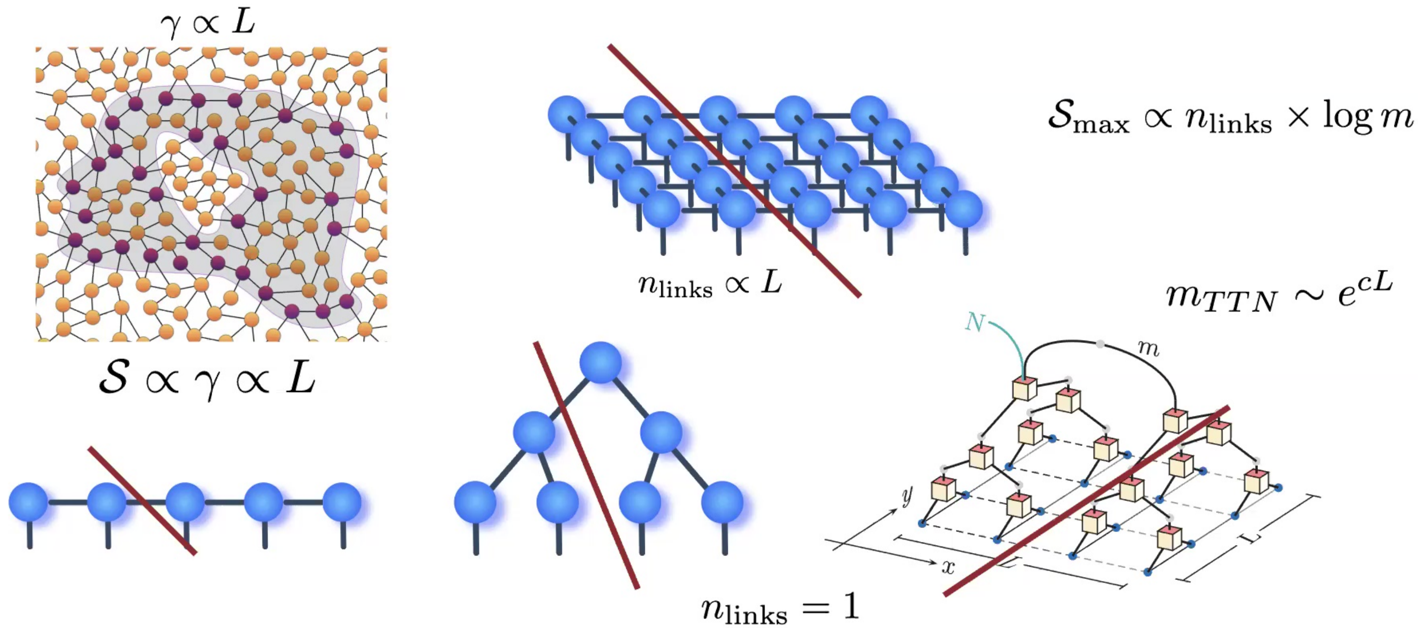
L. Arceci, P. Silvi, and S. Montangero arXiv:2011.01247

AREA LAWS AND TENSOR NETWORKS

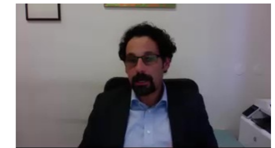


Tensor Network	Complexity	Area law in 2D	Typical Bond dimensions	Exact contractable
MPS / DMRG	$\mathcal{O}\{\chi^3\}$	No (Only in 1D)	> 10.000	Yes ($\mathcal{O}\{\chi^3\}$)
TTN	$\mathcal{O}\{\chi^4\}$	No (Only in 1D)	$\approx 1.000 - 2.000$	Yes ($\mathcal{O}\{\chi^4\}$)
PEPS	$\mathcal{O}\{\chi^{10}\}$	Yes	~ 10	No ($\mathcal{O}\{\chi^L\}$)
MERA	$\mathcal{O}\{\chi^8\}$ (1D), $\mathcal{O}\{\chi^{16}\}$ (2D)	Yes	~ 10	Yes ($\mathcal{O}\{\chi^8\}$)

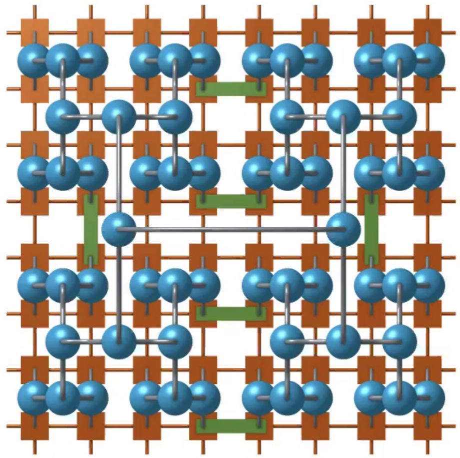
AREA LAWS AND TENSOR NETWORKS



Tensor Network	Complexity	Area law in 2D	Typical Bond dimensions	Exact contractable
MPS / DMRG	$\mathcal{O}\left\{\chi^3\right\}$	No (Only in 1D)	> 10.000	Yes ($\mathcal{O}\left\{\chi^3\right\}$)
TTN	$\mathcal{O}\left\{\chi^4\right\}$	No (Only in 1D)	$\approx 1.000 - 2.000$	Yes ($\mathcal{O}\left\{\chi^4\right\}$)
PEPS	$\mathcal{O}\left\{\chi^{10}\right\}$	Yes	~ 10	No ($\mathcal{O}\left\{\chi^L\right\}$)
MERA	$\mathcal{O}\left\{\chi^8\right\}$ (1D), $\mathcal{O}\left\{\chi^{16}\right\}$ (2D)	Yes	~ 10	Yes ($\mathcal{O}\left\{\chi^8\right\}$)
aTTN	$\mathcal{O}\left\{\chi^4\right\}$	Yes*	≈ 500	Yes ($\mathcal{O}\left\{\chi^4\right\}$)



AUGMENTED TREE TENSOR NETWORKS



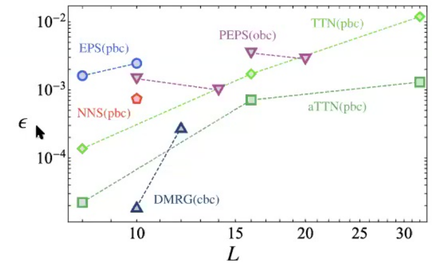
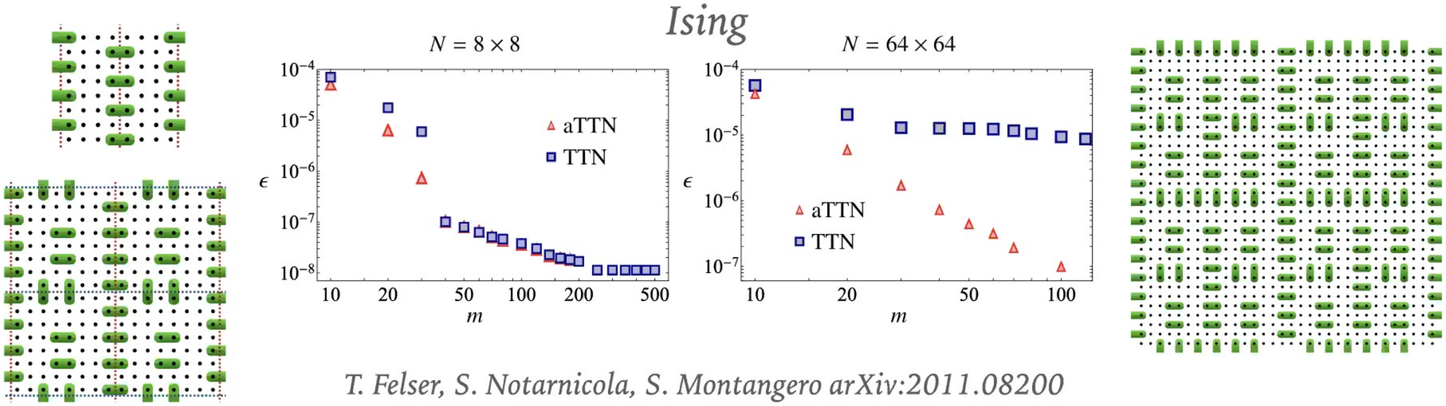


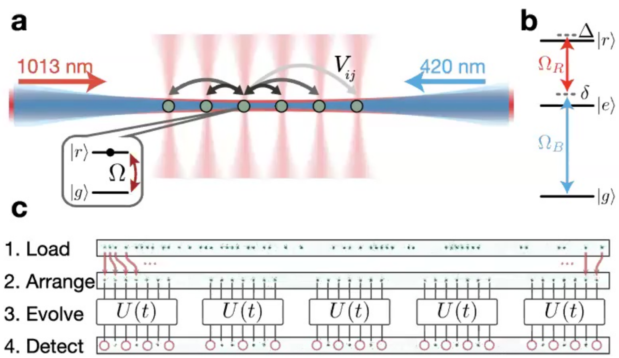
FIG. 2: Relative error ϵ of the 2D Heisenberg ground-state energy as a funciotn of the system linear size L compared with the best available estimates obtained by MC [21] for the TTN, aTTN, NNS [59], EPS [60], PEPS [61], 2D-DMRG [57]. Depending on the method open (obc), cylindrical (cbc) or periodic (pbc) boundary conditions have been chosen. For each datapoint, we compare the Monte Carlo result with the same boundary conditions.

Ising



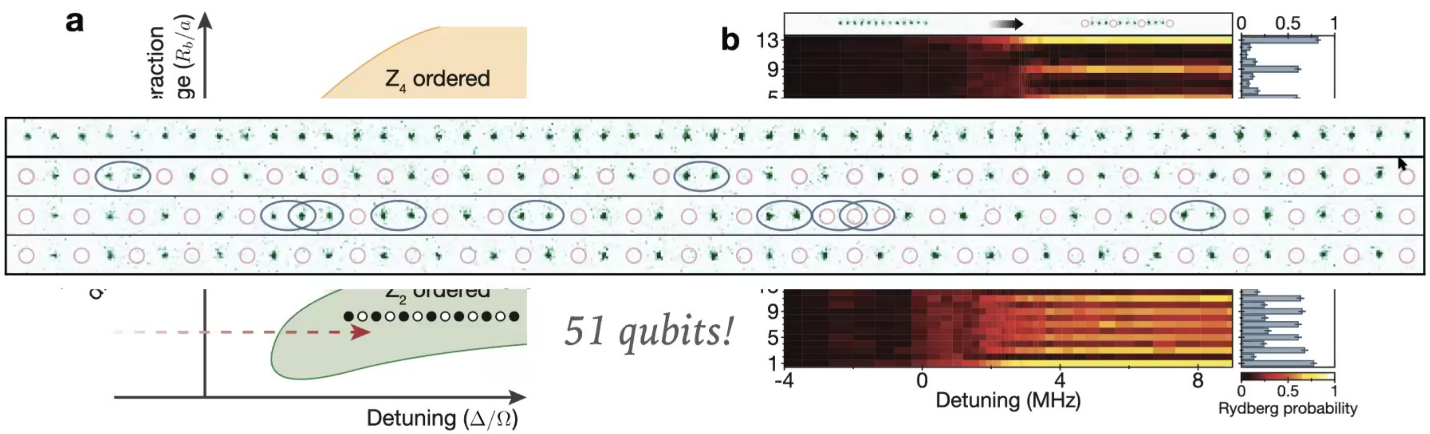
T. Felser, S. Notarnicola, S. Montangero arXiv:2011.08200

QUANTUM SIMULATION OF MANY-BODY CORRELATED DYNAMICS



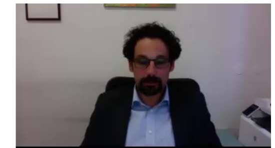
$$\frac{\mathcal{H}}{\hbar} = \sum_i \frac{\Omega_i}{2}\sigma_x^i - \sum_i \Delta_i n_i + \sum_{i<j} V_{ij} n_i n_j,$$

Rydberg Blockade



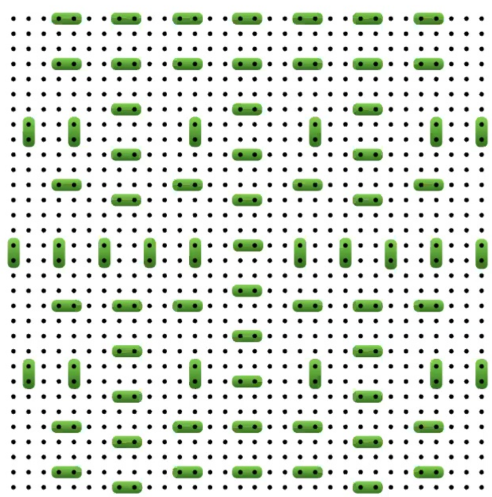
51 qubits!

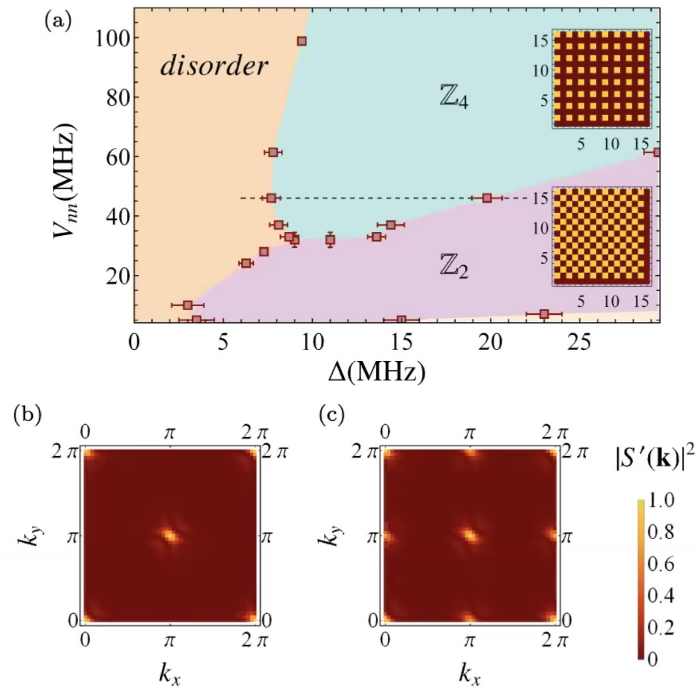
M. Lukin's group ***Nature*** *(2017)*

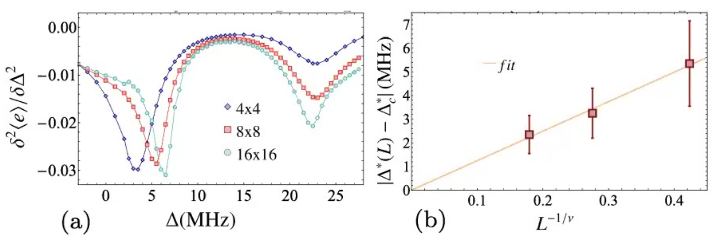


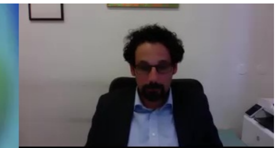
RYDBERG QUANTUM SIMULATOR

32x32 sites









Simulating Lattice Gauge Theories within Quantum Technologies

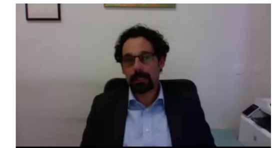
M.C. Bañuls[1,2], R. Blatt[3,4], J. Catani[5,6,7], A. Celi[3,8], J.I. Cirac[1,2], M. Dalmonte[9,10], L. Fallani[5,6,7], K. Jansen[11], M. Lewenstein[8,12,13], S. Montangero[7,14 a], C.A. Muschik[3], B. Reznik[15], E. Rico[16,17 b], L. Tagliacozzo[18], K. Van Acoleyen[19], F. Verstraete[19,20], U.-J. Wiese[21], M. Wingate[22], J. Zakrzewski[23,24], and P. Zoller[3]

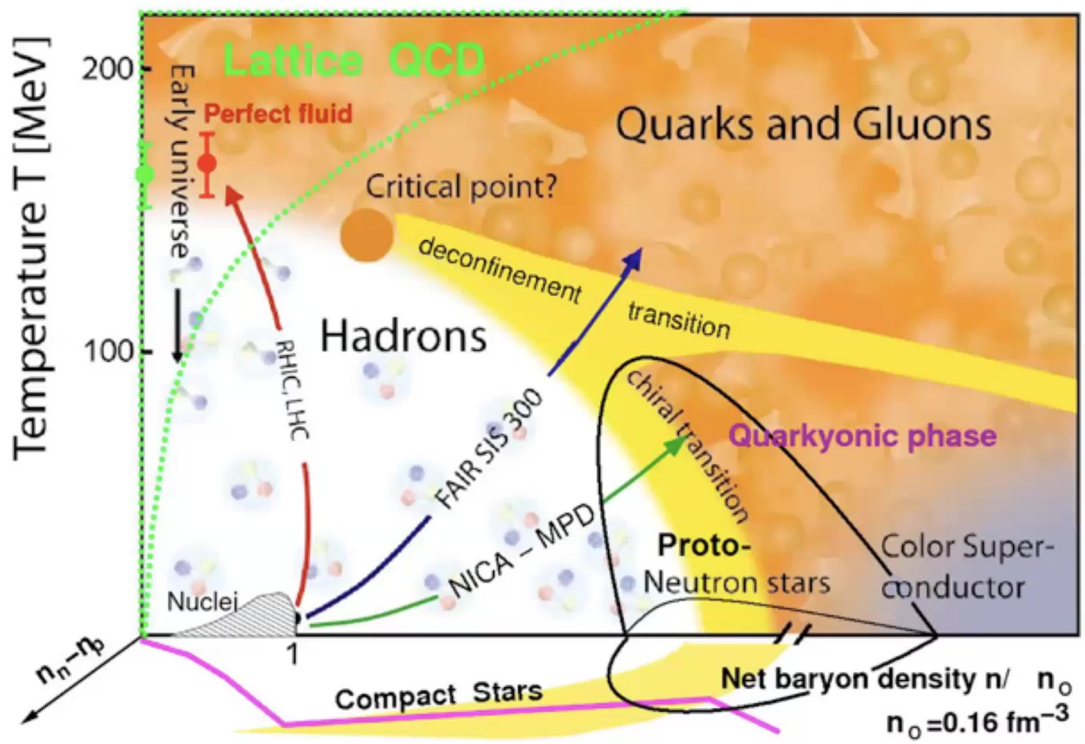
https://qt.eu/qtflag/

EPJD (2020)

QUANTERA

LATTICE GAUGE THEORIES

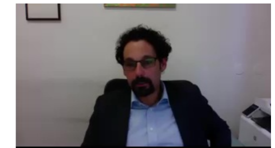




The current wisdom on the phase diagram of nuclear matter.

McLerran, L. Nucl.Phys.Proc.Suppl. 195 (2009) 275-280

LATTICE GAUGE TENSOR NETWORKS



Local degrees of freedom

$$[\psi^a_x, U^{ab}_{x,x+\mu_x}]$$

Matter field   Gauge field

Gauge symmetry generator
(Gauss' law)

$$G_x|\varphi_{phys}\rangle = 0$$

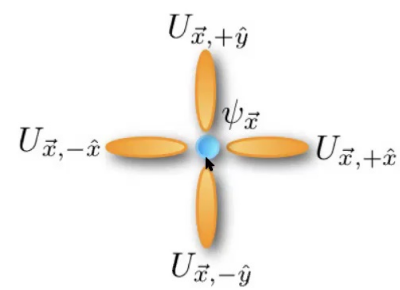
Gauge invariant dynamics

$$H = J\sum_x \left(\psi^\dagger_x U_{x,x+1}\psi_{x+1} + \text{h.c.}\right)$$

abelian

$$H = t\sum_{x,a,b}\left[\psi^{a\dagger}_x U^{ab}_{x,x+1}\psi^b_{x+1} + \text{h.c.}\right]$$

non abelian

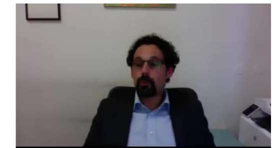


Kogut-Susskind

Hamiltonian formulation of LGT

Dynamics commutes with symmetry generator

$$\left[H^{[\text{QED}]}_{\text{int}}, G_x\right] = 0 \quad \forall\, x$$



QUANTUM LINK AND RISHON REPRESENTATION

Link operator $U_{x,y} \equiv S^{+}_{x,y} = c^{\dagger}_{y} c_{x}$

Electric field [U(1) generator] $E_{x,y} \equiv S^{(3)}_{x,y} = \frac{1}{2}\left[c^{\dagger}_{y} c_{y} - c^{\dagger}_{x} c_{x}\right]$

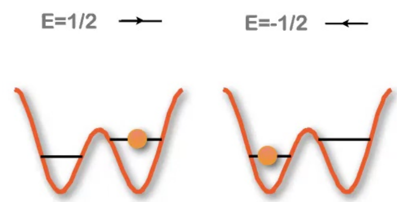
$\{c_x, c^{\dagger}_{y}\} = \delta_{x,y}$ Schwinger fermions (rishons)

$[c_x, c^{\dagger}_{y}] = \delta_{x,y}$ Schwinger bosons

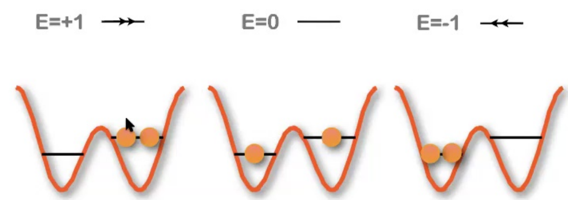
Spin representation:

$N_{x,y} = c^{\dagger}_{y} c_{y} + c^{\dagger}_{x} c_{x}$ $\qquad \left[\vec{S}_{x,y}\right]^2 \equiv \frac{N_{x,y}}{2}\left[\frac{N_{x,y}}{2} + 1\right]$

Spin-½:



Spin-1:



QUANTUM LINK AND RISHON REPRESENTATION

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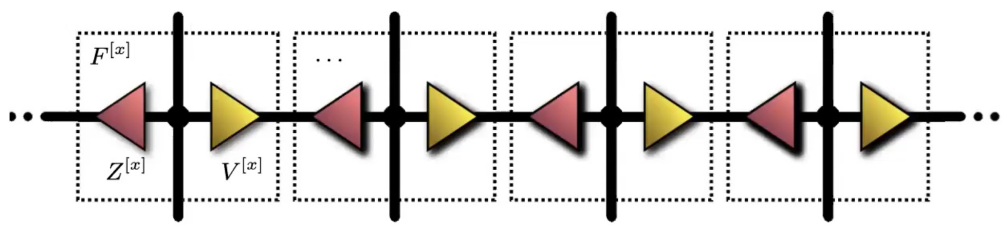


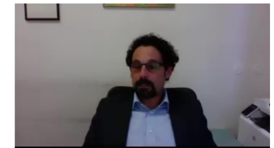
Local projection on a gauge invariant base

$+$

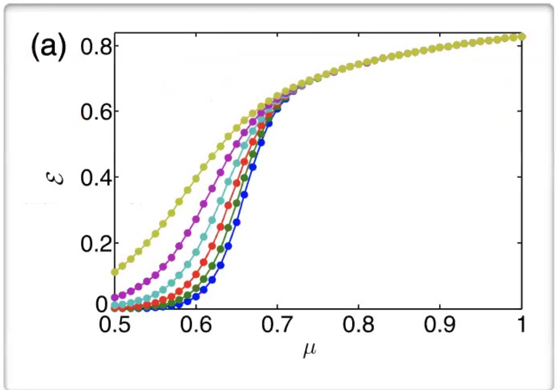
Projection on rishon number

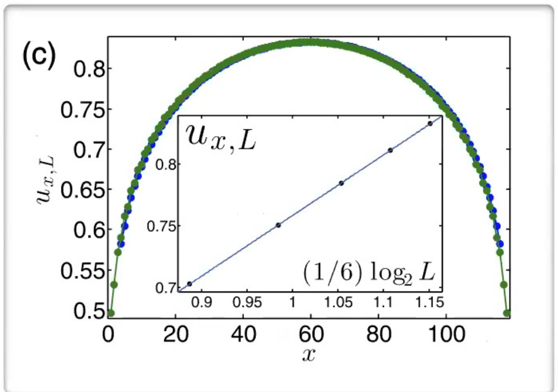
$=$

Matrix product operator



U(1) LATTICE GAUGE THEORY IN 1+1D





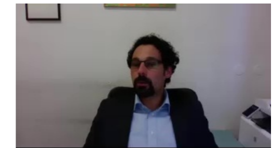
$$H = -t\sum_x \left[\psi_x^\dagger U_{x,x+1}^\dagger \psi_{x+1} + \psi_{x+1}^\dagger U_{x,x+1}\psi_x\right]$$

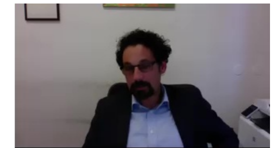
$$+m\sum_x (-1)^x \psi_x^\dagger \psi_x + \frac{g^2}{2}\sum_x E_{x,x+1}^2.$$

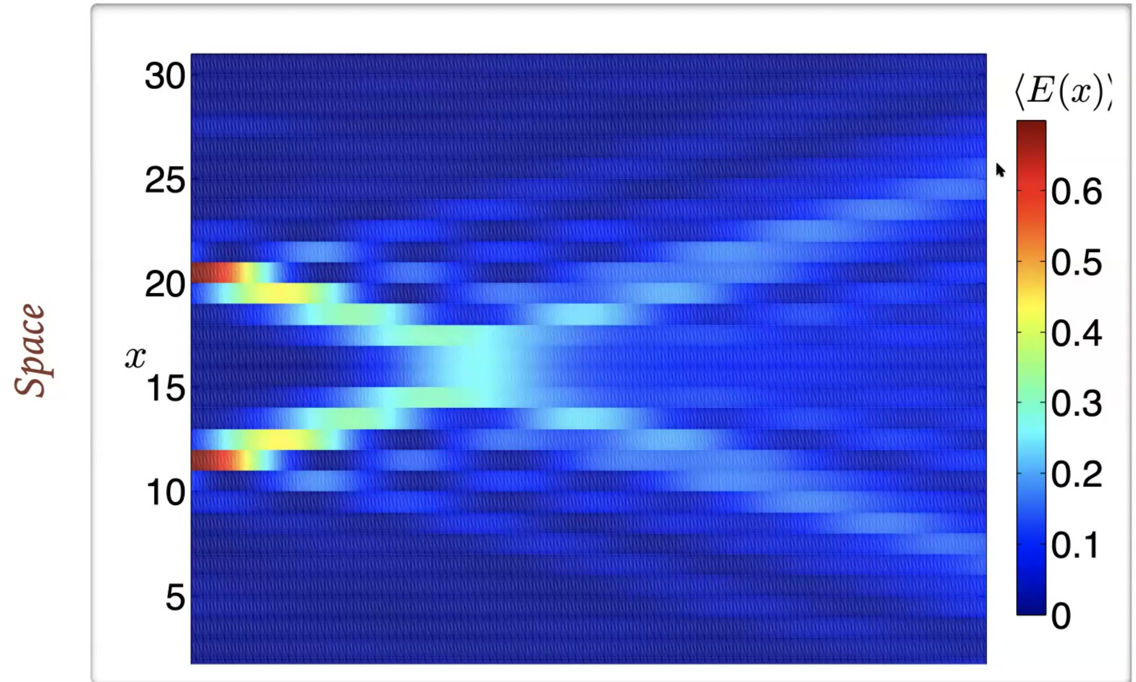
$$\mathcal{E} = \sum_x \langle E_{x,x+1}\rangle / L$$

- *Quantum link representation*
- *Staggered fermions*
- *Ising universality class*
- *Central charge* $c = 0.49 \pm 0.01$
- *Confirmed by higher-link representation*

E. Rico, T. Pichler, M. Dalmonte, P. Zoller, and SM, PRL (2014)



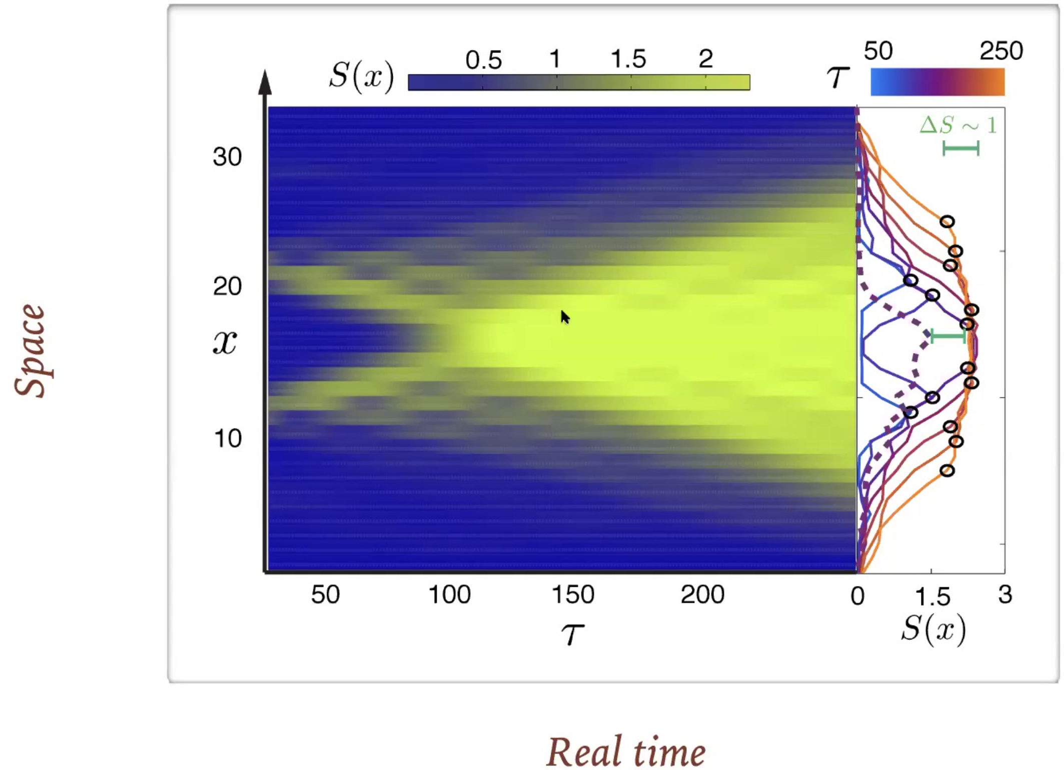




Real time

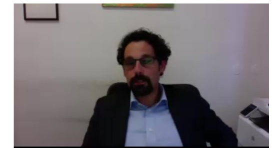
MESONS SCATTERING

T. Pichler, E. Rico, M. Dalmonte, P. Zoller, and SM, PRX (2016)



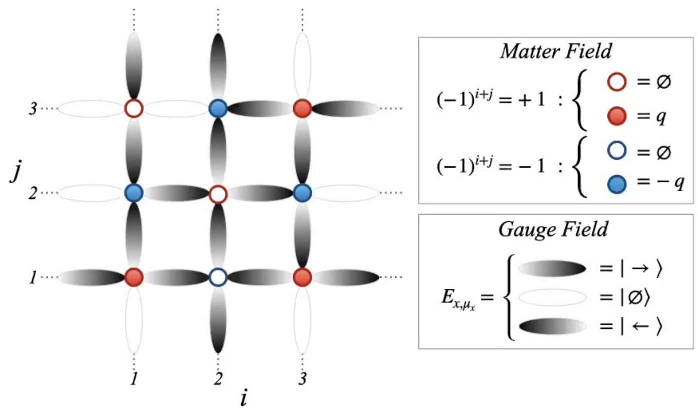
MESONS SCATTERING

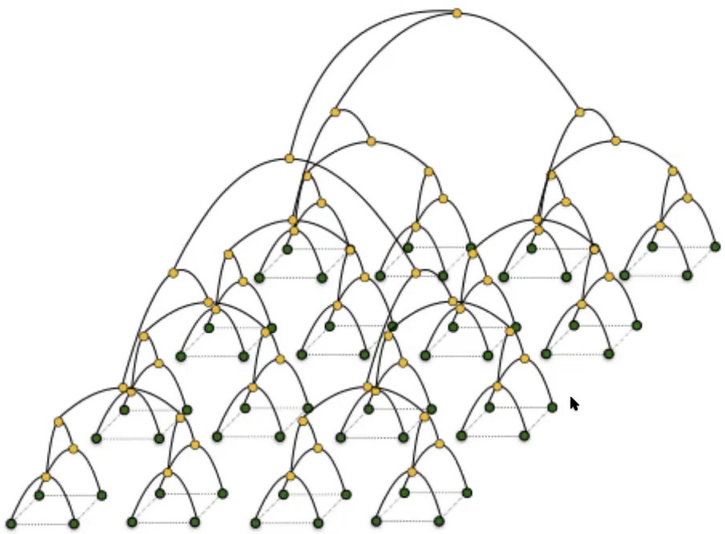
T. Pichler, E. Rico, M. Dalmonte, P. Zoller, and SM, PRX (2016)



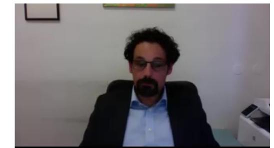
TWO DIMENSIONAL SIMULATION OF A LGT AT FINITE DENSITY

$$
\begin{aligned}
\mathrm{H} = & -t \sum_{x,\mu} \left(\psi_x^\dagger U_{x,\mu} \psi_{x+\mu} + h.c. \right) \\
& + m \sum_x (-1)^x \psi_x^\dagger U_{x,\mu} \psi_x + \frac{g_e^2}{2} \sum_{x,\mu} E_{x,\mu}^2 \\
& - \frac{g_m^2}{2} \sum_x \left(U_{x,\mu_x} U_{x+\mu_x,\mu_y} U^\dagger_{x+\mu_y,\mu_x} U^\dagger_{x,\mu_y} + h.c \right)
\end{aligned}
$$





T. Felser, P. Silvi, M. Collura, S. Montangero.
arXiv:1911.09693
PRX in press



TWO DIMENSIONAL SIMULATION OF A LGT AT FINITE DENSITY

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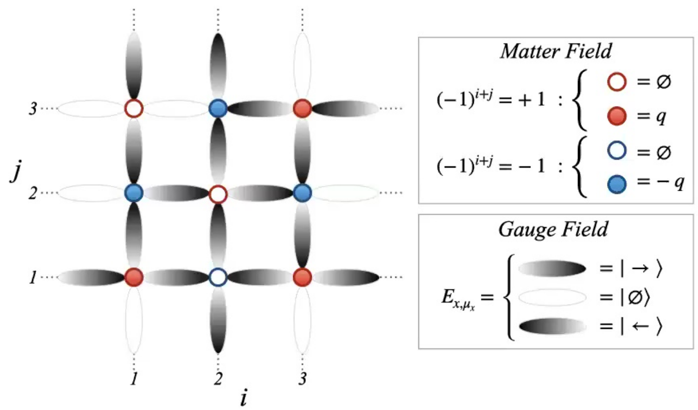
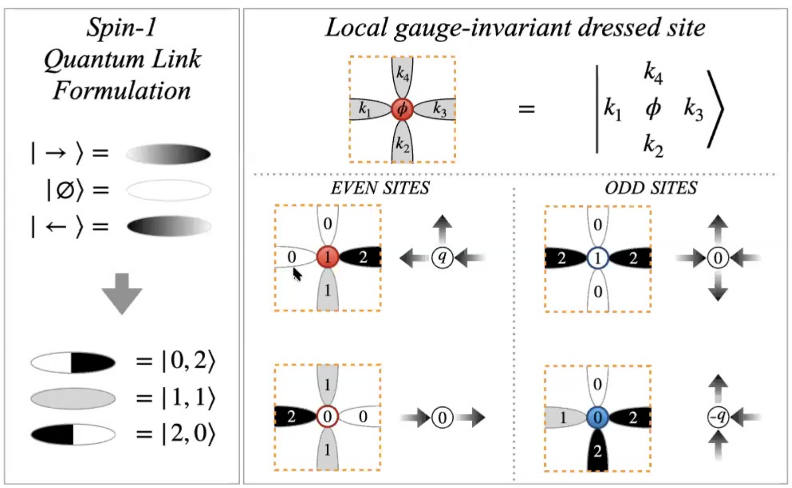
& - \frac{g_m^2}{2}\sum_{x}\left(U_{x,\mu_x}U_{x+\mu_x,\mu_y}U^\dagger_{x+\mu_y,\mu_x}U^\dagger_{x,\mu_y} + h.c\right)
\end{aligned}
$$





T. Felser, P. Silvi, M. Collura, S. Montangero.
arXiv:1911.09693
PRX in press

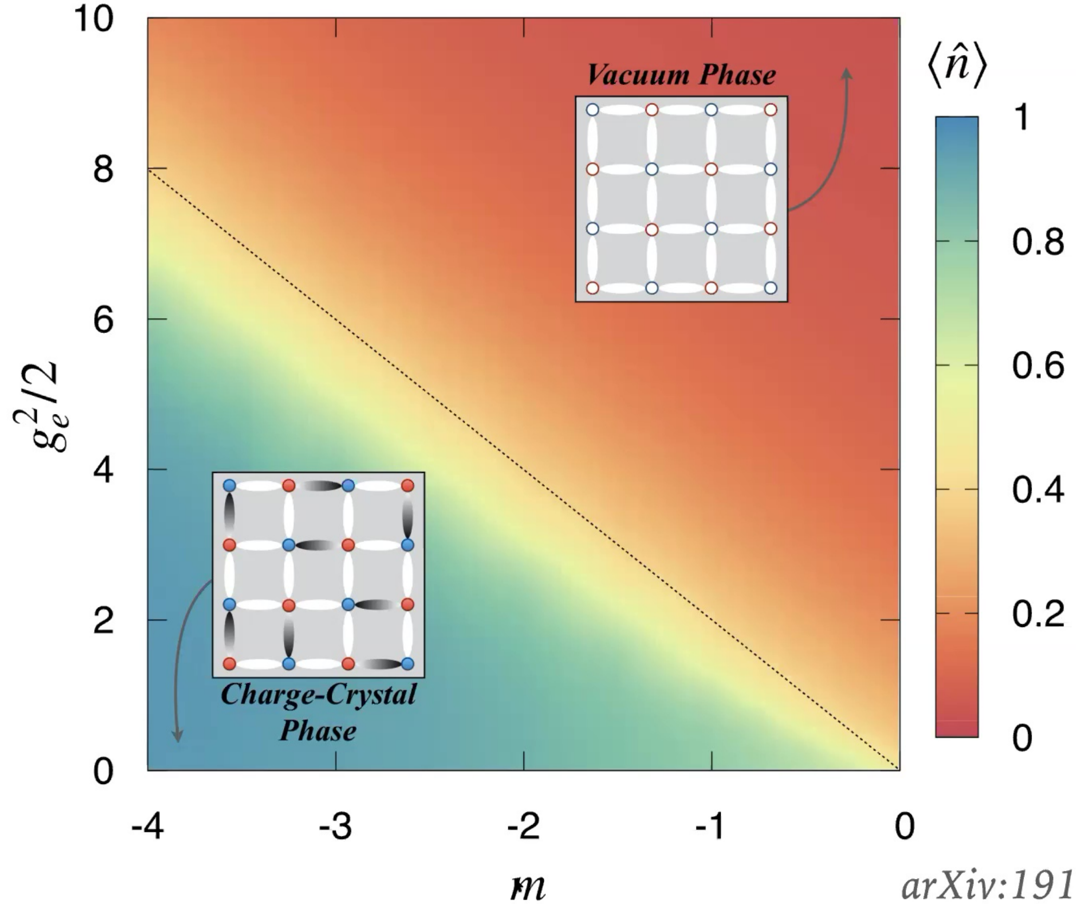
Even number of fermions =

No Jordan-Wigner strings!

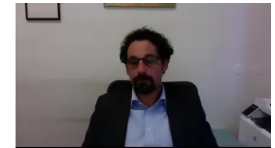
PHASE DIAGRAM

16x16 lattice sites

Hilbert space of ~80x80 qubits

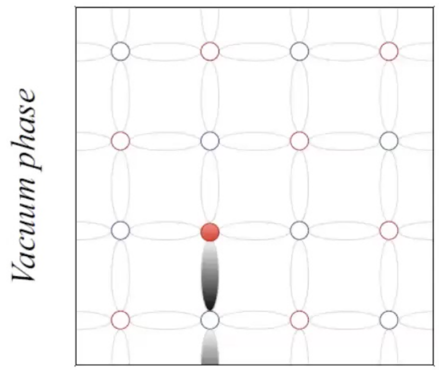


arXiv:1911.09693



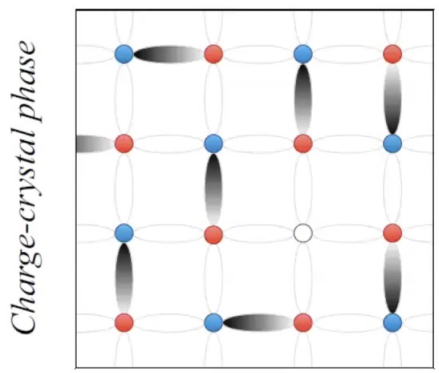
FINITE DENSITY

$$m > \frac{g_e^2}{2}$$

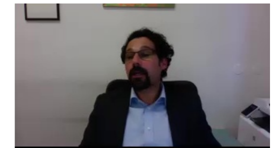


$$\langle \hat{H} \rangle = m + 3g_e^2/4$$

$$m < \frac{g_e^2}{2}$$

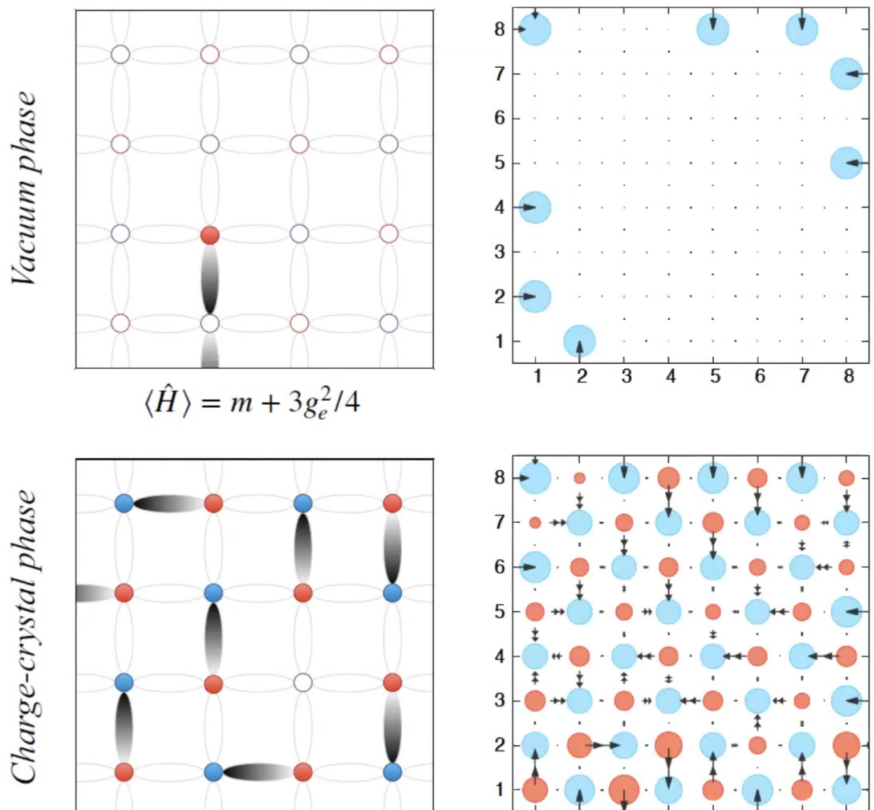


$$\langle \hat{H} \rangle = (L^2/2 - 1/2)(2m + g_e^2/2)$$



FINITE DENSITY

$m > \frac{g_e^2}{2}$

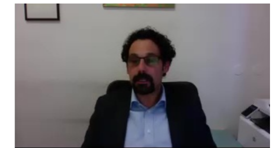


$\langle \hat{H} \rangle = m + 3g_e^2/4$

$m < \frac{g_e^2}{2}$

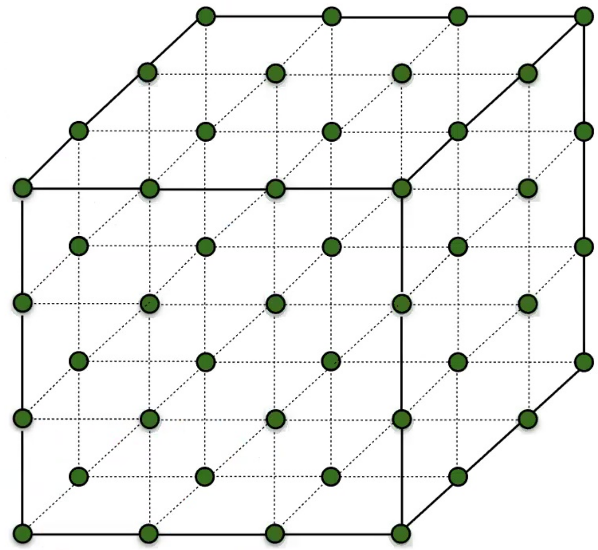
$\langle \hat{H} \rangle = (L^2/2 - 1/2)(2m + g_e^2/2)$

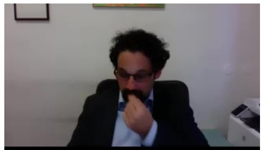
Q=-8



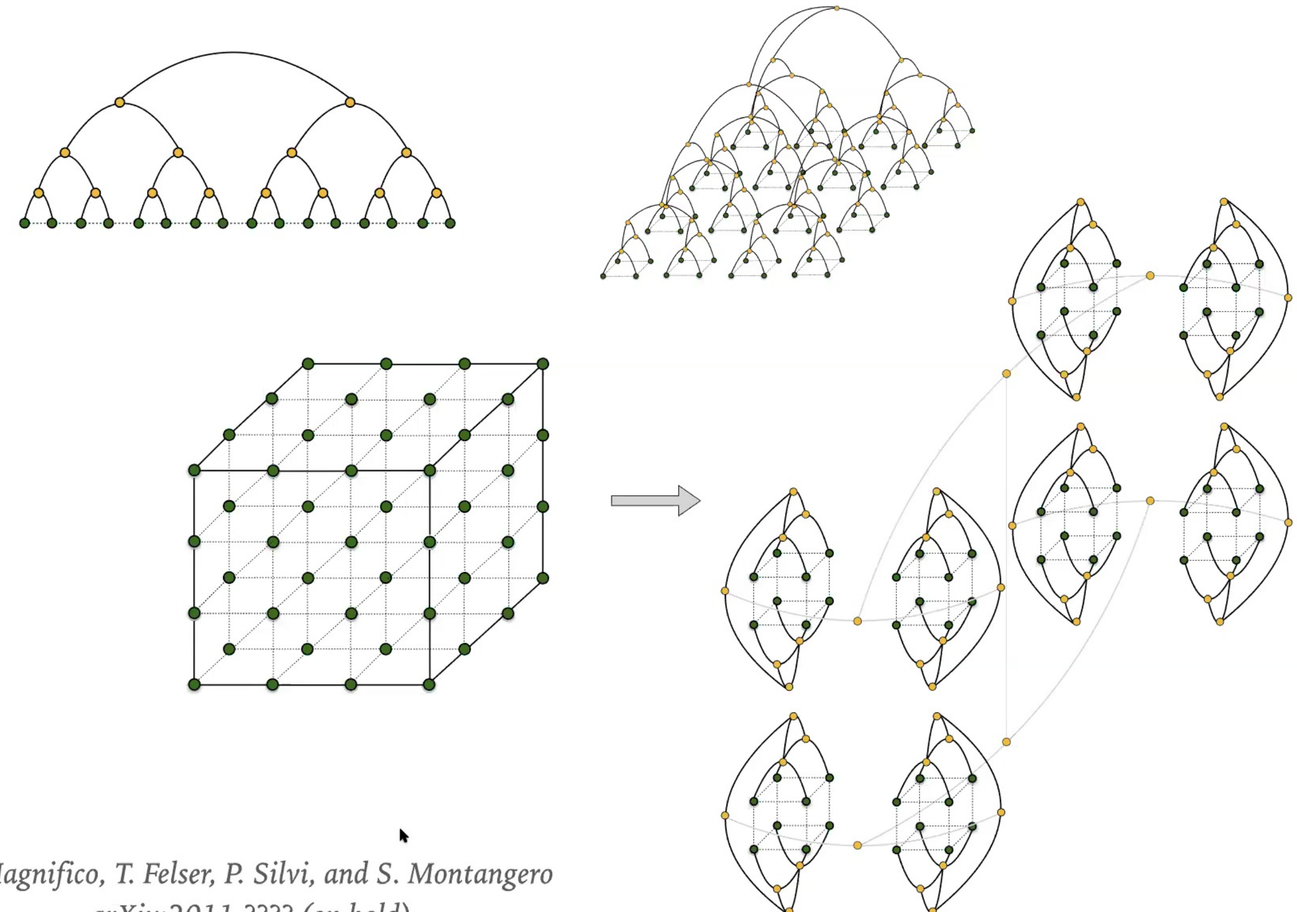
3D LATTICE GAUGE THEORIES

With tree tensor networks

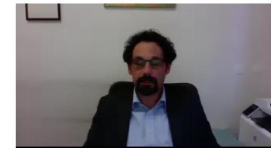


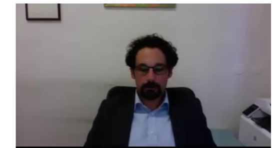


3D TREE TENSOR NETWORK



G. Magnifico, T. Felser, P. Silvi, and S. Montangero
arXiv:2011.???? (on hold)



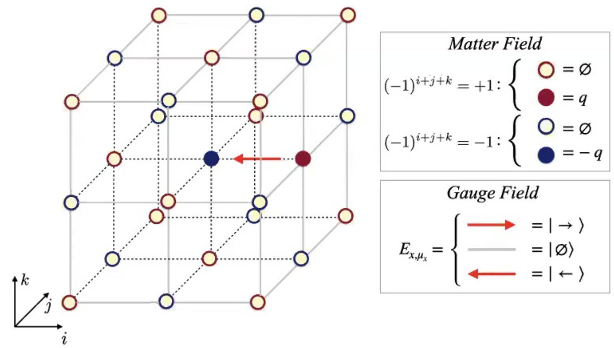


3D QUANTUM-LINK FORMULATION OF QED

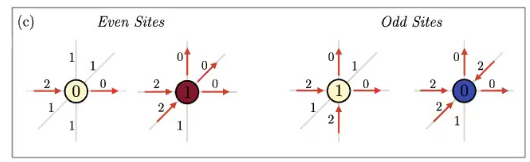
$$\hat{H} = -t \sum_{x,\mu} \left(\hat{\psi}_x^\dagger \, \hat{U}_{x,\mu} \, \hat{\psi}_{x+\mu} + \text{H.c.} \right)$$

$$+ m \sum_x (-1)^x \hat{\psi}_x^\dagger \hat{\psi}_x + \frac{g_e^2}{2} \sum_{x,\mu} \hat{E}_{x,\mu}^2$$

$$- \frac{g_m^2}{2} \sum_x \left(\square_{\mu_x,\mu_y} + \square_{\mu_x,\mu_z} + \square_{\mu_y,\mu_z} + \text{H.c.} \right)$$



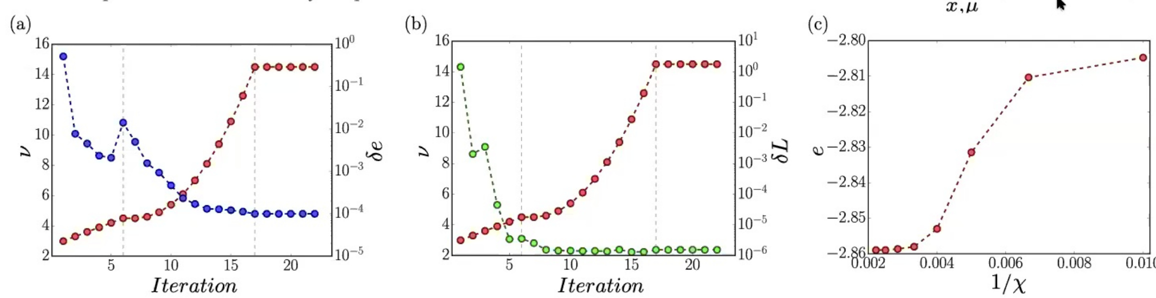
$$\hat{G}_x = \hat{\psi}_x^\dagger \hat{\psi}_x - \frac{1-(-1)^x}{2} - \sum_\mu \hat{E}_{x,\mu}$$



Local dimension 267, up to 12288 Hamiltonian operators

$$H_{pen} = \nu \sum_{x,\mu} \left(1 - \delta_{2,\hat{L}_{x,\mu}} \right)$$

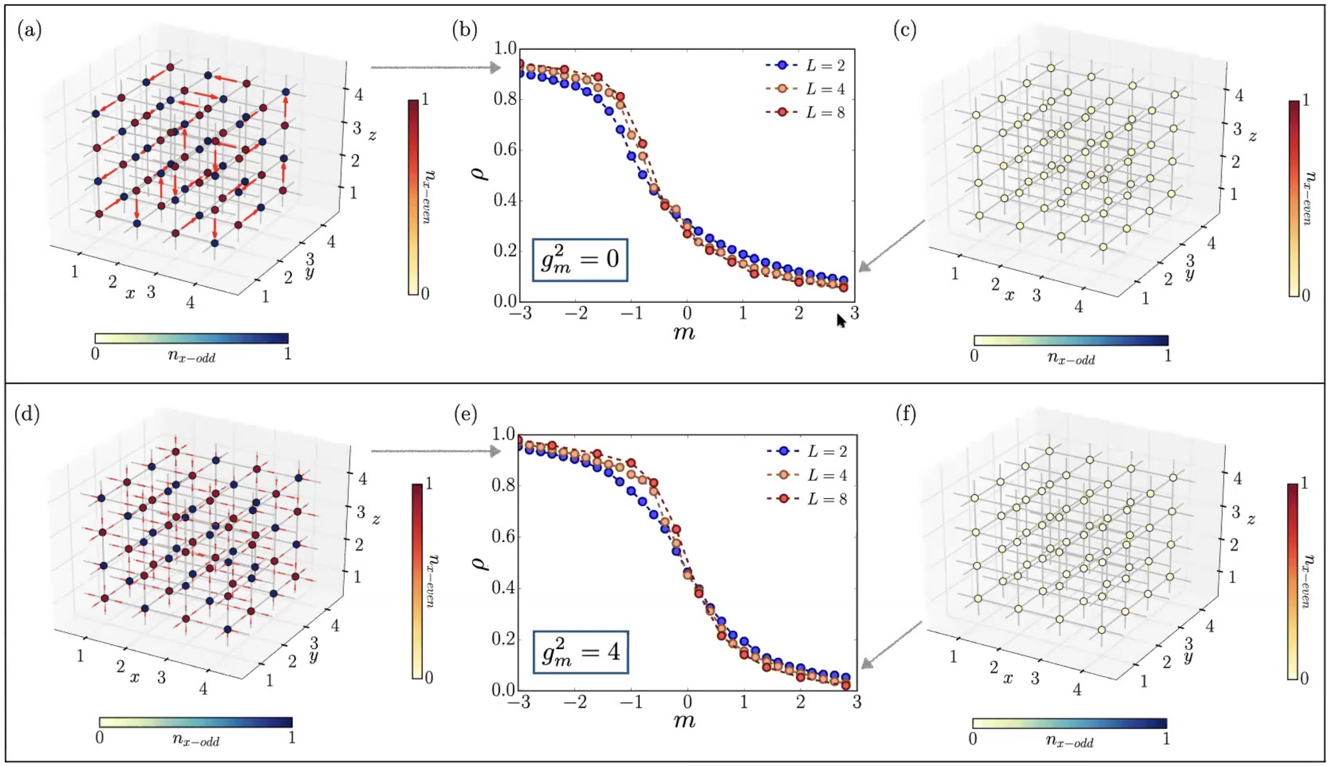
Up to 5 weeks x 64 cores of computational time



QUANTUM PHASES

Hilbert space of

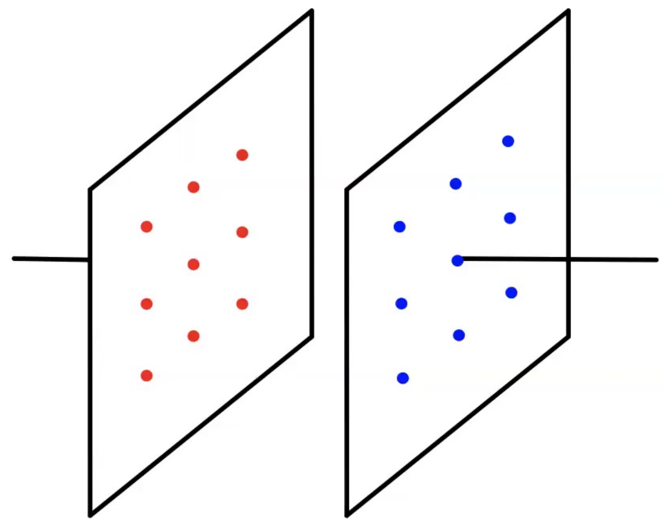
~64x64x64 qubits!



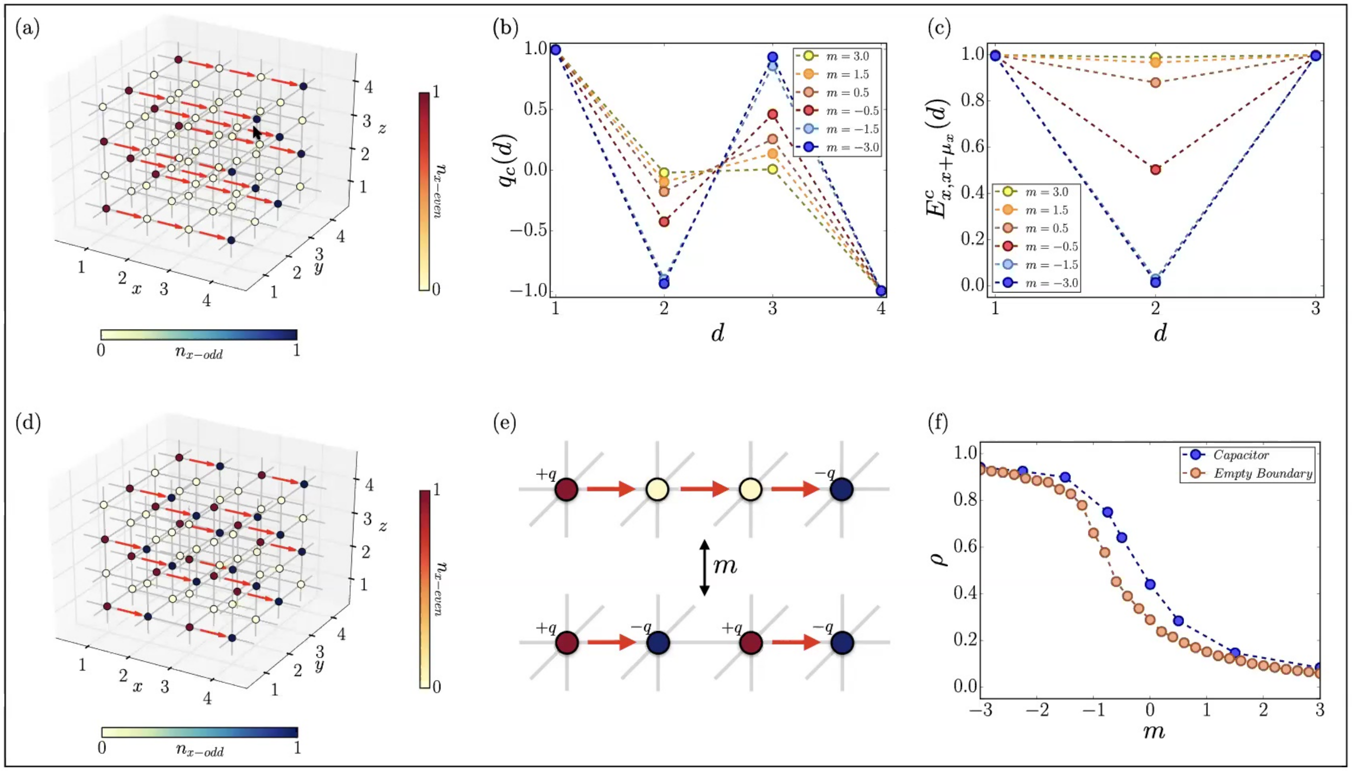
$m_c \approx +0.22$

$g_m^2 = 8/g_e^2$

SCREENING

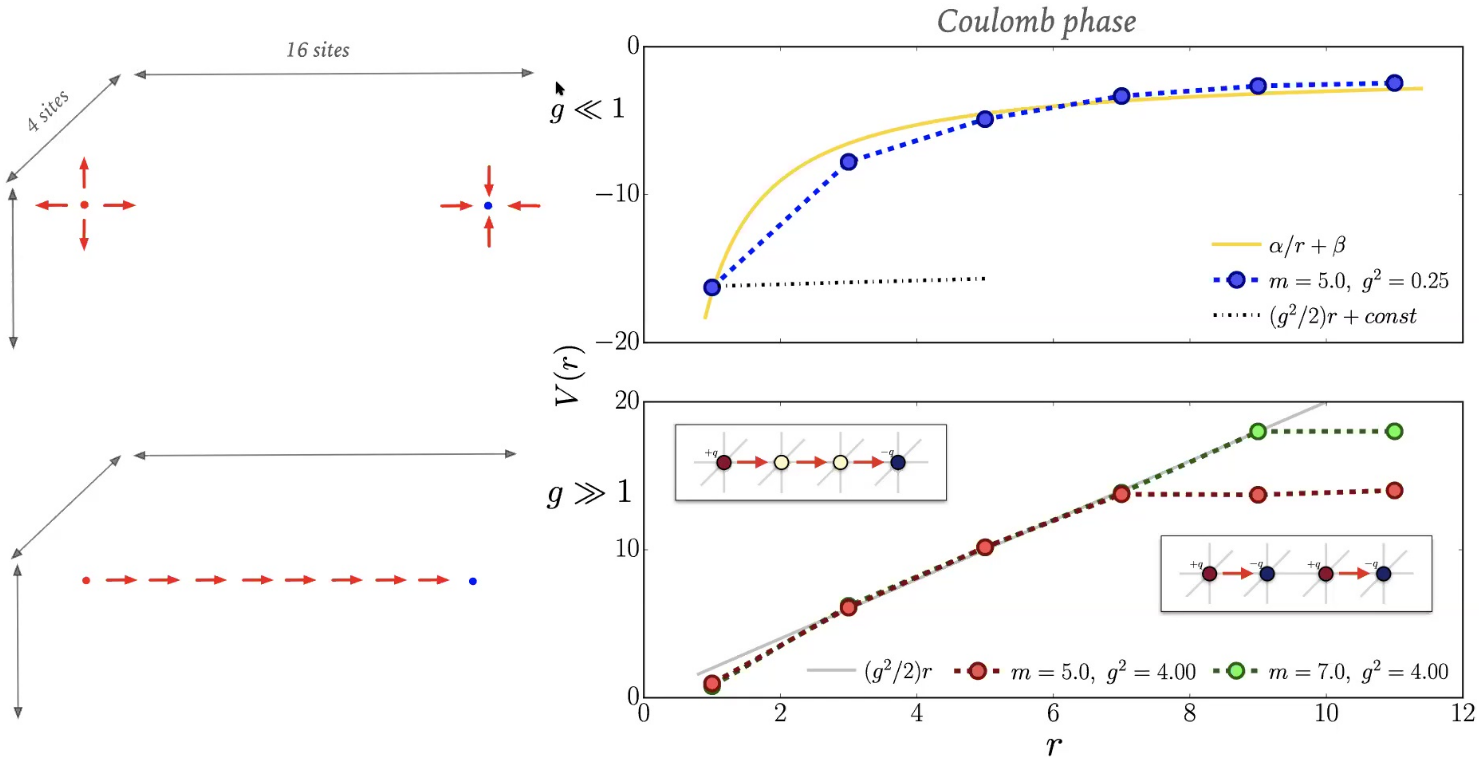


SCREENING



(a)
(b)
(c)
(d)
(e)
(f)
n_{x-even}
n_{x-odd}
$q_c(d)$
d
$m = 3.0$
$m = 1.5$
$m = 0.5$
$m = -0.5$
$m = -1.5$
$m = -3.0$
$E^c_{x,x+\mu_x}(d)$
$+q$
$-q$
m
ρ
Capacitor
Empty Boundary

CONFINEMENT



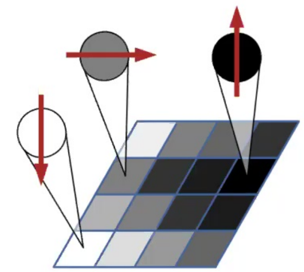
$g_e^2 = g^2/a,\ g_m^2 = 8/(g^2 a)$

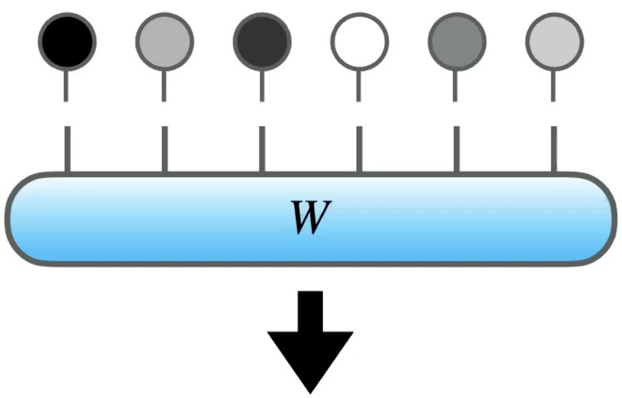
MACHINE LEARNING WITH TENSOR NETWORKS

Raw data

Map to "Spins"

$$\Phi(x_j) = \left[\cos\left(\frac{\pi}{2}x_j\right), \sin\left(\frac{\pi}{2}x_j\right)\right]$$



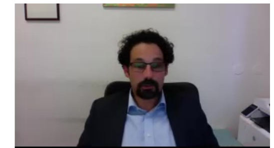


$$f^{\ell}(\bar{x}) = \sum_{\mathbf{s}} W^{\ell}_{s_1 s_2 \ldots s_N} \phi(x_1)^{s_1} \phi(x_2)^{s_2} \ldots \phi(x_N)^{s_N}$$

W : weight tensor

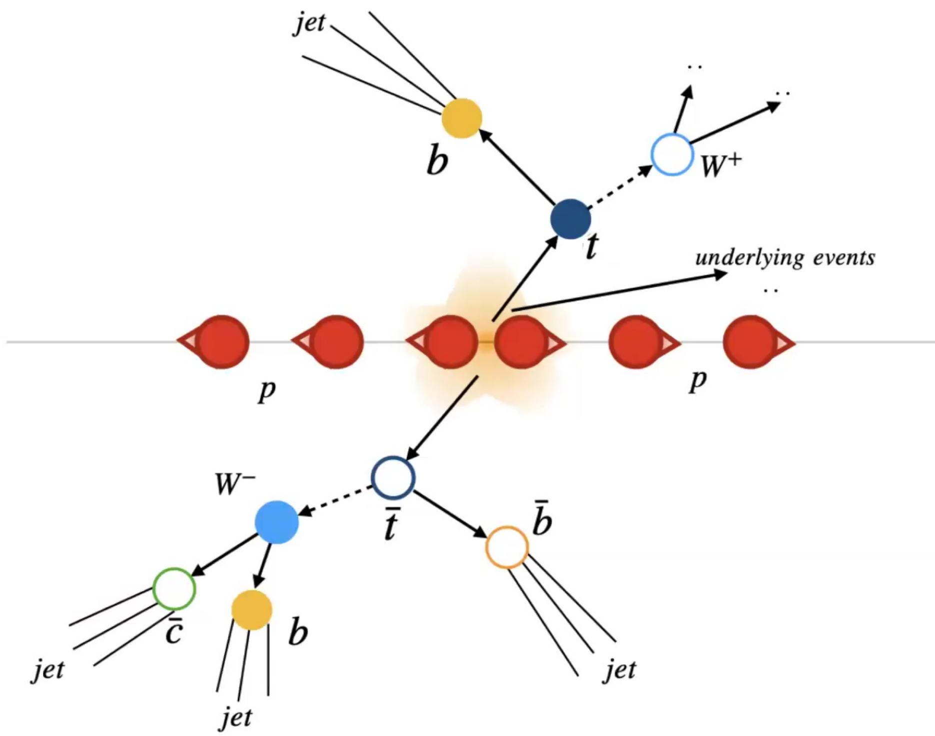
f(x) : decision function

Stoudenmire, Advances in Neural IPS 29, 4799 (2016), arXiv:1605.05775 [stat.ML]



P-P SCATTERING

Typical event in LHC



Quarks

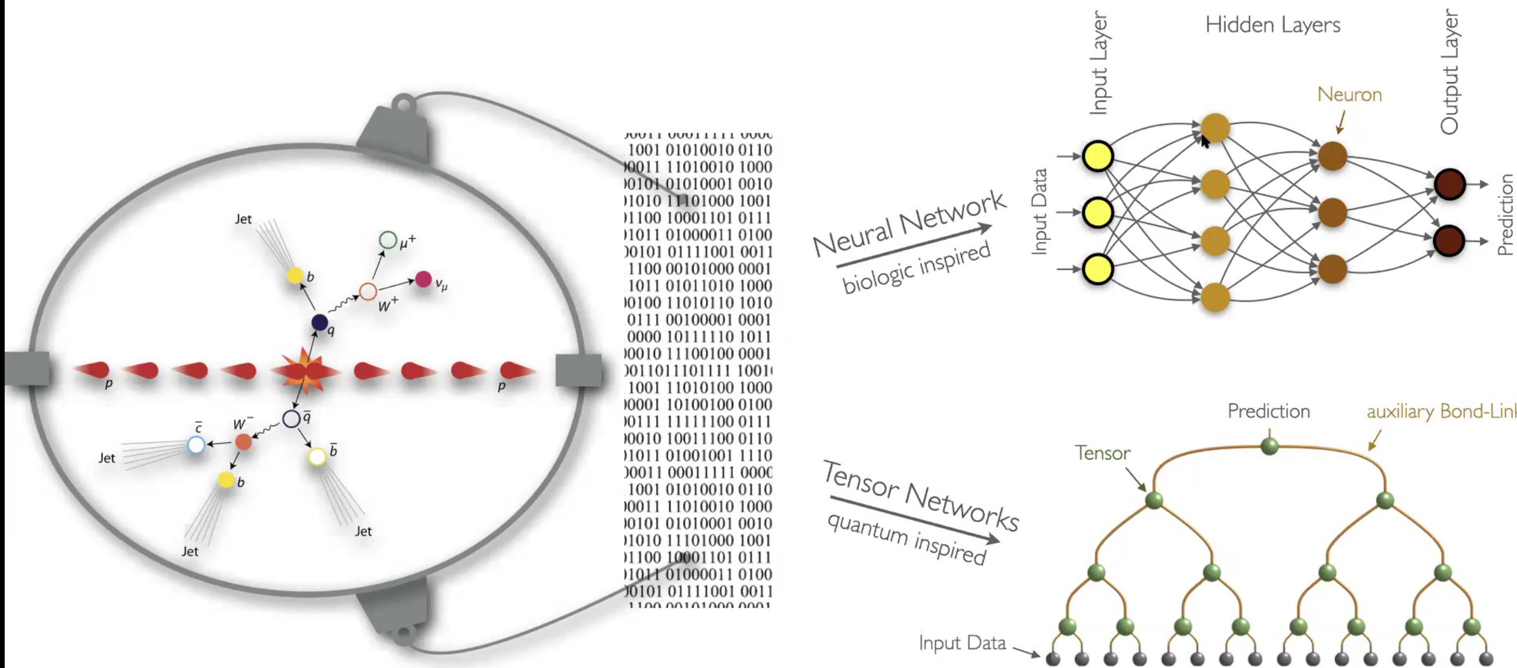
$$q \begin{cases} u \\ d \\ s \end{cases}$$

c

b

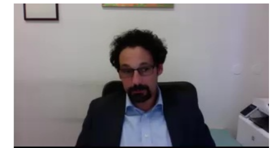
t

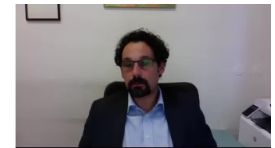
MACHINE LEARNING BASED CLASSIFICATION



In collaboration with A. Gianelle, D. Lucchesi, L. Sestini, D. Zuliani

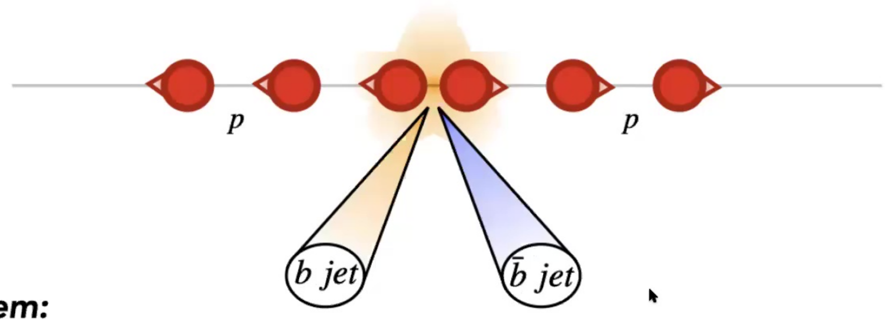
arXiv: 2004.13747





BINARY B BBAR CLASSIFICATION

This kind of events are used to measure **asymmetries** between the charge of b and $\bar{b}$.



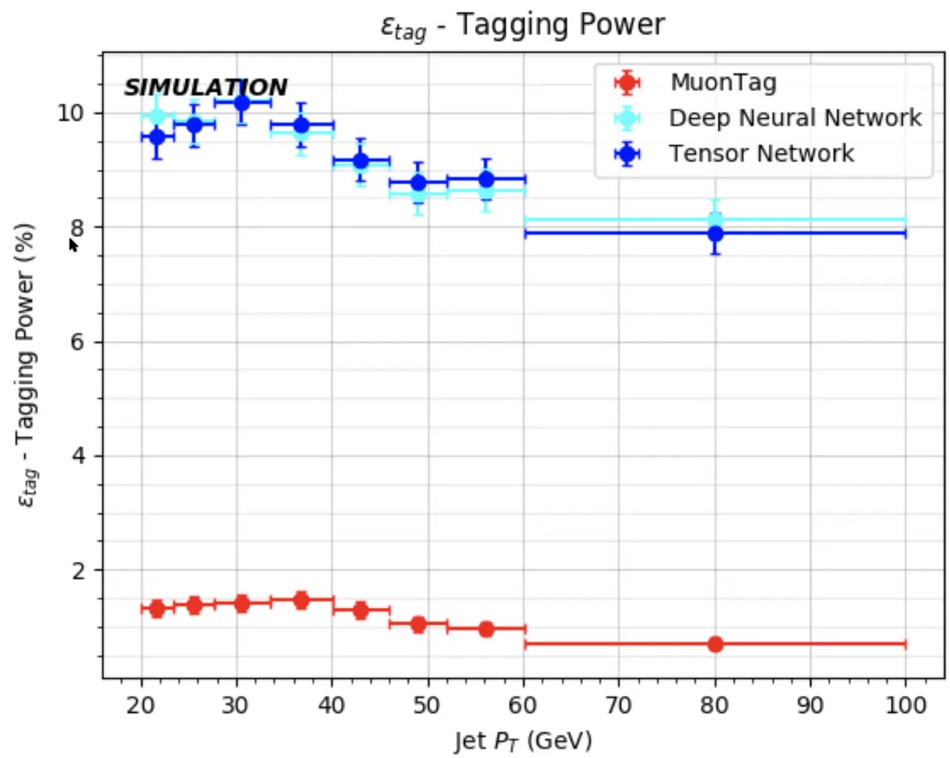
Easier problem:

- ***16 selected features (most physically relevant)***
- ***~10^6 data samples***

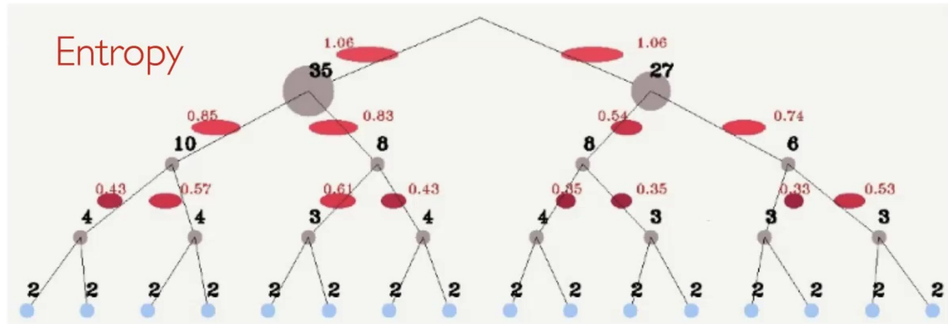
μ k π e p

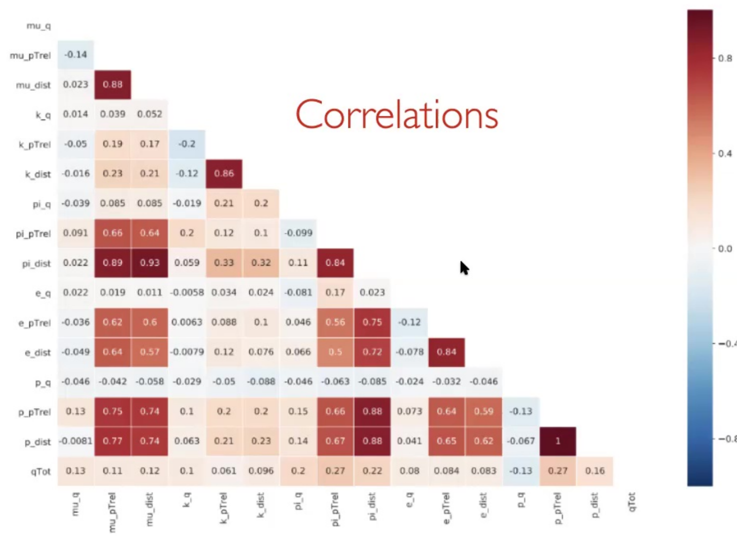
charge momenta direction

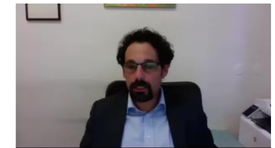
LHCB DATA ANALYSIS



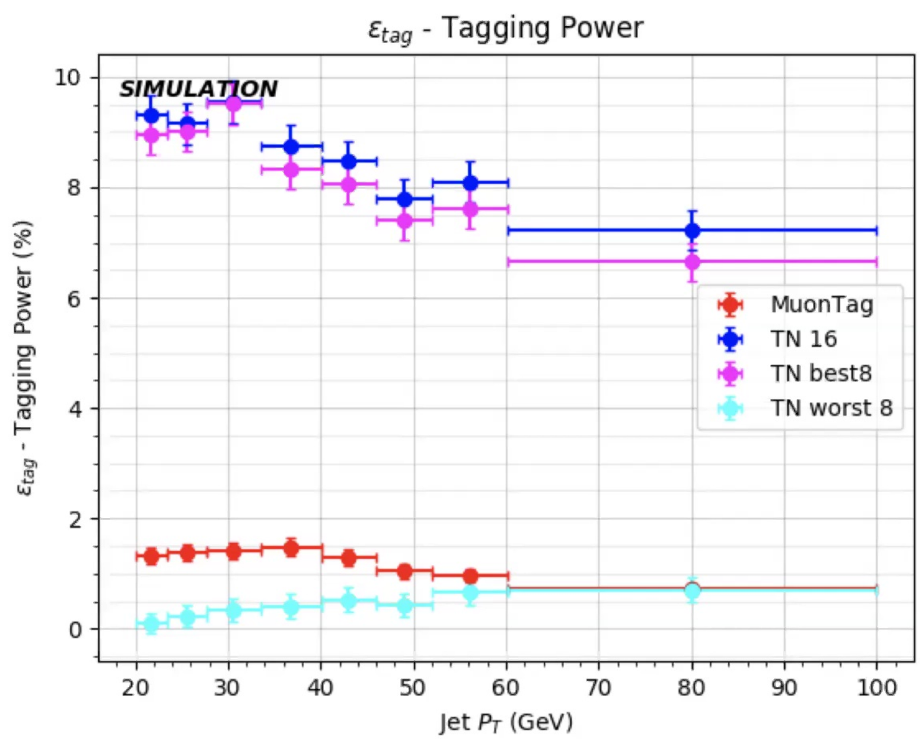
CORRELATIONS





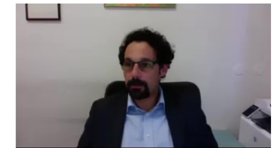


FINAL RESULT



- 4.7 times faster
- Only 0.4% less precise

TAKE HOME MESSAGES



- Tensor network algorithms can be used to benchmark, verify, support and guide quantum simulations/computations
- High-dimensional tensor network simulations are becoming available (PEPS, aTTN,…)
- Entanglement of mixed many-body states can be quantified
- Scalability to HPC is necessary to produce relevant results
- Interaction with HEP is becoming more and more relevant
- Interesting developments also in other directions (classical optimisers/annealers)
- Tensor network machine learning is competitive with DNN

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Ottocento anni di libertà e futuro

Thank you for your attention!

Simone Montangero
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Simone Notarnicola
Luca Arceci
Ferdinand Tschirsich
Timo Felser
Matthias Gerster
Phila Rembold
Marco Rossignolo
Marco Trenti
Marco Rigobello
Samuele Cavinato

Quantum Flagship · QuantERA · INFN · DFG Deutsche Forschungsgemeinschaft · QuSCo · PASQuanS · MIUR · QTFLAG · QuantHEP · Fondazione Cassa di Risparmio di Padova e Rovigo · Google · CINECA · bwGRiD

quantum.dfa.unipd.it

QuantHEP Seminar

ECT* Ph.D. School
Trento Summer 2021
https://indico.ectstar.eu/event/72/

Dipartimento di Fisica e Astronomia Galileo Galilei

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