Gaussian states for the variational study of (1+1)-dimensional lattice gauge models

arXiv:1805.05190

Stefan Kühn

PERIMETER INSTITUTE

in collaboration with

Pablo Sala	Technical University of Munich
Tao Shi	Chinese Academy of Science
Mari Carmen Bañuls	Max Planck Institute of Quantum Optics
Eugene Demler	Harvard University
J. Ignacio Cirac	Max Planck Institute of Quantum Optics

Motivation

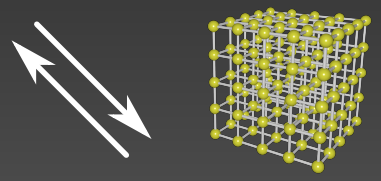
Lattice gauge theories

- Nonperturbative regime
- Analytical access hard

Motivation

Lattice gauge theories

- Nonperturbative regime
- Analytical access hard



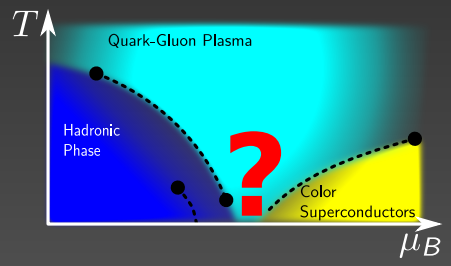
Classical simulation

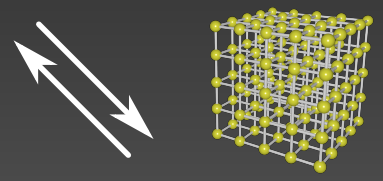
- Monte Carlo methods in euclidean space-time

Motivation

Lattice gauge theories

- Nonperturbative regime
- Analytical access hard





Classical simulation

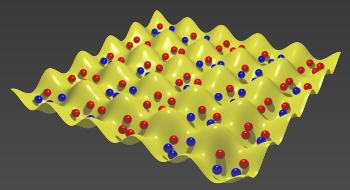
- Monte Carlo methods in euclidean space-time
  - No real-time dynamics
  - Sign problem

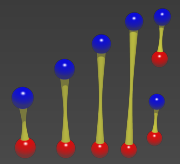
K. Fukushima, T. Hatsuda, Rep. Prog. Phys. 74, 014001 (2011)

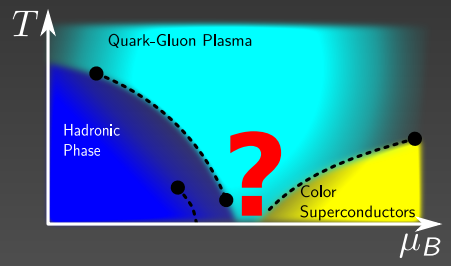
Motivation

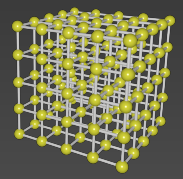
Lattice gauge theories

- Nonperturbative regime
- Analytical access hard









Quantum simulation

- Many promising experimental platforms
- Free from purely numerical limitations

Classical simulation

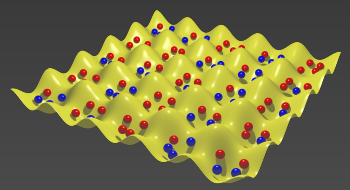
- Monte Carlo methods in euclidean space-time
  - No real-time dynamics
  - Sign problem

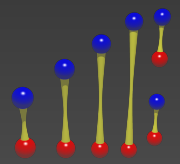
K. Fukushima, T. Hatsuda, Rep. Prog. Phys. 74, 014001 (2011)
E. A. Martinez et al., Nature (London) 534, 516 (2016)

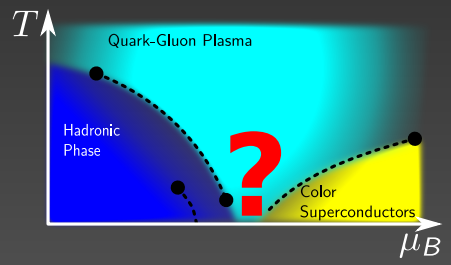
Motivation

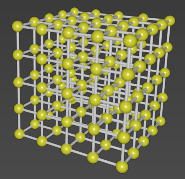
Lattice gauge theories

- Nonperturbative regime
- Analytical access hard









Quantum simulation

- Many promising experimental platforms
- Free from purely numerical limitations

Classical simulation

- Tensor Networks

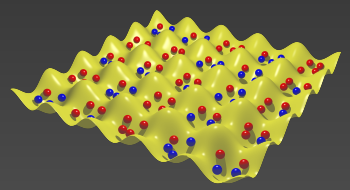
→ Plenary talk by Dr. Bañuls on Saturday

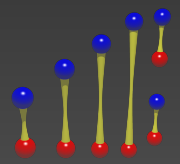
K. Fukushima, T. Hatsuda, Rep. Prog. Phys. 74, 014001 (2011)
E. A. Martinez et al., Nature (London) 534, 516 (2016)

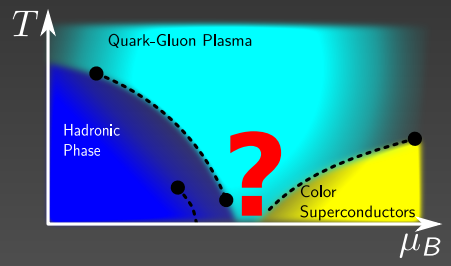
Motivation

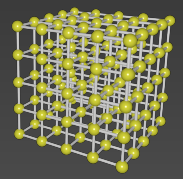
Lattice gauge theories

- Nonperturbative regime
- Analytical access hard









Quantum simulation

- Many promising experimental platforms
- Free from purely numerical limitations

Classical simulation

- Tensor Networks

→ Plenary talk by Dr. Bañuls on Saturday

- **Variational** ansatz based on **Gaussian states**

K. Fukushima, T. Hatsuda, Rep. Prog. Phys. 74, 014001 (2011)
E. A. Martinez et al., Nature (London) 534, 516 (2016)

Outline

2.

Hamiltonian lattice formulation

Lattice Hamiltonian formulation

- Kogut-Susskind staggered fermions in temporal gauge $A^0 = 0$

$$H = \varepsilon \sum_{n=1}^{N-1} \left(\phi_n^\dagger \, U_n \, \phi_{n+1} + \text{H.c.} \right) + m \sum_{n=1}^{N} (-1)^n \phi_n^\dagger \phi_n + \frac{g^2}{2} \sum_{n=1}^{N-1} L_n^2$$

Kinetic part + coupling to gauge field

Staggered mass term

(Color)-electric energy

J. Kogut and L. Susskind, Phys. Rev. D **11**, 395

Hamiltonian lattice formulation

Lattice Hamiltonian formulation

- Kogut-Susskind staggered fermions in temporal gauge $A^0 = 0$

$$H = \varepsilon \sum_{n=1}^{N-1} \left(\phi_n^\dagger \, U_n \, \phi_{n+1} + \text{H.c.} \right) + m \sum_{n=1}^{N} (-1)^n \phi_n^\dagger \phi_n + \frac{g^2}{2} \sum_{n=1}^{N-1} L_n^2$$

Kinetic part + coupling to gauge field — Staggered mass term — (Color)-electric energy

- Gauss law for physical states $G_n^a |\psi\rangle = 0$

$$G_n^a = L_n^a - R_{n-1}^a - \mathcal{Q}_n^a, \quad \mathcal{Q}_n = Q_n + q_n$$

dynamical charge — external charge

J. Kogut and L. Susskind, Phys. Rev. D 11, 395

Hamiltonian lattice formulation

Lattice Hamiltonian formulation

- Kogut-Susskind staggered fermions in temporal gauge $A^0 = 0$

$$H = \varepsilon \sum_{n=1}^{N-1} \left(\phi_n^\dagger \, U_n \, \phi_{n+1} + \text{H.c.} \right) + m \sum_{n=1}^{N} (-1)^n \phi_n^\dagger \phi_n + \frac{g^2}{2} \sum_{n=1}^{N-1} \boldsymbol{L}_n^2$$

Kinetic part + coupling to gauge field — Staggered mass term — (Color)-electric energy

- Gauss law for physical states $G_n^a |\psi\rangle = 0$

$$G_n^a = L_n^a - R_{n-1}^a - \mathcal{Q}_n^a, \quad \boldsymbol{\mathcal{Q}}_n = \boldsymbol{Q}_n + \boldsymbol{q}_n$$

U(1), Schwinger model

- ▷ Single component fermionic field: ϕ_n
- ▷ $Q_n = \phi_n^\dagger \phi_n - \frac{1}{2}(1 - (-1)^n)$
- ▷ $q_n \in \mathbb{R}$

SU(2)

- ▷ Two colors of fermions: $\phi_n^\dagger = (\phi_n^{r,\dagger}, \phi_n^{g,\dagger})$
- ▷ $Q_n^a = \frac{1}{2} \phi_n^\dagger \sigma^a \phi_n$
- ▷ $q_n^a = \frac{1}{2} \sigma^a$

J. Kogut and L. Susskind, Phys. Rev. D 11, 395

Hamiltonian lattice formulation

Disentangling the gauge field

- Transformation disentangling the gauge degrees of freedom

$$\Theta = \prod_{k=1}^{\rightarrow} \exp\left(i\theta_k^a \sum_{m>k} \mathcal{Q}_m^a\right)$$

- Hamiltonian in the rotated frame $H_\Theta = \Theta H \Theta^\dagger$

$$H_\Theta = \varepsilon \sum_n \left(\phi_n^\dagger \phi_{n+1} + \text{H.c.}\right) + m \sum_n (-1)^n \phi_n^\dagger \phi_n + \sum_a \sum_{n,m} \mathcal{Q}_n^a V_{n,m} \mathcal{Q}_m^a$$

- In the sector of vanishing total charge $\sum_n \mathcal{Q}_n = 0$

$$V_{n,m} = -\frac{1}{2}|n-m|$$

- H_Θ depends only on the fermionic content and is nonlocal

F. Lenz, H.W.L. Naus, M. Thies, Ann. Phys. 233, 317 (1994)
B. Bringoltz, Phys. Rev. D 79, 105021 (2009)

3.

Variational ansatz

Variational ansatz

- Pure Gaussian state

$$|\mathrm{GS}\rangle = C \times \exp\left(-\frac{1}{2}\Phi^\dagger \xi \Phi\right)|\Omega\rangle$$

with $\Phi^\dagger = (\phi_1^\dagger, \ldots, \phi_M^\dagger, \phi_1, \ldots, \phi_M)$
$\phi_j |\Omega\rangle = 0$, ξ hermitian $2M \times 2M$ matrix

- Characterized by its covariance matrix

$$\Gamma = \left\langle \Phi\Phi^\dagger \right\rangle$$

- Variational ansatz in the original frame

$$|\psi\rangle = \Theta^\dagger |\mathrm{GS}\rangle |0\rangle_{\mathrm{gauge}}$$

$\Rightarrow$ Non-Gaussian ansatz

S. Bravyi, arXiv:quant-ph/0507282 (2005)
S. Bravyi, Quantum Inf. and Comp. 5, 216 (2005)
C. Weedbrook et al., Rev. Mod. Phys. 84, 621 (2012)
C. V. Kraus, M. M. Wolf, J. I. Cirac, G. Giedke, Phys. Rev. A 79, 012306 (2009)

Variational ansatz

Variational ansatz

- Pure Gaussian state

$$|\mathrm{GS}\rangle = C \times \exp\left(-\frac{1}{2}\Phi^\dagger \xi \Phi\right)|\Omega\rangle$$

with $\Phi^\dagger = (\phi_1^\dagger, \ldots, \phi_M^\dagger, \phi_1, \ldots, \phi_M)$
$\phi_j |\Omega\rangle = 0$, ξ hermitian $2M \times 2M$ matrix

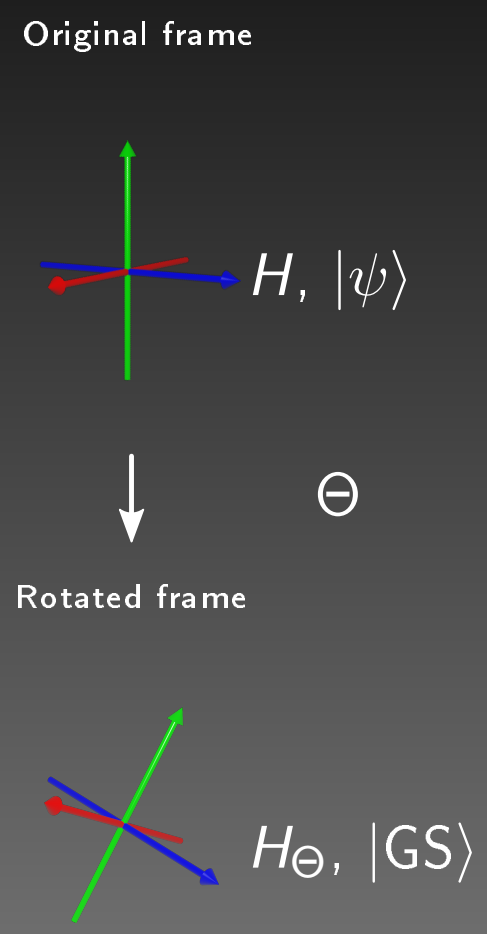
- Characterized by its covariance matrix

$$\Gamma = \left\langle \Phi\Phi^\dagger \right\rangle$$

- Variational ansatz in the original frame

$$|\psi\rangle = \Theta^\dagger |\mathrm{GS}\rangle |0\rangle_{\mathrm{gauge}}$$

$\Rightarrow$ Non-Gaussian ansatz

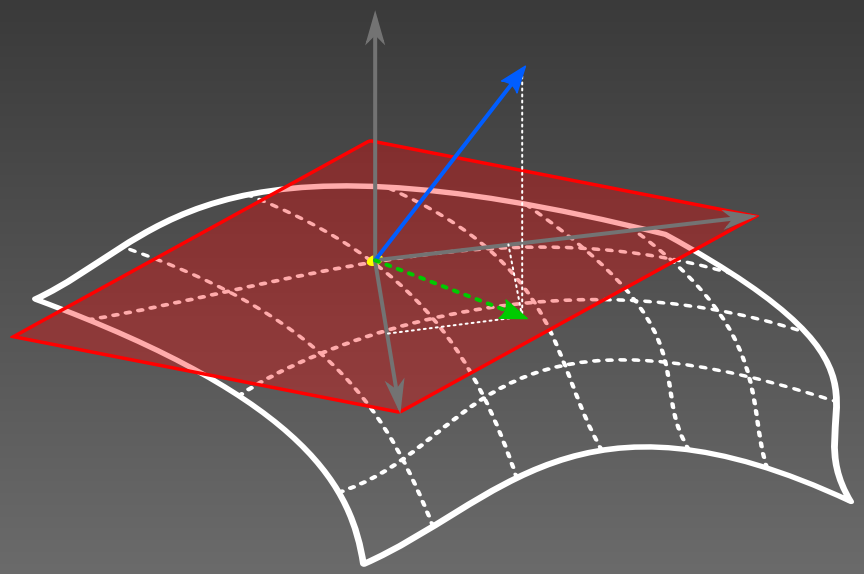


S. Bravyi, arXiv:quant-ph/0507282 (2005)
S. Bravyi, Quantum Inf. and Comp. 5, 216 (2005)
C. Weedbrook et al., Rev. Mod. Phys. 84, 621 (2012)
C. V. Kraus, M. M. Wolf, J. I. Cirac, G. Giedke, Phys. Rev. A 79, 012306 (2009)

Variational ansatz

Time-dependent variational principle

- Compute the evolution of a given initial Gaussian state under $H_\ominus$ in the manifold of Gaussian states

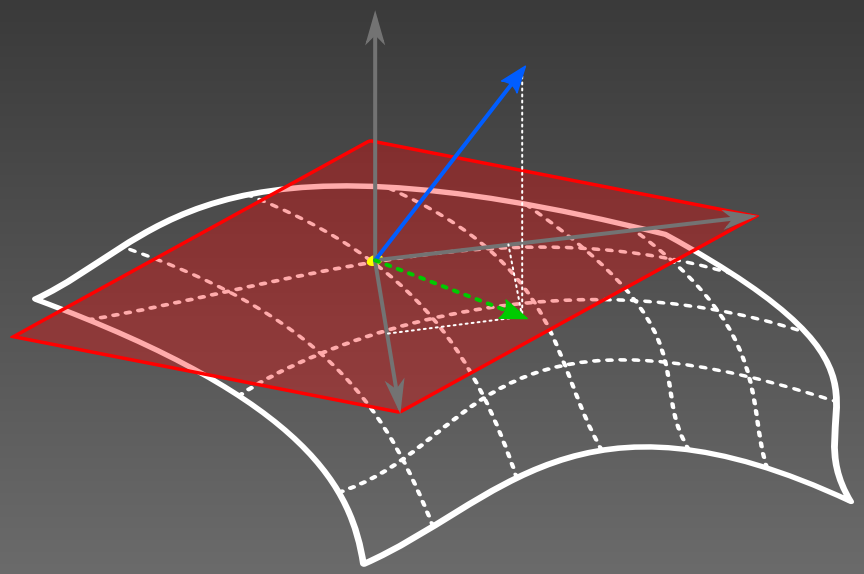


T. Shi, E. Demler, J. I. Cirac, Ann. Phys. 390, 245 (2018)

Variational ansatz

Time-dependent variational principle

- Compute the evolution of a given initial Gaussian state under H_Θ in the manifold of Gaussian states
- Time-dependent variational principle applied to Gaussian states yields



▷ Imaginary-time evolution:

$$\frac{d}{d\tau}\Gamma(\tau) = \{\Gamma, \mathcal{H}(\Gamma)\} - 2\Gamma\ \mathcal{H}(\Gamma)\Gamma$$

▷ Real-time evolution:

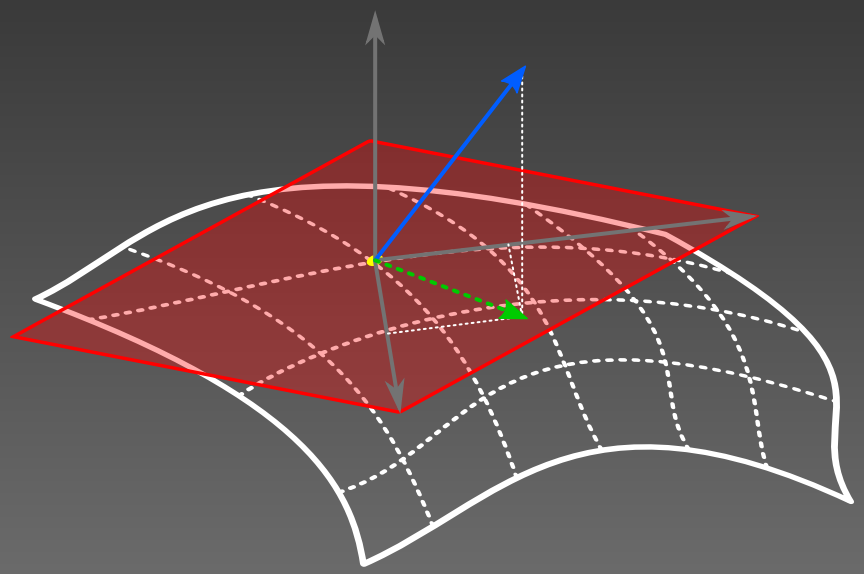
$$i\frac{d}{dt}\Gamma(t) = [\mathcal{H}(\Gamma), \Gamma]$$

T. Shi, E. Demler, J. I. Cirac, Ann. Phys. 390, 245 (2018)

Variational ansatz

Time-dependent variational principle

- Compute the evolution of a given initial Gaussian state under $H_\ominus$ in the manifold of Gaussian states
- Time-dependent variational principle applied to Gaussian states yields



▷ Imaginary-time evolution:

$$\frac{d}{d\tau}\Gamma(\tau) = \{\Gamma, \mathcal{H}(\Gamma)\} - 2\Gamma\ \mathcal{H}(\Gamma)\Gamma$$

▷ Real-time evolution:

$$i\frac{d}{dt}\Gamma(t) = [\mathcal{H}(\Gamma), \Gamma]$$

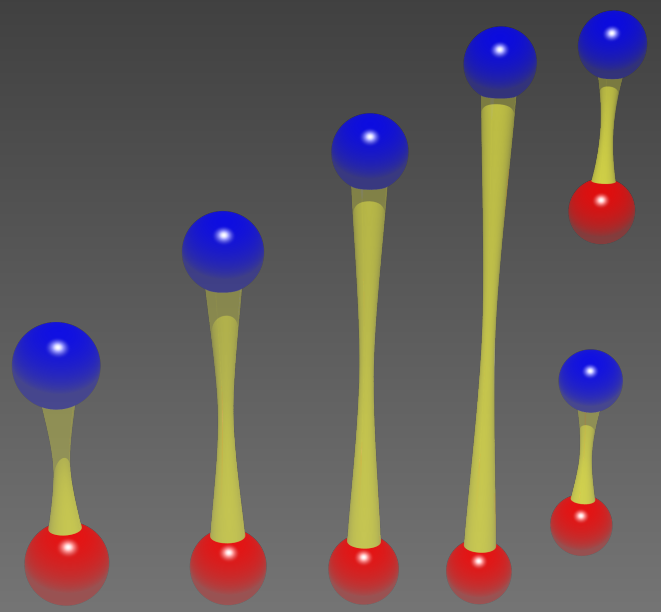
$\Rightarrow$ Allows us to compute ground states/real-time dynamics

- From Γ we can efficiently obtain averages of (local) observables

T. Shi, E. Demler, J. I. Cirac, Ann. Phys. 390, 245 (2018)

4.

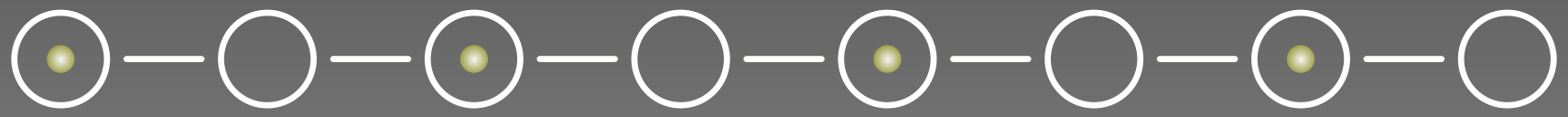
String breaking in the Schwinger model



Results: Schwinger model

Static potential

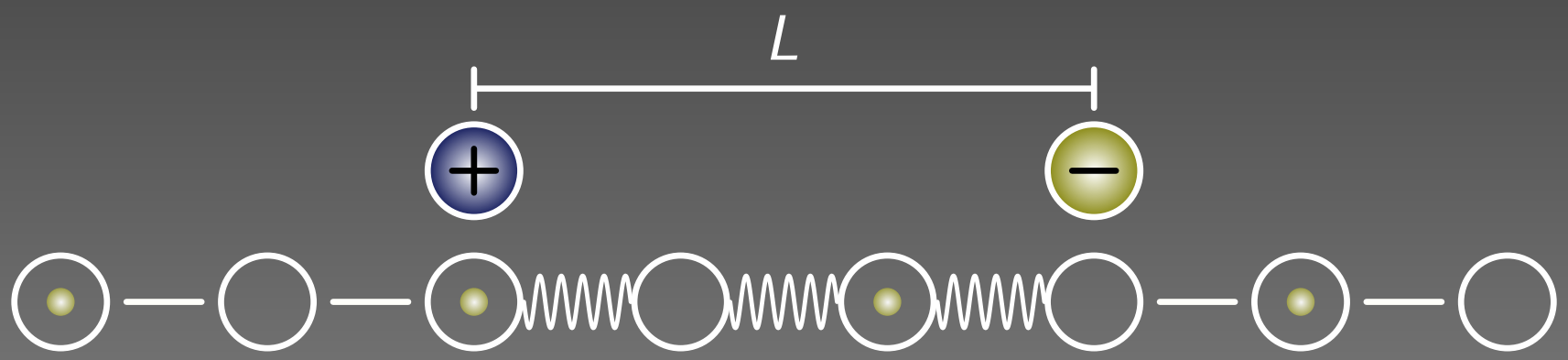
- Start from the strong-coupling vacuum



Results: Schwinger model

Static potential

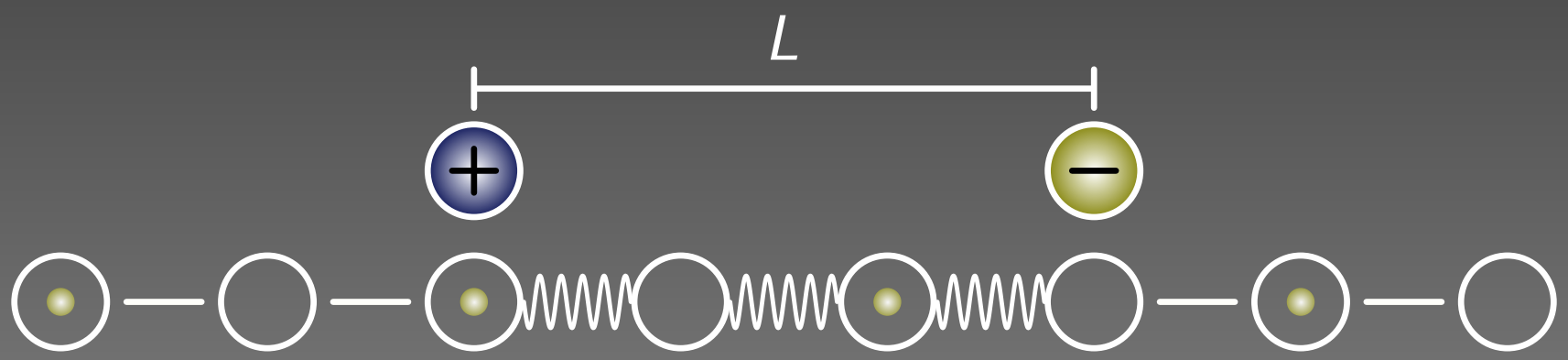
- Start from the strong-coupling vacuum
- Impose a flux string between static external charges separated by a length L on top
- Evolve in imaginary time and determine the ground-state energy $E_Q(L)$



Results: Schwinger model

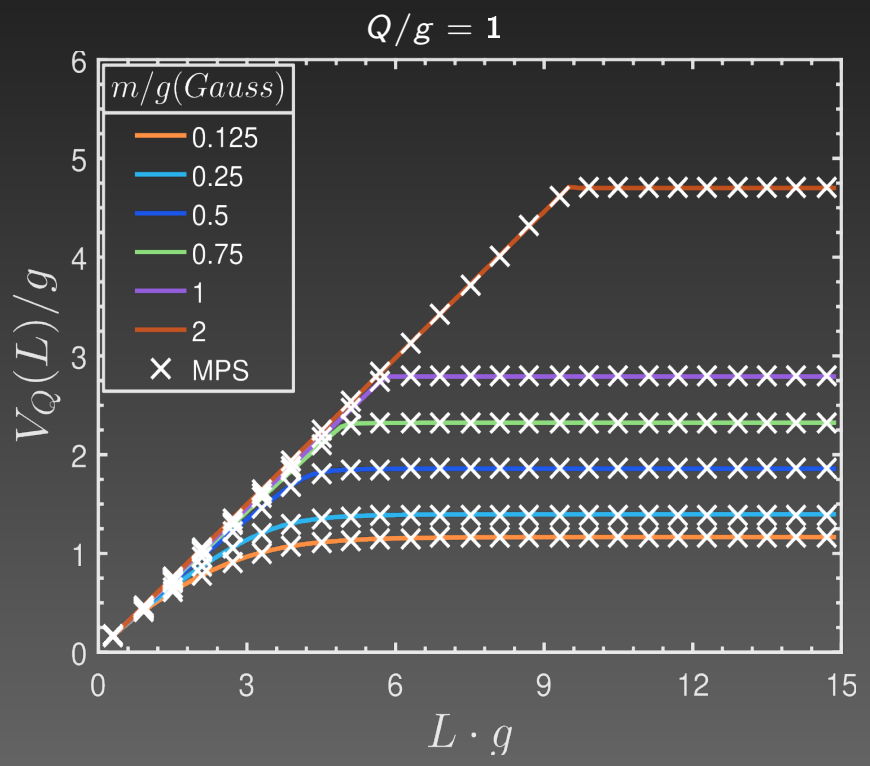
Static potential

- Start from the strong-coupling vacuum
- Impose a flux string between static external charges separated by a length L on top
- Evolve in imaginary time and determine the ground-state energy $E_Q(L)$
- Measure the static potential $V_Q(L) = E_Q(L) - E_{\text{vac}}$



Results: Schwinger model

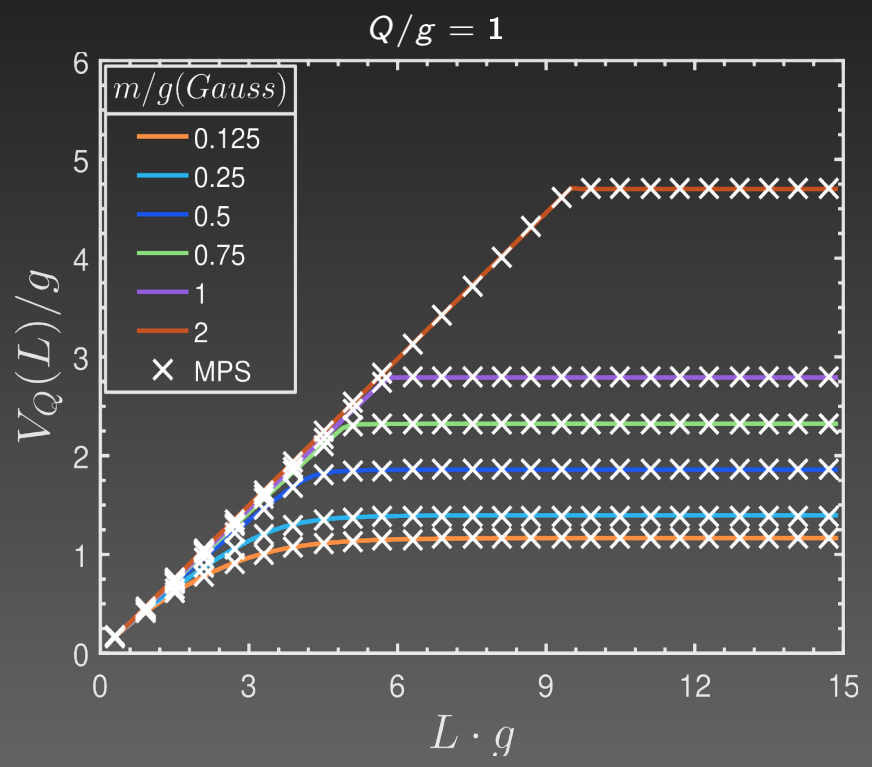
Static potential

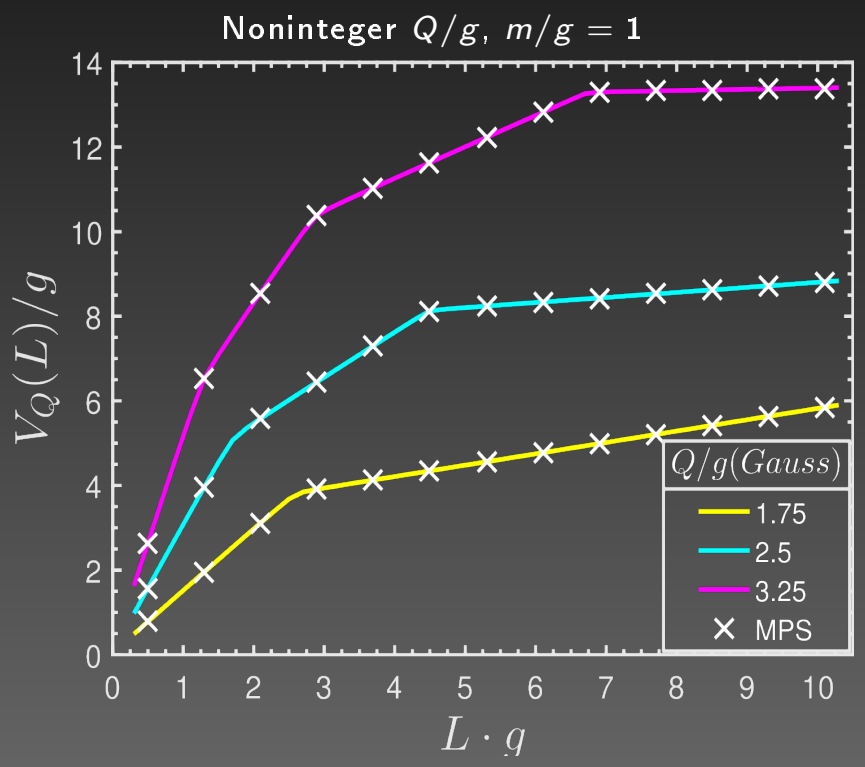


B. Buyens, J. Haegeman, H. Verschelde. F. Verstraete, K. Van Acoleyen. Phys. Rev. X 6, 041040 (2016)

Results: Schwinger model

Static potential





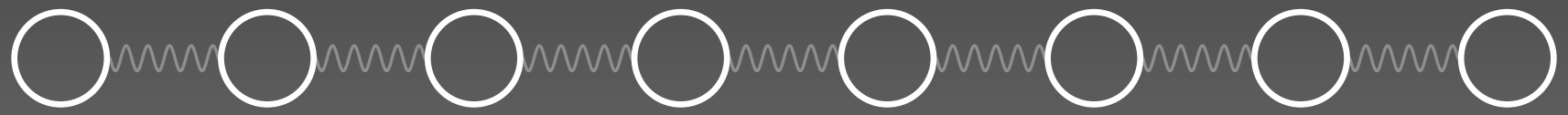
$\Rightarrow$ Excellent agreement with results from Tensor Network calculations

B. Buyens, J. Haegeman, H. Verschelde. F. Verstraete, K. Van Acoleyen. Phys. Rev. X 6, 041040 (2016)

Results: Schwinger model

Out-of-equilibrium dynamics

- Compute the interacting vacuum of the theory or start on the strong-coupling vacuum



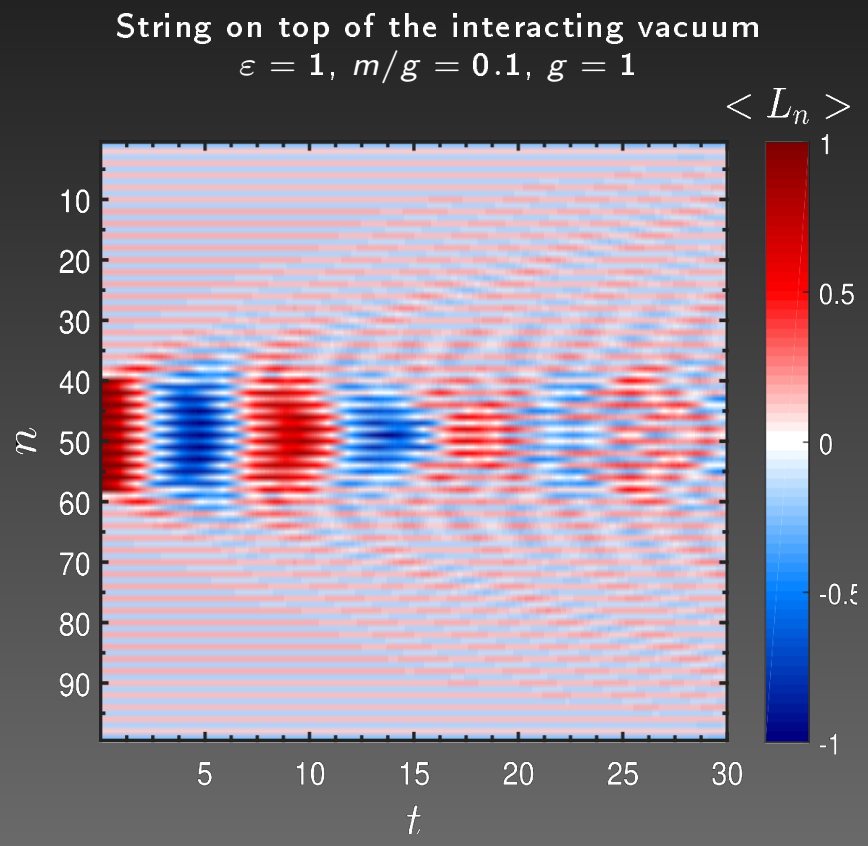
Results: Schwinger model

Out-of-equilibrium dynamics

- Compute the interacting vacuum of the theory or start on the strong-coupling vacuum
- Impose a flux string of length L on top
- Evolve in real time and monitor the site resolved average electric field $\langle L_n^2 \rangle$

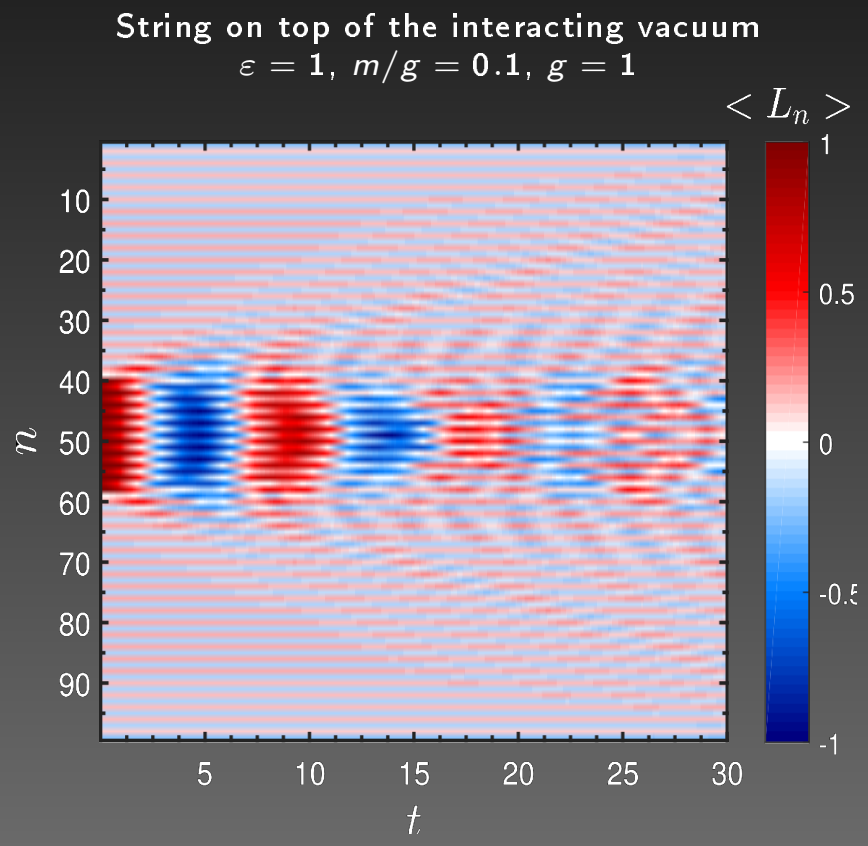
Results: Schwinger model

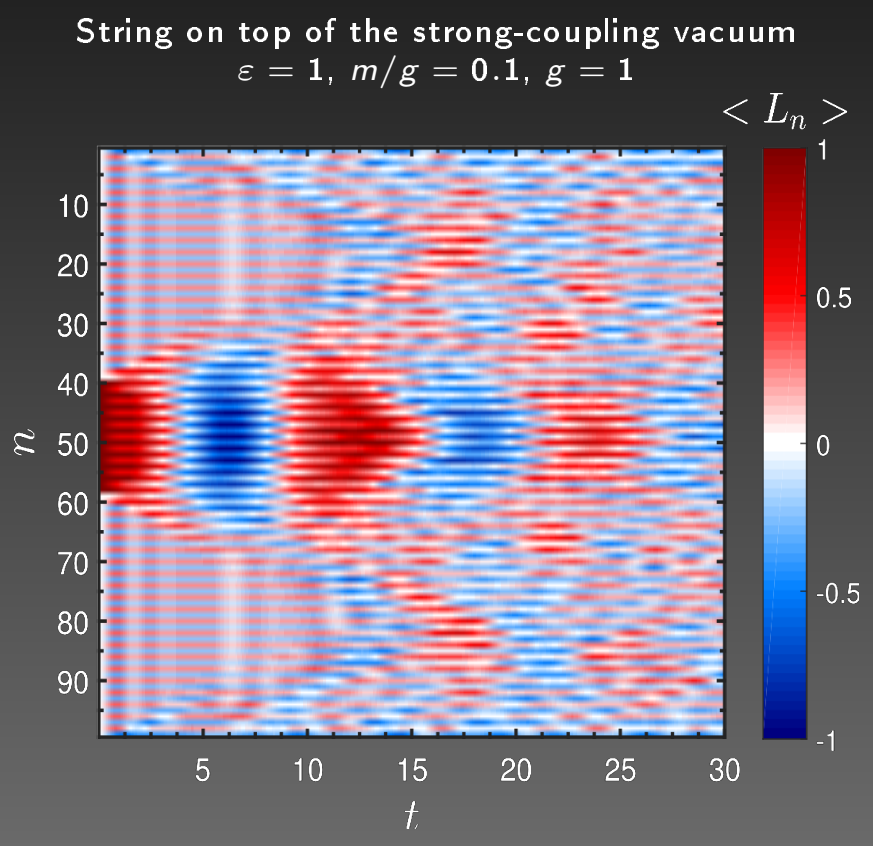
Out-of-equilibrium dynamics



Results: Schwinger model

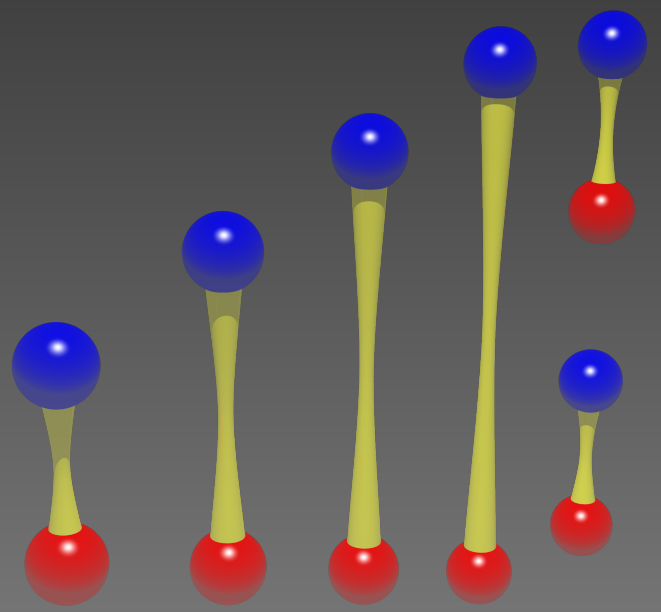
Out-of-equilibrium dynamics





$\Rightarrow$ Reliable simulations even in the situation of a global quench

String breaking in a SU(2) lattice gauge theory



Results: SU(2) lattice gauge theory

Static potential

- External charges are described by $q^a = \frac{1}{2}\sigma^a$
  $\Rightarrow$ Gauge invariant color-neutral state is not a Gaussian state
- Parity symmetries of H_Θ allow for finding unitary transformations V_1 and V_2 which decouple the external charges

$$\overline{H}_\Theta(s_1, s_2) = V_2 V_1 H_\Theta V_1^\dagger V_2^\dagger$$

Results: SU(2) lattice gauge theory

Static potential

- External charges are described by $q^a = \frac{1}{2}\sigma^a$
  $\Rightarrow$ Gauge invariant color-neutral state is not a Gaussian state
- Parity symmetries of H_Θ allow for finding unitary transformations V_1 and V_2 which decouple the external charges

$$\overline{H}_\Theta(s_1, s_2) = V_2 V_1 H_\Theta V_1^\dagger V_2^\dagger$$

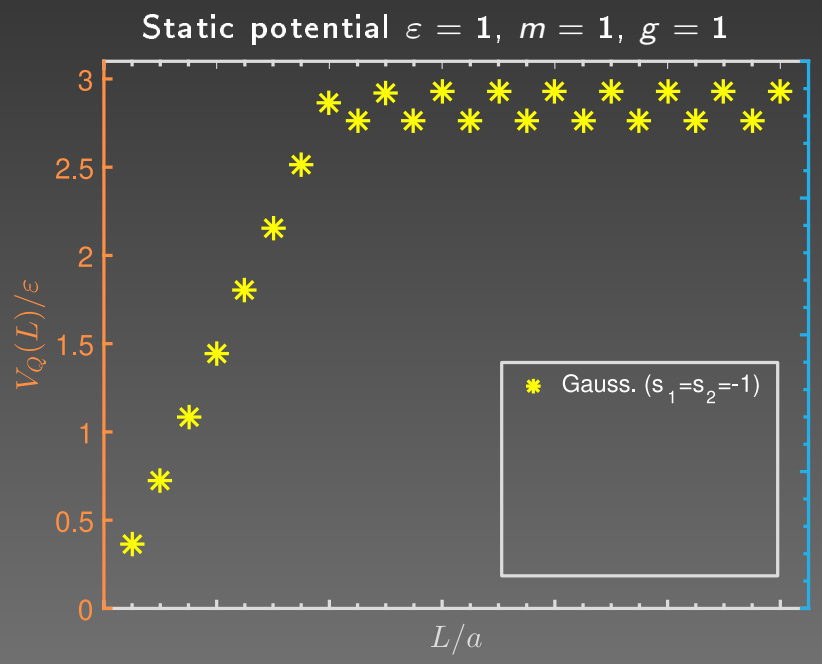
- $s_1, s_2 \in \{-1, 1\}$: Eigenvalues of the parity operators in the rotated frame
- Gauge invariant correlation function to characterize the entanglement between the static external charges

$$C_2(n_1, n_2) = \sum_{a,b} \left\langle q^a_{n_1} \left(U^{\mathrm{Adj.},\dagger}_{n_1} \cdots U^{\mathrm{Adj.},\dagger}_{n_2-1} \right)_{a,b} q^b_{n_2} \right\rangle$$

Results: SU(2) lattice gauge theory

Static potential

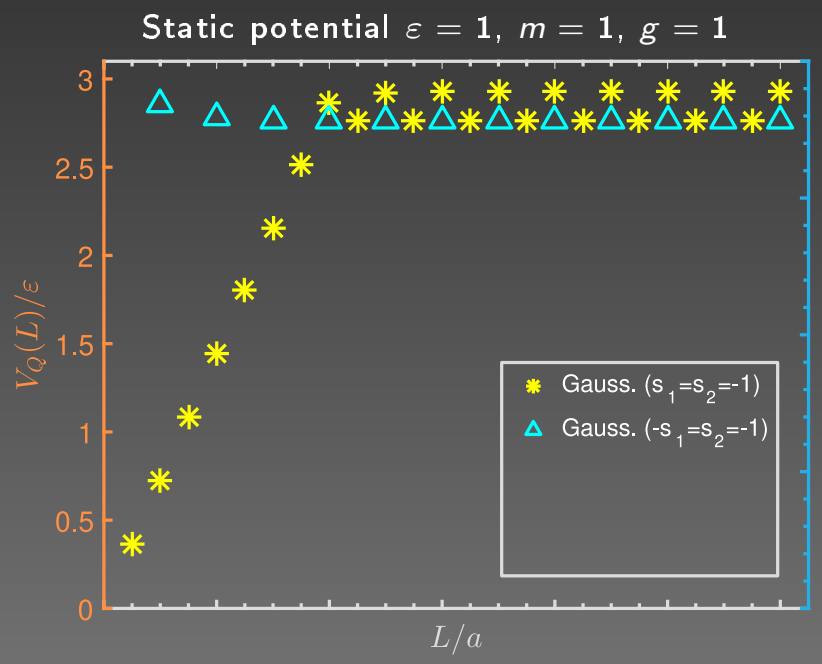
- Analogous to the U(1) case start with the strong-coupling vacuum
- Impose a color-flux string of length L on top
- Compute the ground state via imaginary time evolution



Results: SU(2) lattice gauge theory

Static potential

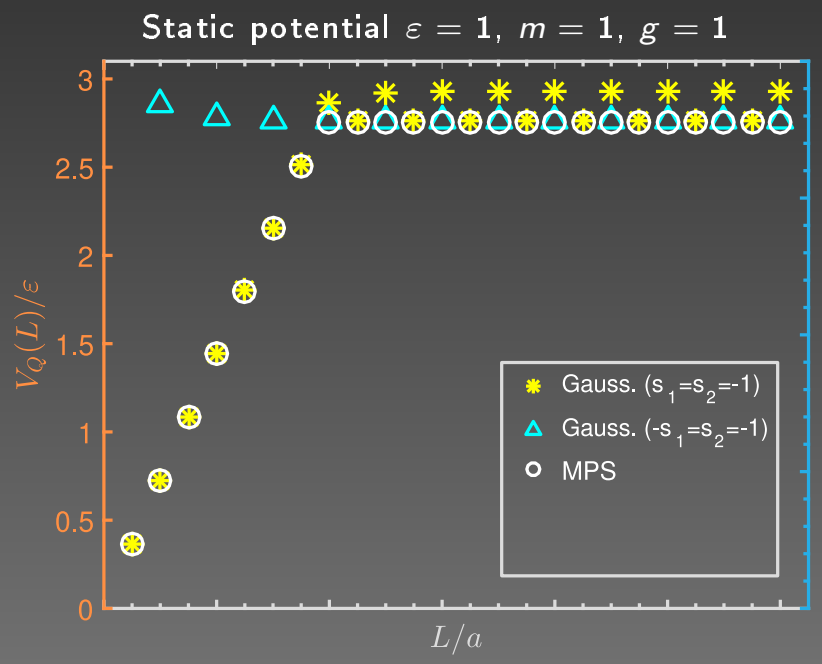
- Analogous to the U(1) case start with the strong-coupling vacuum
- Impose a color-flux string of length L on top
- Compute the ground state via imaginary time evolution



Results: SU(2) lattice gauge theory

Static potential

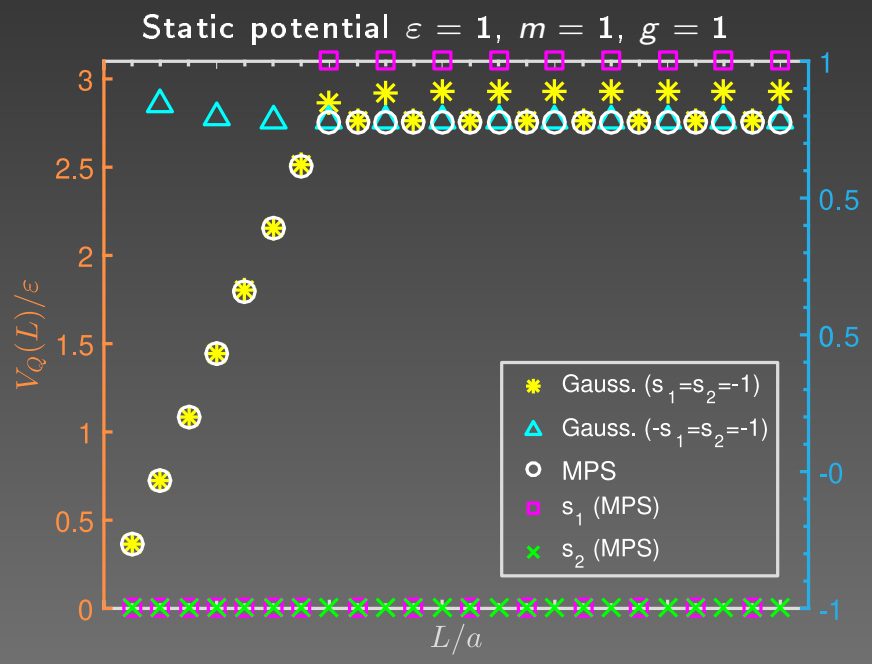
- Analogous to the U(1) case start with the strong-coupling vacuum
- Impose a color-flux string of length L on top
- Compute the ground state via imaginary time evolution



Results: SU(2) lattice gauge theory

Static potential

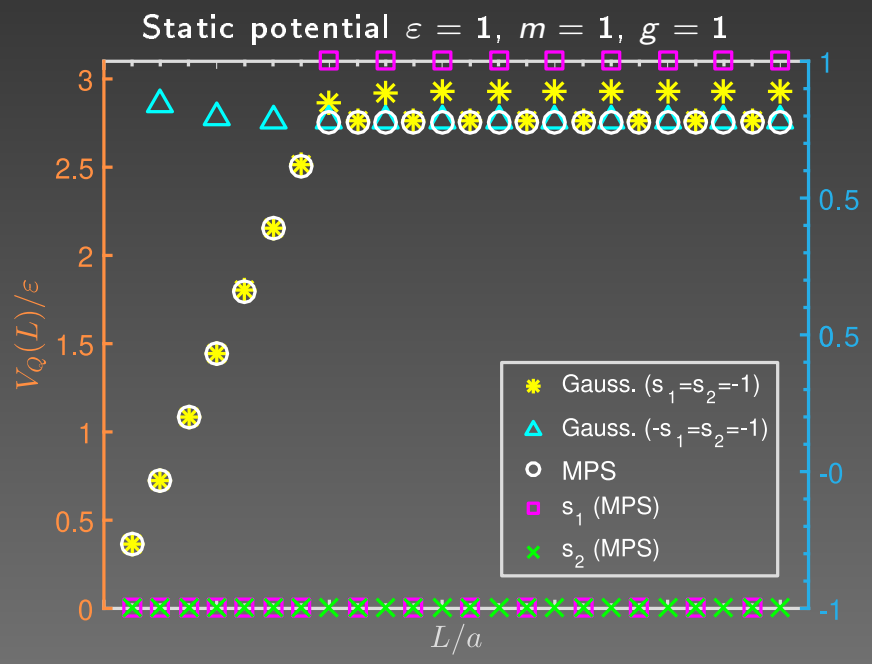
- Analogous to the U(1) case start with the strong-coupling vacuum
- Impose a color-flux string of length L on top
- Compute the ground state via imaginary time evolution

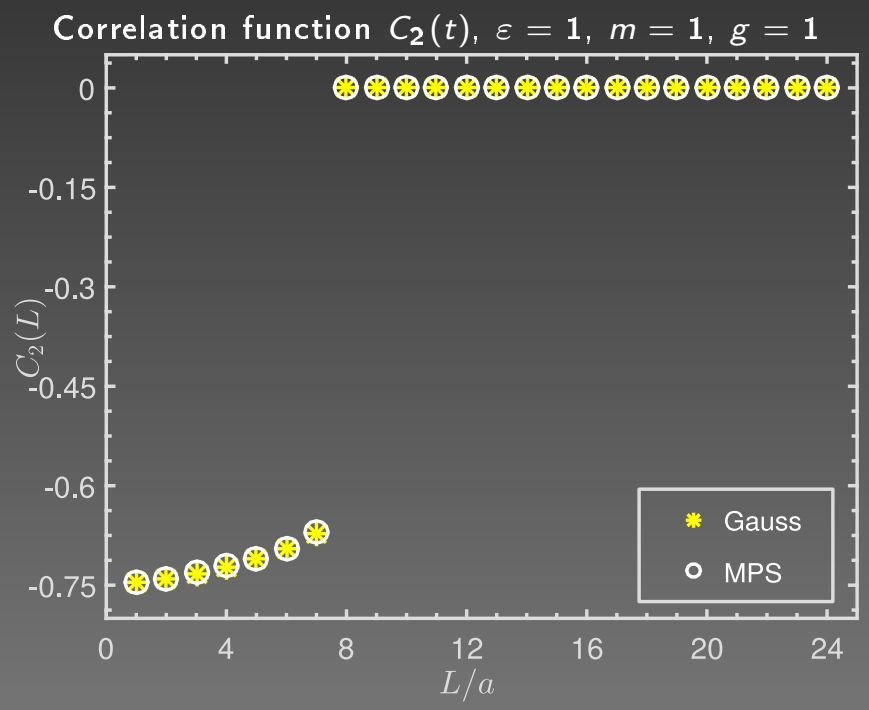


Results: SU(2) lattice gauge theory

Static potential

- Analogous to the U(1) case start with the strong-coupling vacuum
- Impose a color-flux string of length L on top
- Compute the ground state via imaginary time evolution

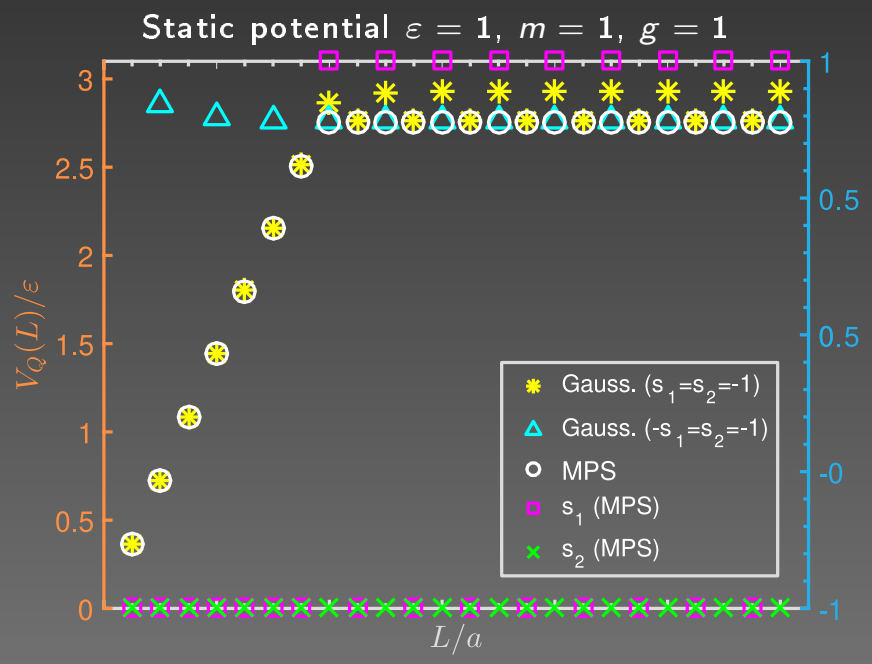


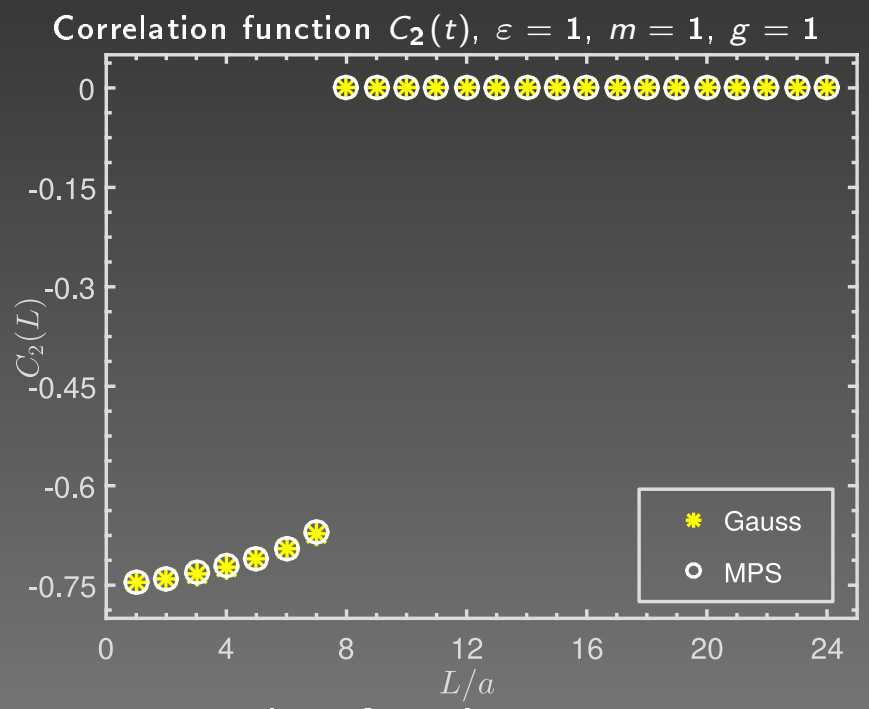


Results: SU(2) lattice gauge theory

Static potential

- Analogous to the U(1) case start with the strong-coupling vacuum
- Impose a color-flux string of length L on top
- Compute the ground state via imaginary time evolution



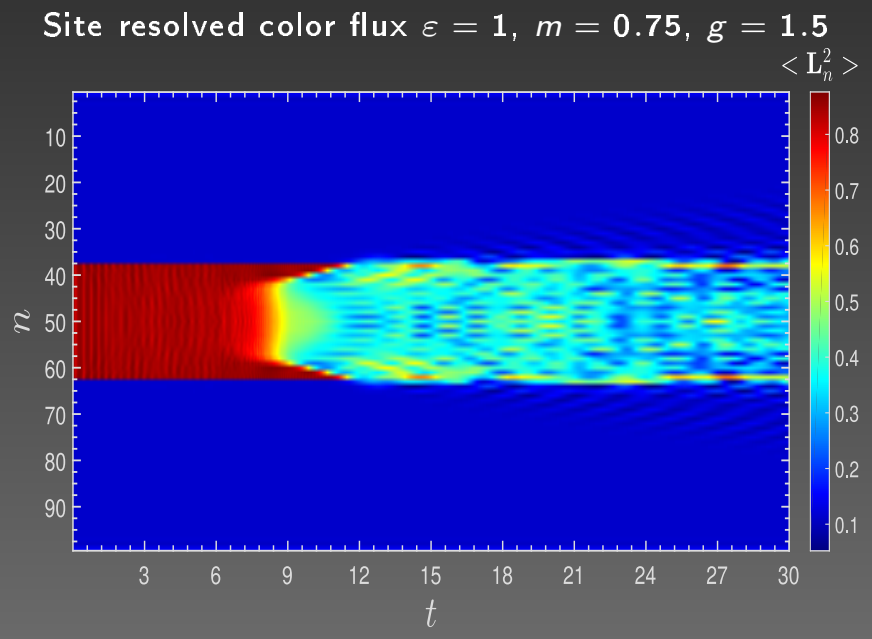


$\Rightarrow$ Reliable simulations of static properties also for the non-Abelian cases

Results: SU(2) lattice gauge theory

Out-of-equilibrium dynamics

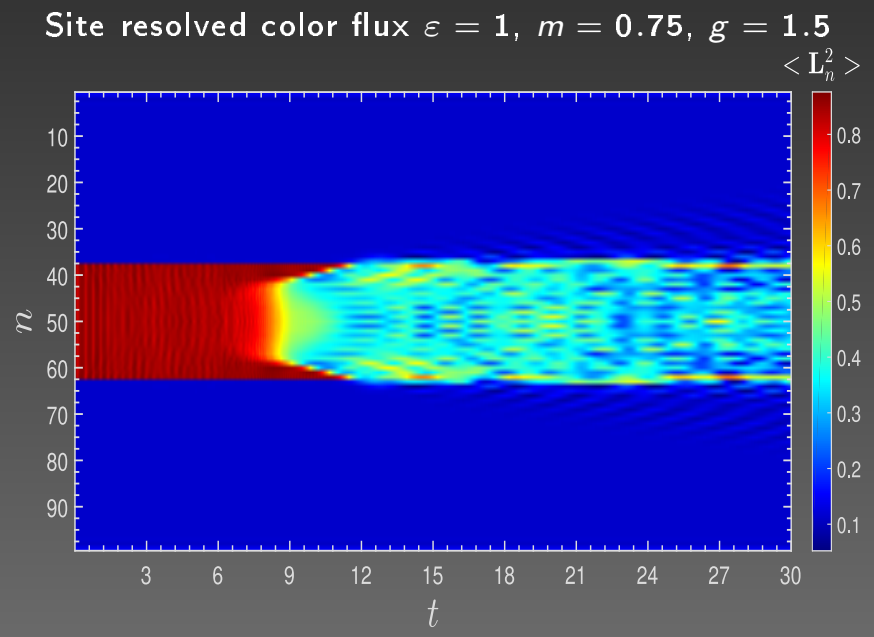
- Similar to the U(1) case we compute the interacting vacuum
- Impose a string between static external charges on top

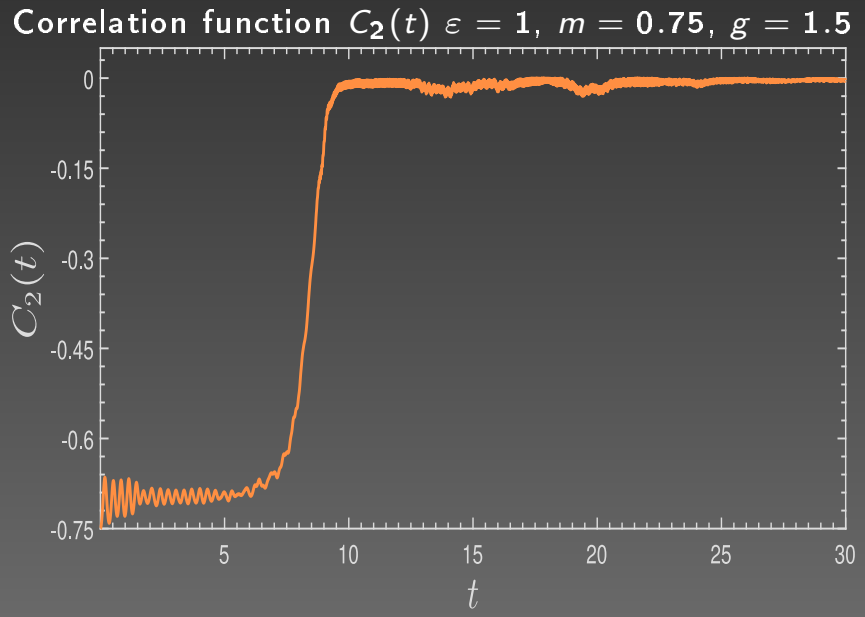


Results: SU(2) lattice gauge theory

Out-of-equilibrium dynamics

- Similar to the U(1) case we compute the interacting vacuum
- Impose a string between static external charges on top





$\Rightarrow$ Reliable simulations of dynamics also for the non-Abelian cases

5.

Conclusion & Outlook

Conclusion

- Ansatz captures the relevant features
  - Static properties
  - Out-of-equilibrium dynamics
- Good agreement with Tensor Network results

Outlook

- Finite density
- Finite temperature
- Higher dimensions
- Formulation $H_\ominus$ might be useful for other applications
  - Tensor Networks
  - Quantum simulation

Thank you for your attention!

arXiv:1805.05190

A. Variational ansatz for the case of SU(2)

Parity symmetries of the Hamiltonian

- Parity symmetry of H_Θ: $[P_1, H_\Theta] = 0$
  with $P_1 = \sigma_1^z \sigma_2^z P_z$ and $P_z = \exp\left[i\frac{\pi}{2}\sum_n \phi_n^\dagger(\sigma^z + \mathbb{1})\phi_n\right]$
- Unitary transformation rotating P_1 to σ_1^x

$$V_1 = \frac{1}{\sqrt{2}}(1 - i\sigma_1^y \sigma_2^z P_z),$$

$\Rightarrow$ In the rotated frame σ_1^x is conserved, classical variable s_1

- Parity symmetry of $P_1^\dagger H_\Theta P_1$: $[P_2, P_1^\dagger H_\Theta P_1] = 0$
  with $P_2 = \sigma_2^x P_x$ and $P_x = \exp\left[i\frac{\pi}{2}\sum_n \phi_n^\dagger(\sigma^x + \mathbb{1})\phi_n\right]$
- Unitary transformation rotating P_2 to $-\sigma_2^z$

$$V_2 = \frac{1}{\sqrt{2}}(1 - i\sigma_2^y P_x)$$

$\Rightarrow$ In the rotated frame σ_2^z is conserved, classical variable s_2

A. Variational ansatz for the case of SU(2)

Variational ansatz

- Ansatz in the rotated frame

$$\left|\overline{\psi}\right\rangle = \left|\mathrm{GS}\right\rangle \left|s_1\right\rangle \left|s_2\right\rangle$$

- Ansatz in the original frame

$$\begin{aligned}
\left|\psi\right\rangle = & \frac{1}{4\sqrt{2}}\Theta^\dagger \Big[\left(\left|\uparrow\right\rangle_z + s_1 \left|\downarrow\right\rangle_z\right)\left[(1+s_2)\left|\uparrow\right\rangle_z + (1-s_2)\left|\downarrow\right\rangle_z\right] \\
& + s_2\left(s_1\left|\uparrow\right\rangle_z - \left|\downarrow\right\rangle_z\right)\left[(1+s_2)\left|\uparrow\right\rangle_z + (1-s_2)\left|\downarrow\right\rangle_z\right] P_z \\
& - s_2\left(\left|\uparrow\right\rangle_z + s_1\left|\downarrow\right\rangle_z\right)\left[(1-s_2)\left|\uparrow\right\rangle_z + (1+s_2)\left|\downarrow\right\rangle_z\right] P_x \\
& + \left(s_1\left|\uparrow\right\rangle_z - \left|\downarrow\right\rangle_z\right)\left[(1-s_2)\left|\uparrow\right\rangle_z + (1+s_2)\left|\downarrow\right\rangle_z\right] i^{\mathcal{N}} P_y \Big] \\
& \times \left|\mathrm{GS}\right\rangle \left|0\right\rangle_{\mathrm{gauge}}
\end{aligned}$$

- If $\left|\mathrm{GS}\right\rangle$ is chosen to be the Dirac sea
  - Singlet between external charges for $s_1 = s_2 = -1$
  - Triplet for any other choice of s_1 and s_2