Gauge-invariant PEPS for pure Z_2 gauge theory and its entanglement

Etsuko Itou (YITP, Kyoto U./ RIKEN iTHEMS)

work in progress, collaboration with T. Okubo (U. of Tokyo/ Niigata U.)

The 43rd International Symposium on Lattice Field Theory(Lattice 2026), University of Maryland, 2026/07/28

Lattice gauge theory in Hamiltonian formalism

- So far, 1+1d gauge theories (Schwinger model) well-investigated in QC and TN
  The gauge d.o.f. in (1+1)d can be eliminated by using Gauss' law and OBC
- In general, the gauge d.o.f. needs an infinite-dimensional Hilbert space.
- 2+1d Hamiltonian lattice gauge theory is still challenging
- Finding a suitable formulation/truncation that preserves gauge symmetry
- Developing computational methods suited to the chosen formulation/truncation

Outline

- Z2 gauge theory in (2+1)dim. and topological entanglement
- Gauged Gaussian fermionic PEPS (GGFPEPS) ansatz (review)
- Algorithms (Grassmann TN and HOTRG methods)
- Numerical results
- Summary

Z2 theory in (2+1) dim.
and its entanglement

Z2 gauge theory in 2+1dim

D. Horn et al., PRD (1979)
E. Zohar, M. Burrello, T. B. Wahl, and J. I. Cirac,(2015,2016)

- $$H= \underbrace{\frac{\lambda}{2}\sum_l [2-(P_l+P_l^\dagger)]}_{\text{electric part}} + \underbrace{\frac{2}{\lambda}\sum_p [2-(Q_{p_1}^\dagger Q_{p_2}^\dagger Q_{p_3} Q_{p_4} + h.c.)]}_{\text{magnetic part}}$$

  $\mathbb{Z}_2$gauge theory: $P=P^\dagger=\sigma_z, Q=Q^\dagger=\sigma_x$

Toric code + external mag. field

$$H_{TC} = -\sum_s \prod_{i\in s}\sigma_i^z - \sum_p \prod_{i\in p}\sigma_i^x$$

$$H=(1-x)H_{TC} - x\sum_{i=1}^{N}\sigma_i^z$$

- Ground state of Hamiltonian

  P-eigenstate (P-basis): $\lambda=\infty$: $|\psi(\lambda=\infty)\rangle = \otimes_l |p=0\rangle_l \equiv |\psi_E\rangle$

  (all link variables take |0>, simple ground state in confined phase = Wilson loop: area law)

  Q-eigenstate (Q-basis) : $\lambda=0: |\psi(\lambda=0)\rangle \propto \prod_p (1+Q_{p_1}Q_{p_2}Q_{p_3}Q_{p_4})|\psi_E\rangle$

  (toric code ground state, topological (deconfined) phase = Wilson loop: perimeter law)

- A second-order transition between confined and topological (deconfined) phases occurs

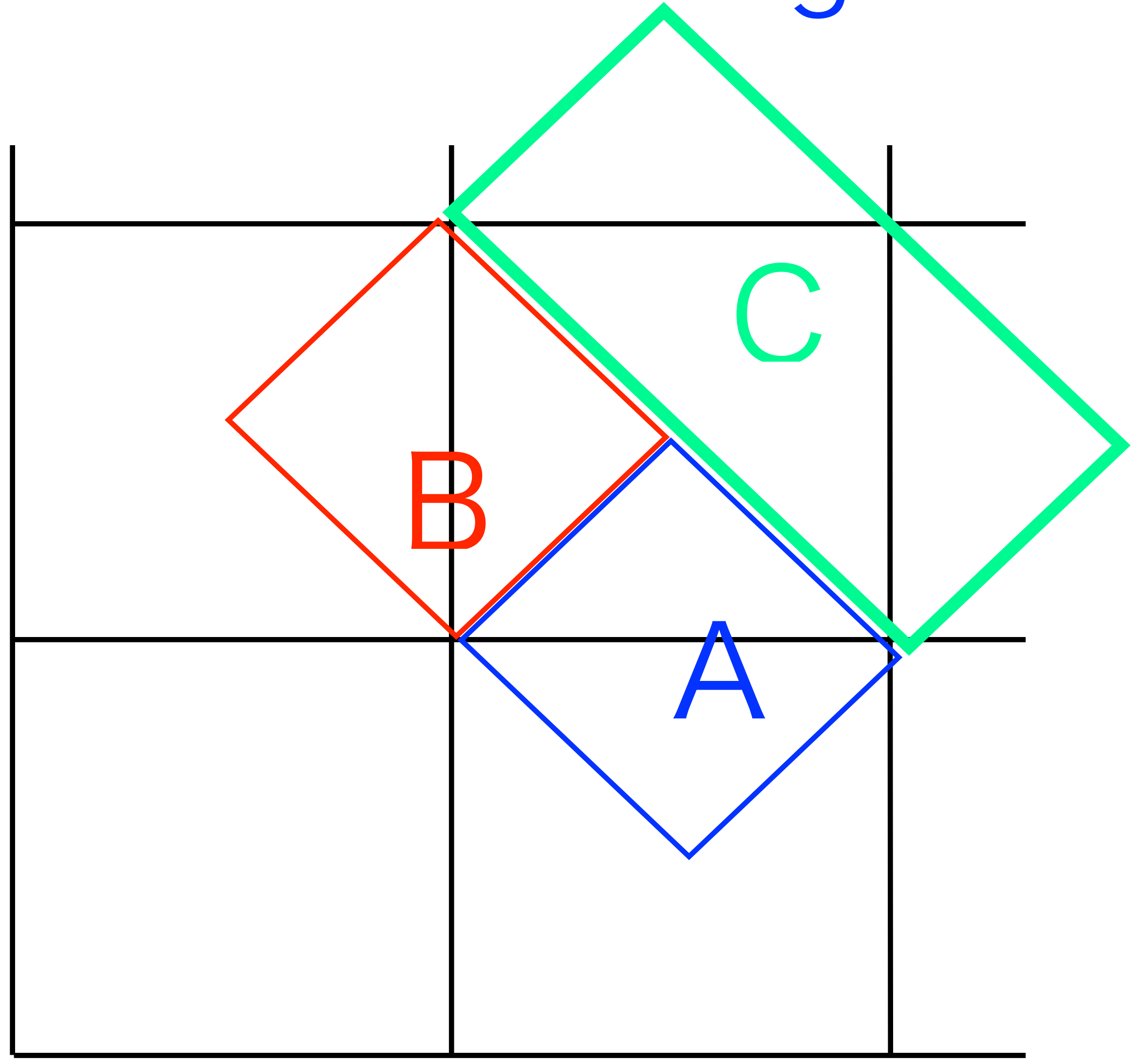
2+1 dim. entanglement entropy

Kitaev and Preskill, PRL (2006)
Levin and Wen, PRL (2006)

- Some 2+1d gauge theory (Z_N gauge) has the quantum phase transition at T=0

- It can be observed by a constant term of EE: $S_A = c\frac{l}{a} + S_{topo}$

"connected along a **link**" def.



"area" is counted by the # of links

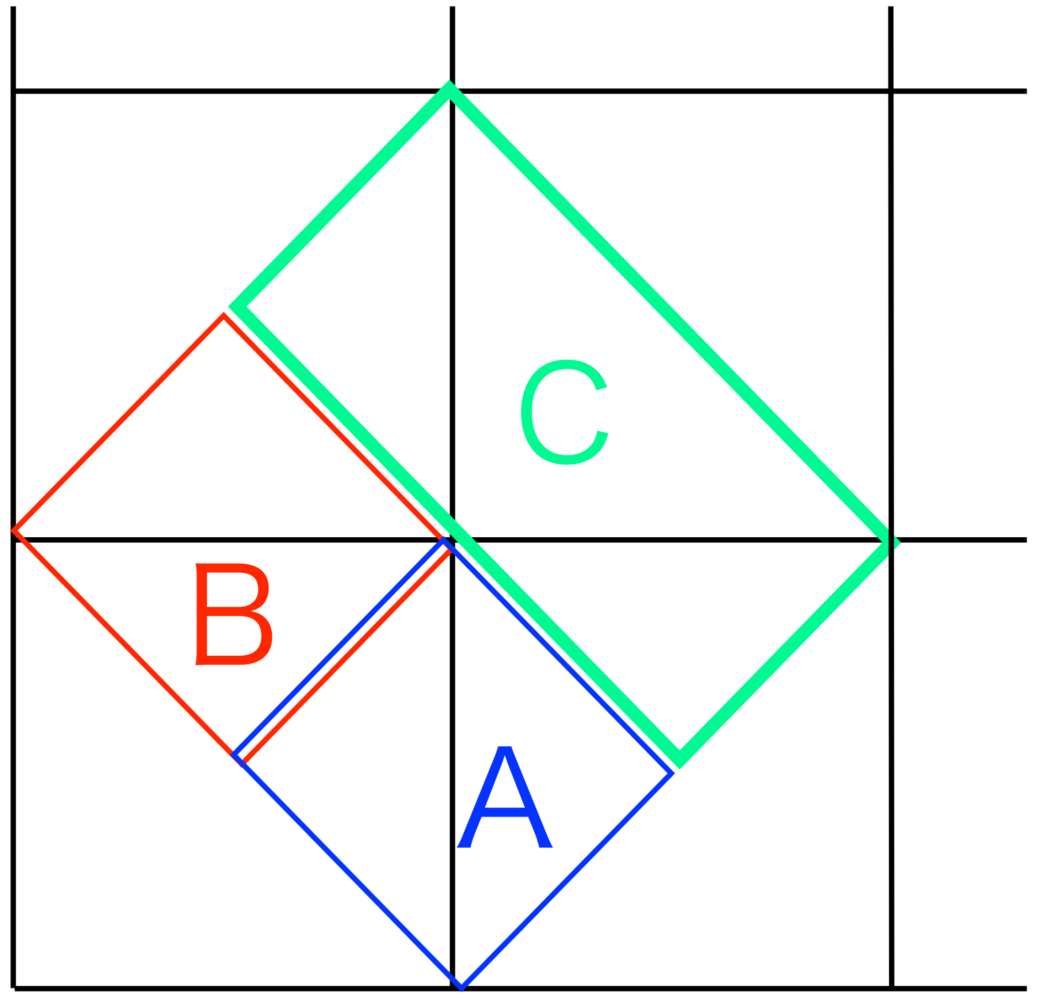
S_A, S_B : 1

S_C, S_{AB} : 2

S_{AC}, S_{BC}: 3

S_{ABC} : 4

"meet at a **site**" def.



"area" is counted by the # of edges

S_A, S_B : 2

S_C, S_{AB} : 3

S_{AC}, S_{BC}, S_{ABC}: 4

- topological EE (TEE): $S_{topo} = S_A + S_B + S_C - S_{AB} - S_{BC} - S_{AC} + S_{ABC}$

Toric code ground state: $S_{topo} = -\ln(2)$

cf.) entropic c-fn. for 3d Z_2 gauge theory
A. Bulgarelli and M. Panero, (2024)

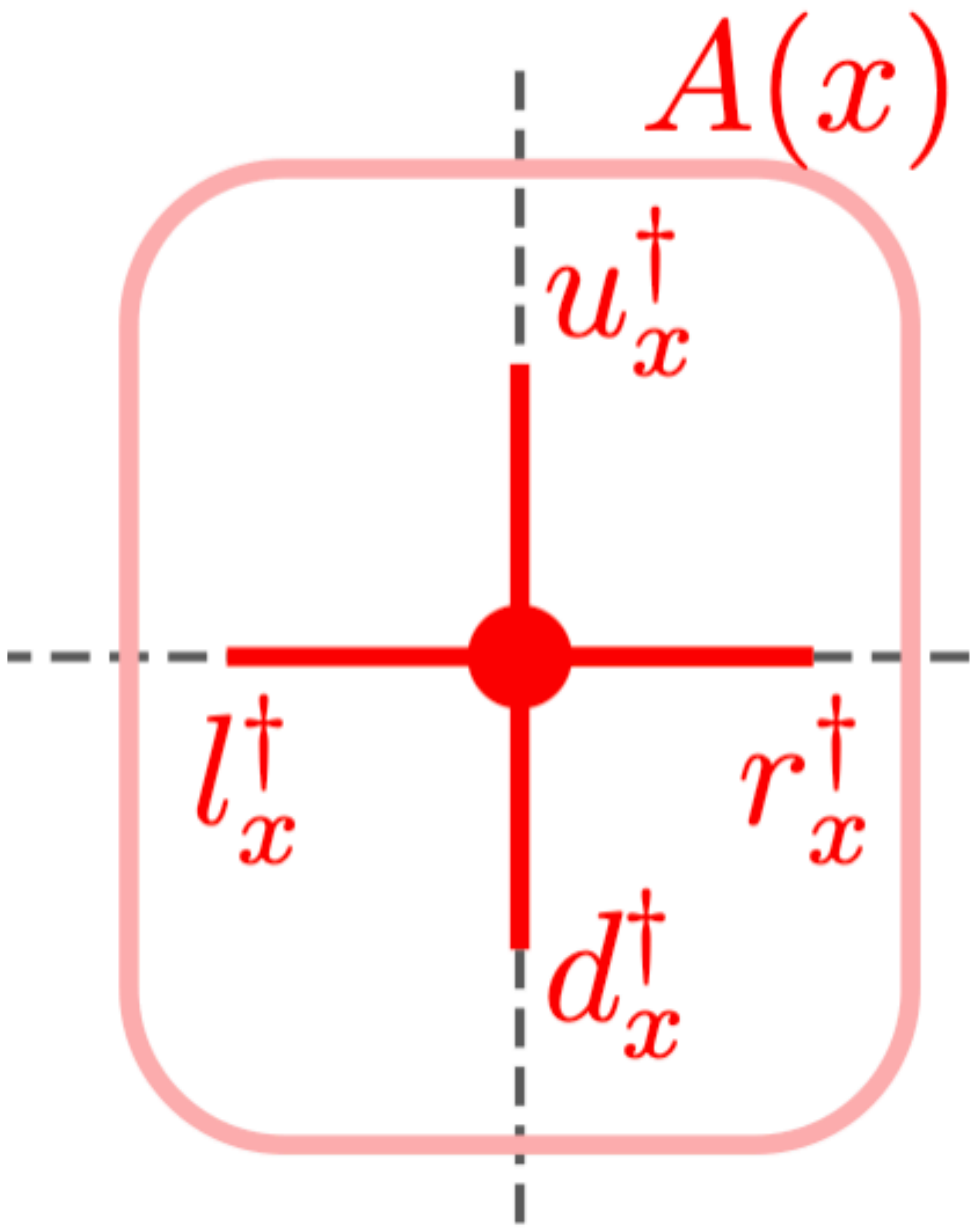
GGFPEPS ansatz state

Patrick Emonts, Mari Carmen Bañuls, Ignacio Cirac and Erez Zohar, PRD (2020)
Patrick Emonts et al., PRD(2023)
Review paper: Ariel Kelman et al., PRD(2024)
fermionic PEPS: C.V. Kraus, N. Schuch, F. Verstraete, and J. I. Cirac, PRA(2010)

Plenary talk by Erez Zohar
(9 am, Fri.)

Gauged Gaussian fermionic PEPS (GGFPEPS) ansatz

- Express link variable using Gaussian form of virtual fermions ops. (r, u, l, d). We put A(x) tensor on each site.



$$A(\mathbf{x}) = \exp\left(T_{\alpha\beta} a_\alpha^\dagger(\mathbf{x})\, a_\beta^\dagger(\mathbf{x})\right)$$

$$a_\alpha = \{r_1, u_1, l_1, d_1, \cdots, r_F, u_F, l_F d_F\}$$

- F sets of virtual fermions
  The size of the variational state is controlled by the parameter F.
  F : dim. of rep. matrix of gauge field
  (# of virtual fermion= 4F)

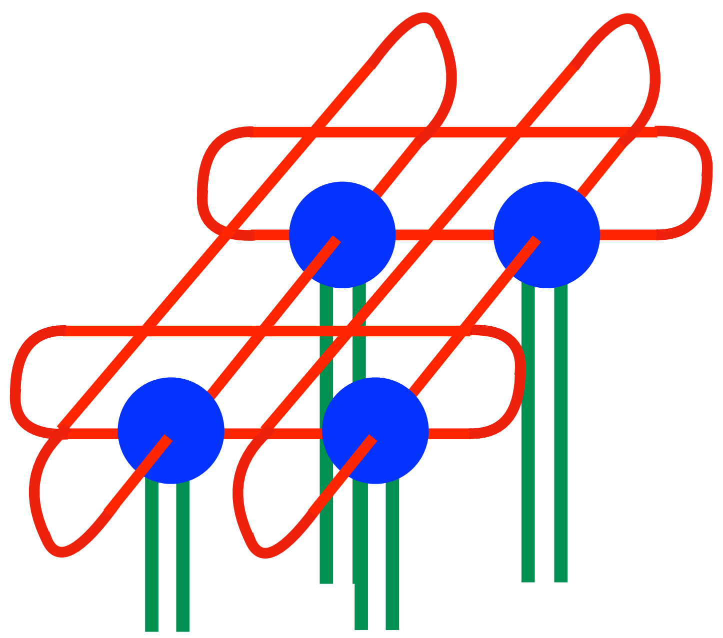
- Imposing translational invariance,
  F=1 : 2 complex parameters (minimal ansatz)
  F=2 : 8 complex parameters

Gauged Gaussian fermionic PEPS (GGFPEPS) ansatz

- GGFPEPS ansatz

$$|\psi\rangle = \langle\Omega| \prod_{x,i} w^\dagger(x,i)\mathscr{U}_{\mathscr{G}} \prod_{x} A(x)|\Omega\rangle|\psi_E\rangle$$

state $|\psi\rangle$



- All tensors, A(x), Uq(x,1), w(x,1), are Gaussian form of virtual fermion

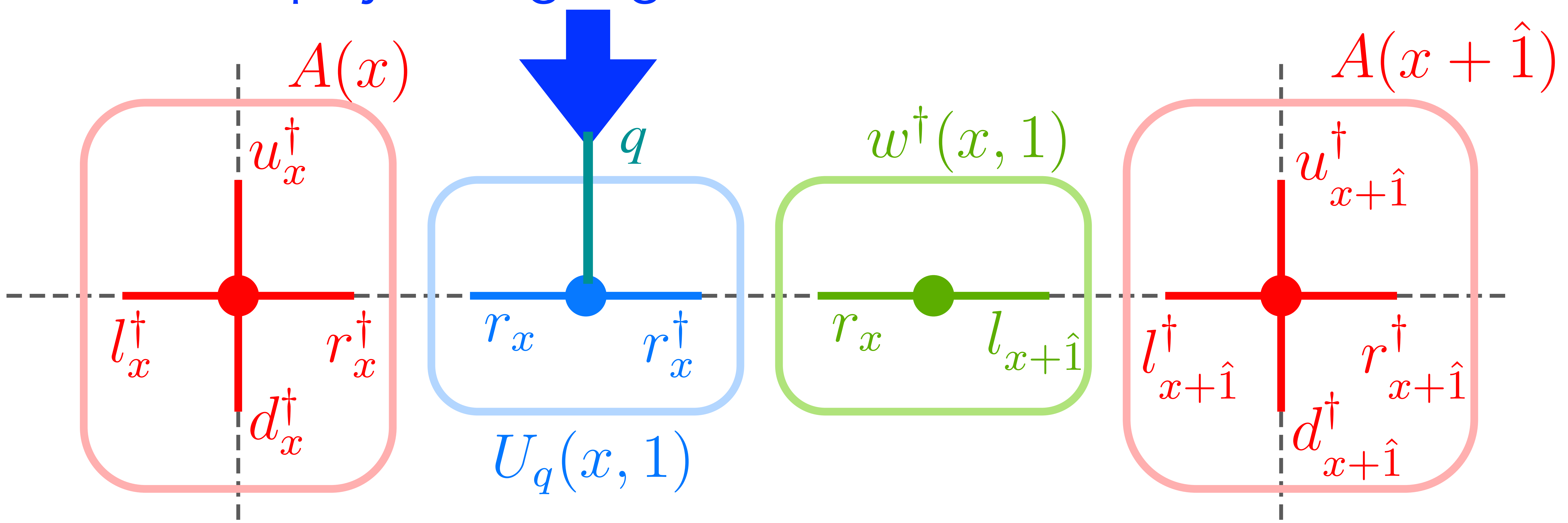
Uq tensor :

Link variable (phys. gauge filed)

w/ charge q=(0,1) in Z_2 gauge

$$\mathcal{U}_q(\mathbf{x},1) = \exp\left(i\pi q \sum_{\alpha=1}^{F} \boxed{r_\alpha^\dagger(\mathbf{x})\, r_\alpha(\mathbf{x})}\right)$$

Number op.

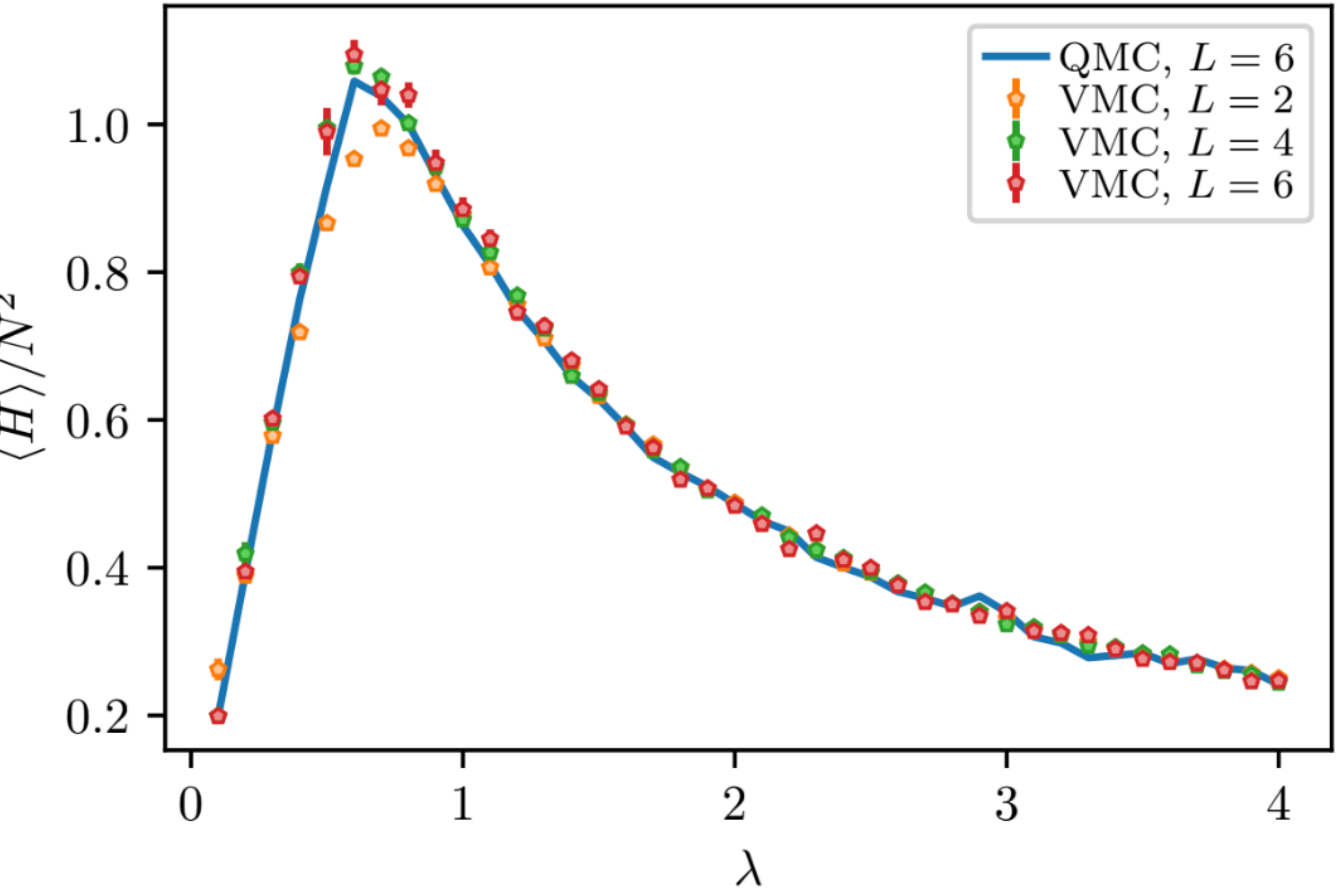


- Traceout all virtual legs, and remain only physical legs
- The formulation is gauge-invariant.

Algorithms
(Grassmann TN and HOTRG)

A previous study by VMC method

F=2 ansatz
(using QMC and VMC)



Patrick Emonts, Mari Carmen Bañuls,
Ignacio Cirac and Erez Zohar, PRD (2020)

- Difficulty of fermionic PEPS (in general):

  To calc. $\langle \Omega | \hat{a}^\dagger_\alpha(x_i) \cdots \hat{a}_\beta(x_j) \cdots \hat{a}^\dagger_\gamma(x_k) | \Omega \rangle$

  Align these ops. in the order "anni, → creat."
  Each exchange introduces a factor of (-1).
  Keeping track of it makes TN calc. complicated.

- So far, to calc <O>, VMC method has used, but statistical errors in MC make it difficult to optimize the variational parameters

- Can we perform more precise calculations and check whether the ansatz works well even near the critical point?

Grassmann tensor network

- An effective approach to extending conventional TN for bosonic sys. to fermionic sys.

- fermionic operator -> (classical) Grassmann number

  Z.-C. Gu, F. Verstraete, X.-G. Wen, arXiv:1004.2563
  S. Akiyama and D. Kadoh, JHEP(2021)

  $\{\hat{a}_i^\dagger, \hat{a}_j\} = \delta_{ij}$ -> $\{\theta_i^*, \theta_j\} = 0$ (const. term vanishes)

- Contraction -> Grassmann integration (formally)
  which automatically accounts for fermionic sign factors

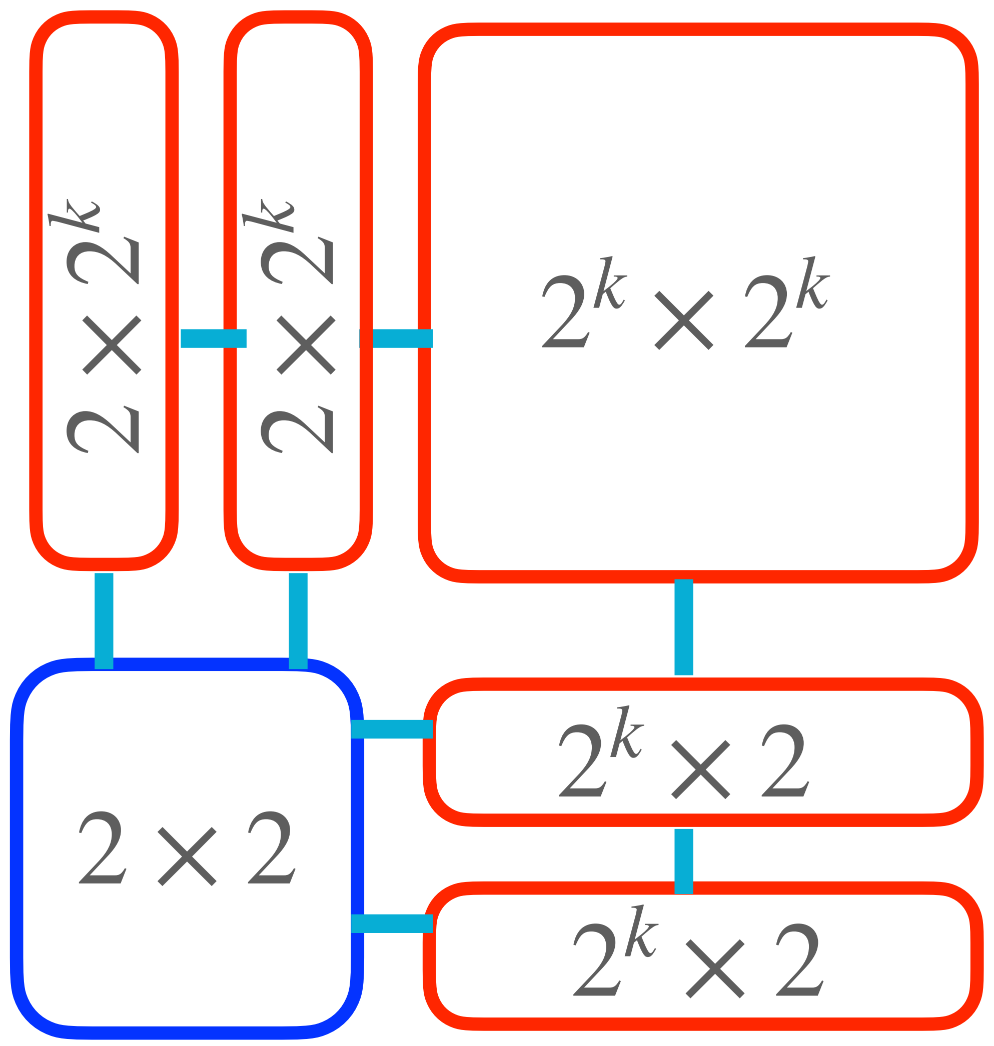
- Procedures of Grassmann TN
  (1) Arrange fermionic ops in the order "annihilation → creation" |vac>
  (Gaussian PEPS almost like that)
  (2) Count the number of (−1) factors from operator exchanges
  (3) Do the contraction by Grassmann integration

- By applying SVD, we can compress the tensor rank

- A package: GrassmannTN: a Python package for Grassmann tensor network computations

SciPost Phys. Codebases 20 (2023), arXiv:2309.07557

Large volume calculations with HOTRG

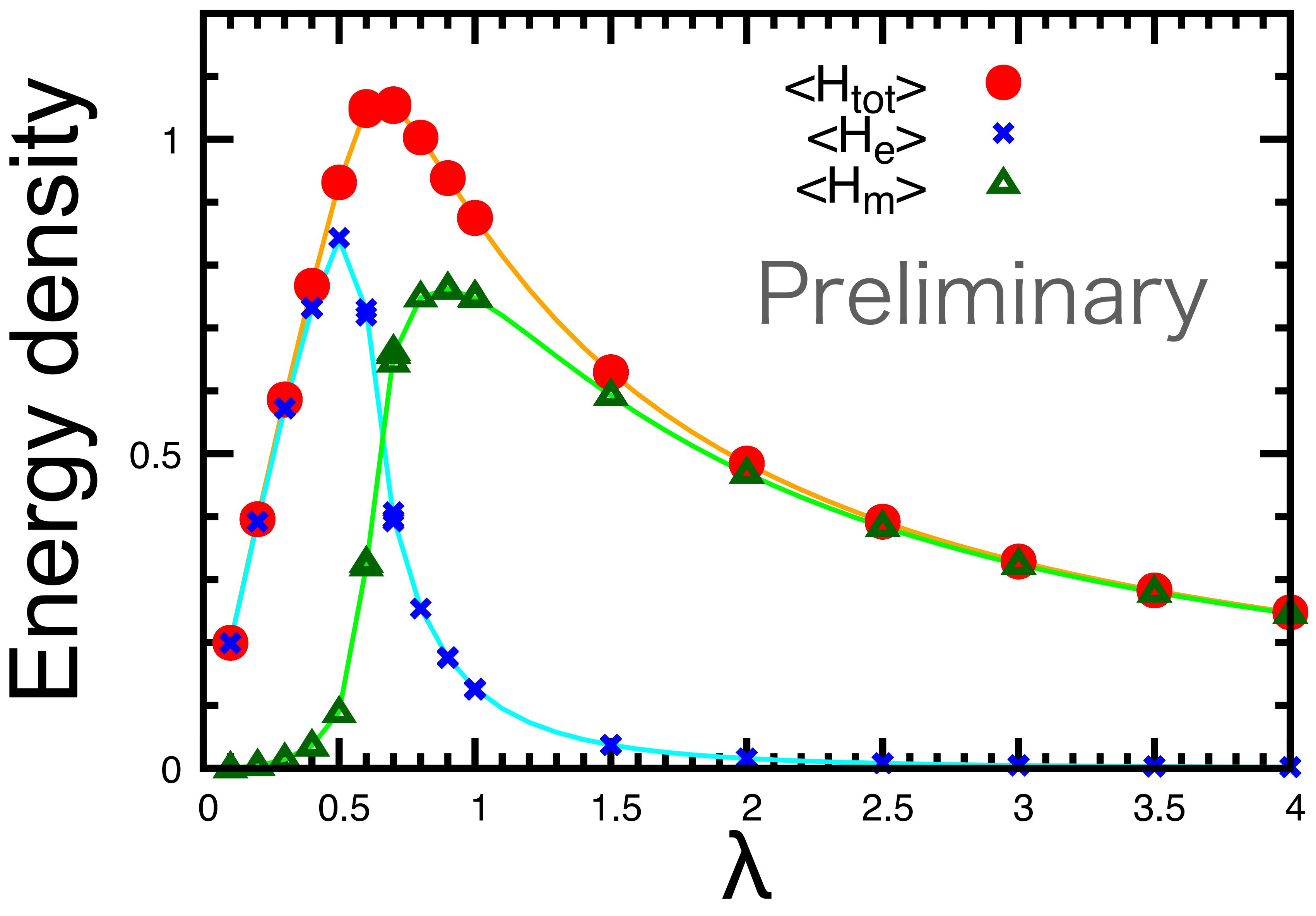


k=0 -> L=4x4
k=1 -> L=6x6
k=2 -> L=10x10
k=3 -> L=18x18
k=4 -> L=34x34

- Used in the contraction of virtual fermions.
  Here, we impose PBC for the lattices
- Local tensor and environment tensors
- Higher-Order Tensor Renormalization Group (HOTRG)
  Efficient computation of environment tensors using HOTRG
- HOTRG recursively
  - coarse-grains 2^k tensors
  - truncating the enlarged bond space (=dcut) by SVD
  - keeping only the dominant SV

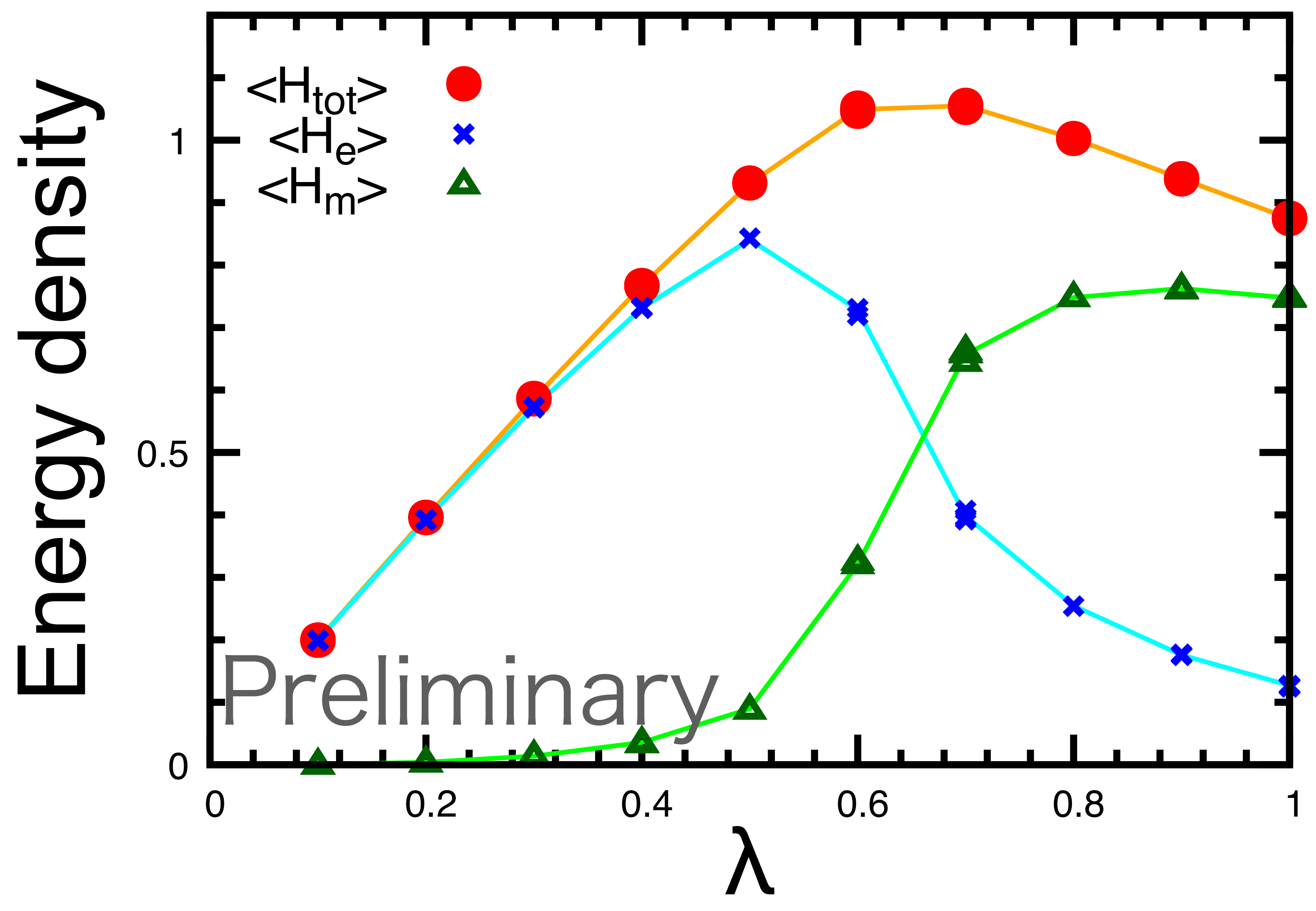
Numerical results

<H> and Topological EE: L = 4 x 4 (HOTRG)



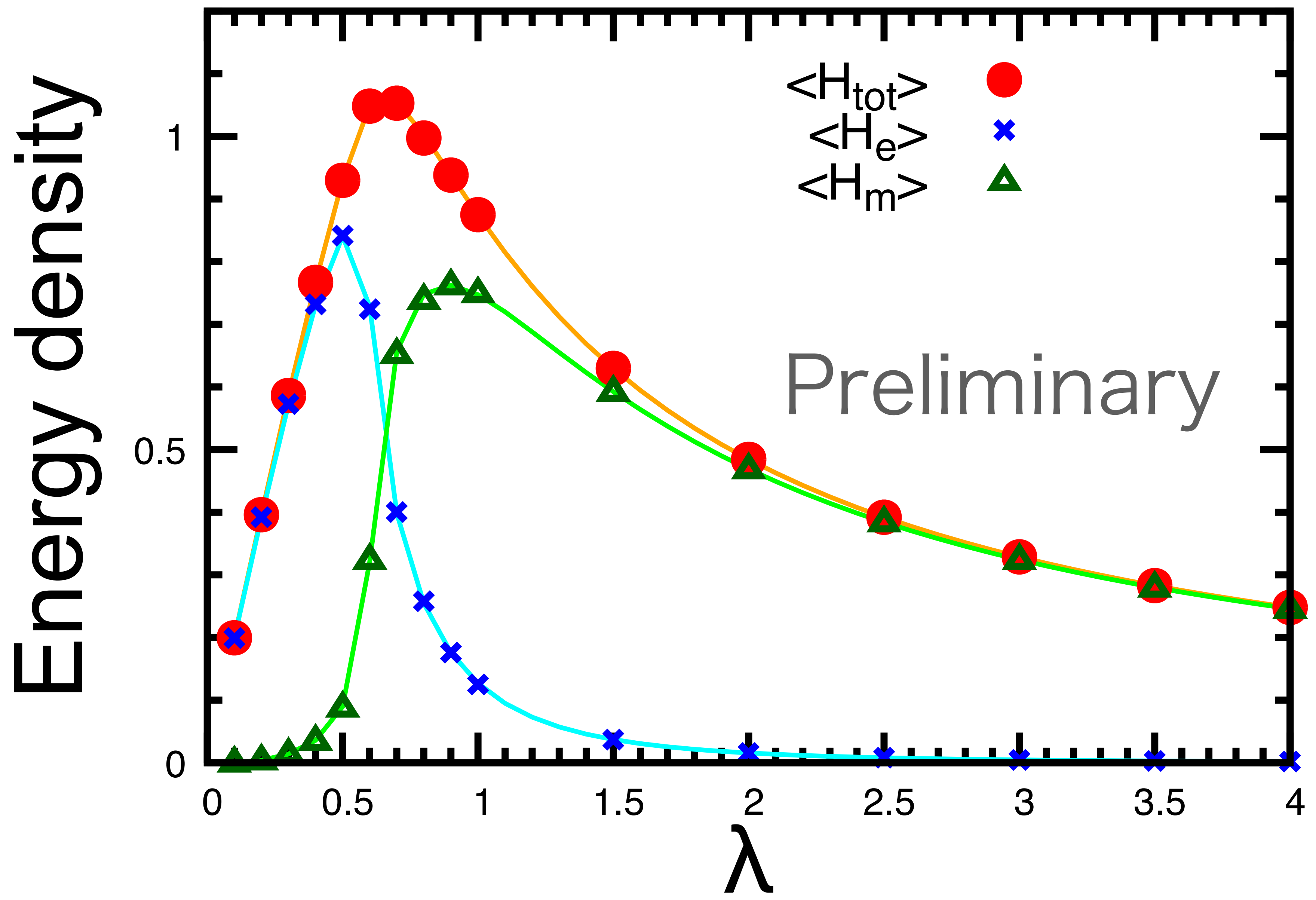
- total Energy
  magnetic Energy
  electric Energy
  Comparison with ED results (solid curves)

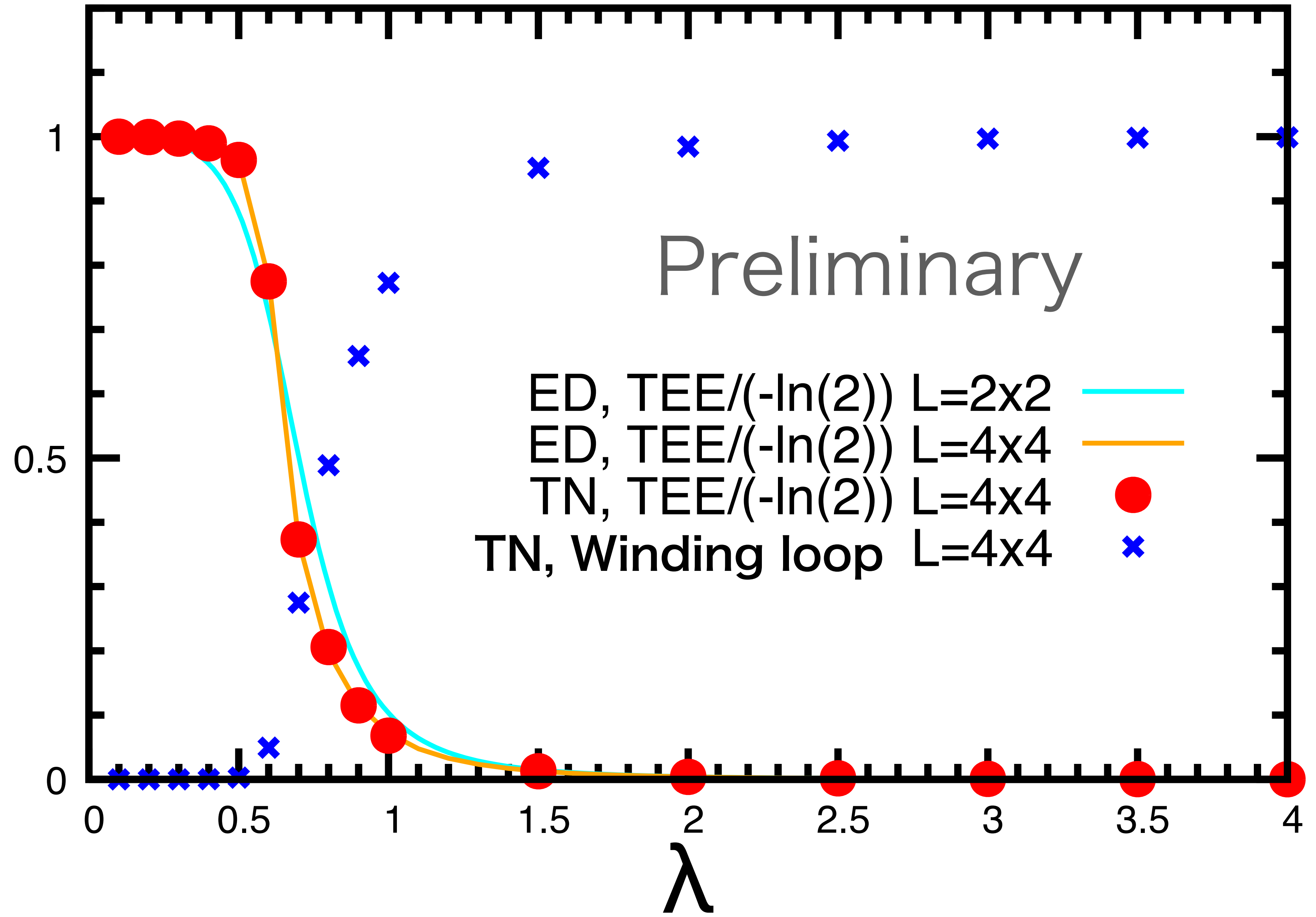
Enlarged plot around λ_c



- Around the critical regime, it works very well if we include seed-dependence of otimization processes as a statistical error. (10 seeds)

<H> and Topological EE: L = 4 x 4 (HOTRG)





- total Energy
  magnetic Energy
  electric Energy
  Comparison with ED results (solid curves)

- Bottom panel:
  Topological EE/(-ln(2))
  S_{topo} = -ln(2): TEE for toric code ground state
  Winding loop : $\langle\psi| \prod_{n_x} P_l(n_x, n_y = 0) |\psi\rangle$
  (approximate order param. of confinement)

- Now, we are doing upto L=34 x 34 lattices calc.

Summary

Summary

- 2+1d Hamiltonian lattice gauge theory is challenging:
  How to represent gauge-invariant states, and what are suitable computational methods?

- Gauged Gaussian Fermionic PEPS ansatz:
  gauge-invariant PEPS ansatz with Gaussian fermionic ops.
  It fits TN and QC

Plenary talk by Erez Zohar
(9 am, Fri.)

- Toward more precise calc. and Validation of the ansatz state near the critical point
  We used the Grassman TN and HOTRG methods

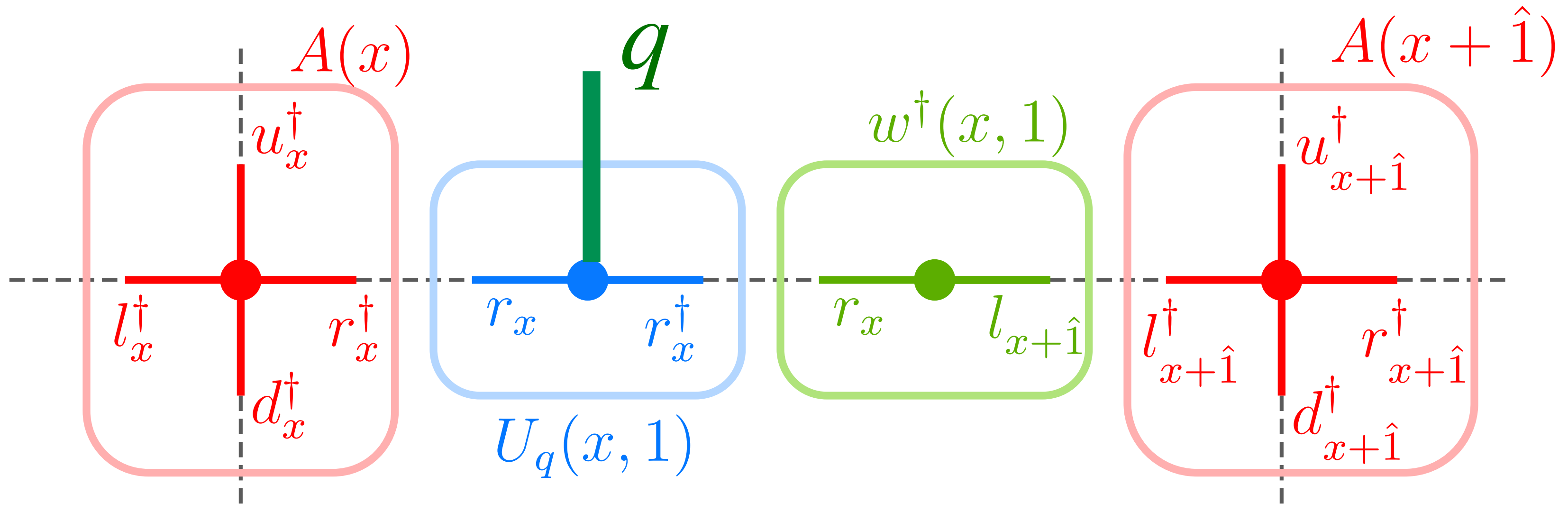
- In 2+1d, Z_2 gauge theory:
  An interesting observable is the Topological EE, which probes of topological transition,
  much like the entropic (c)-function probes confinement in 4d Yang–Mills theory.

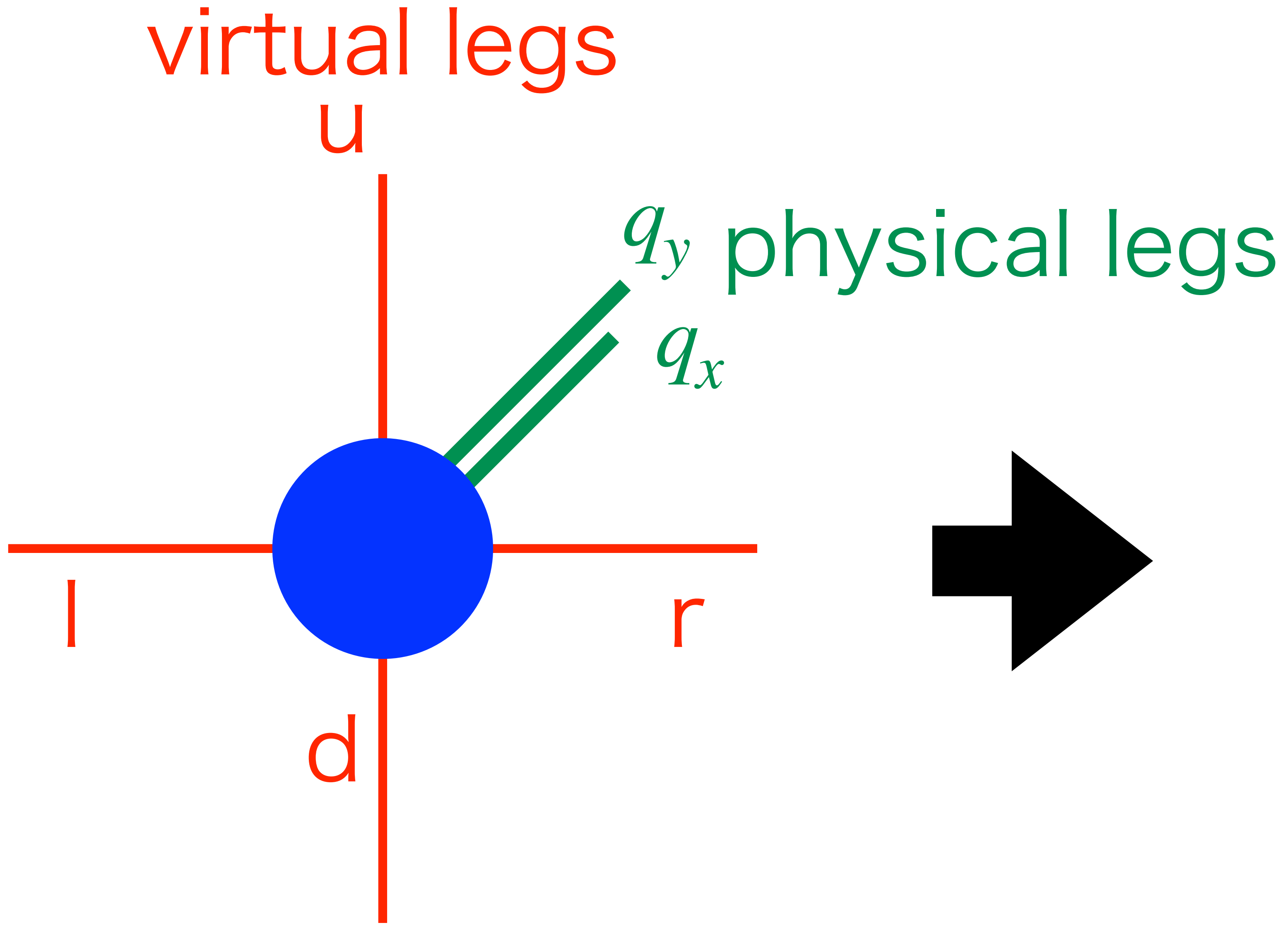
EI, K.Nagata, Y.Nakagawa, A.Nakamura, V.I.Zakhanov
PTEP 2016 (2016) 6, 061B01

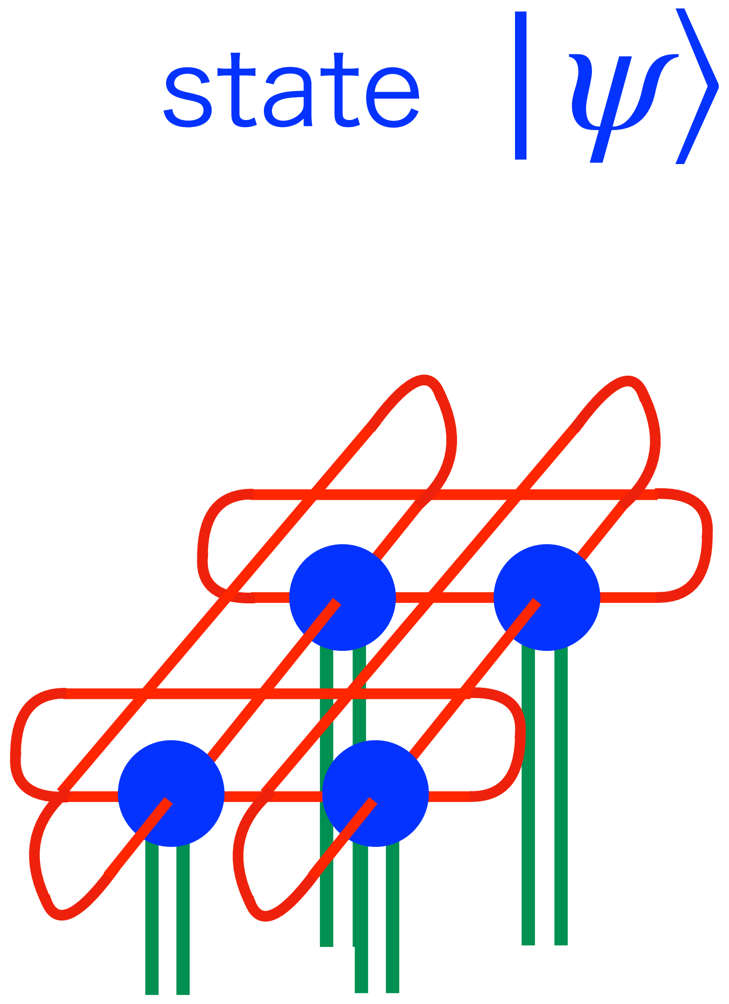
backup

Calculation strategy

State preparation

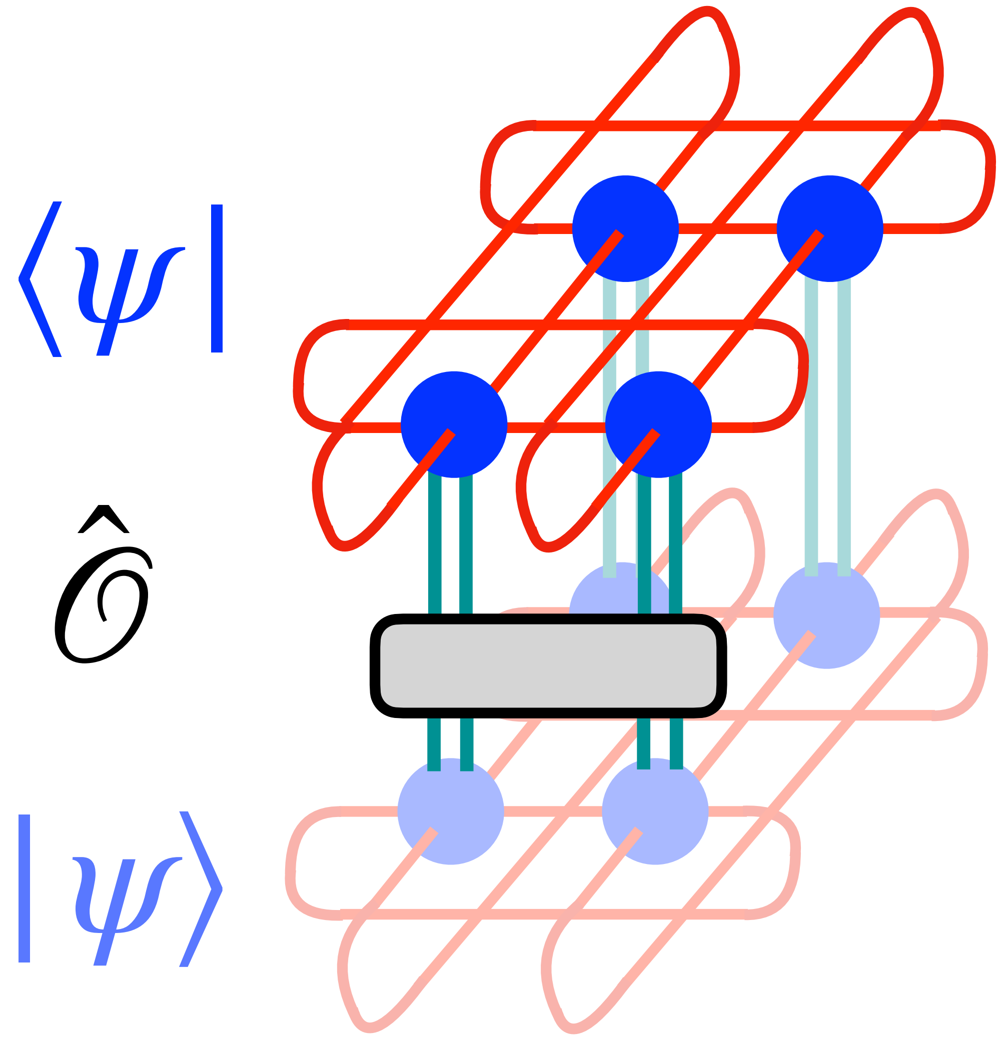






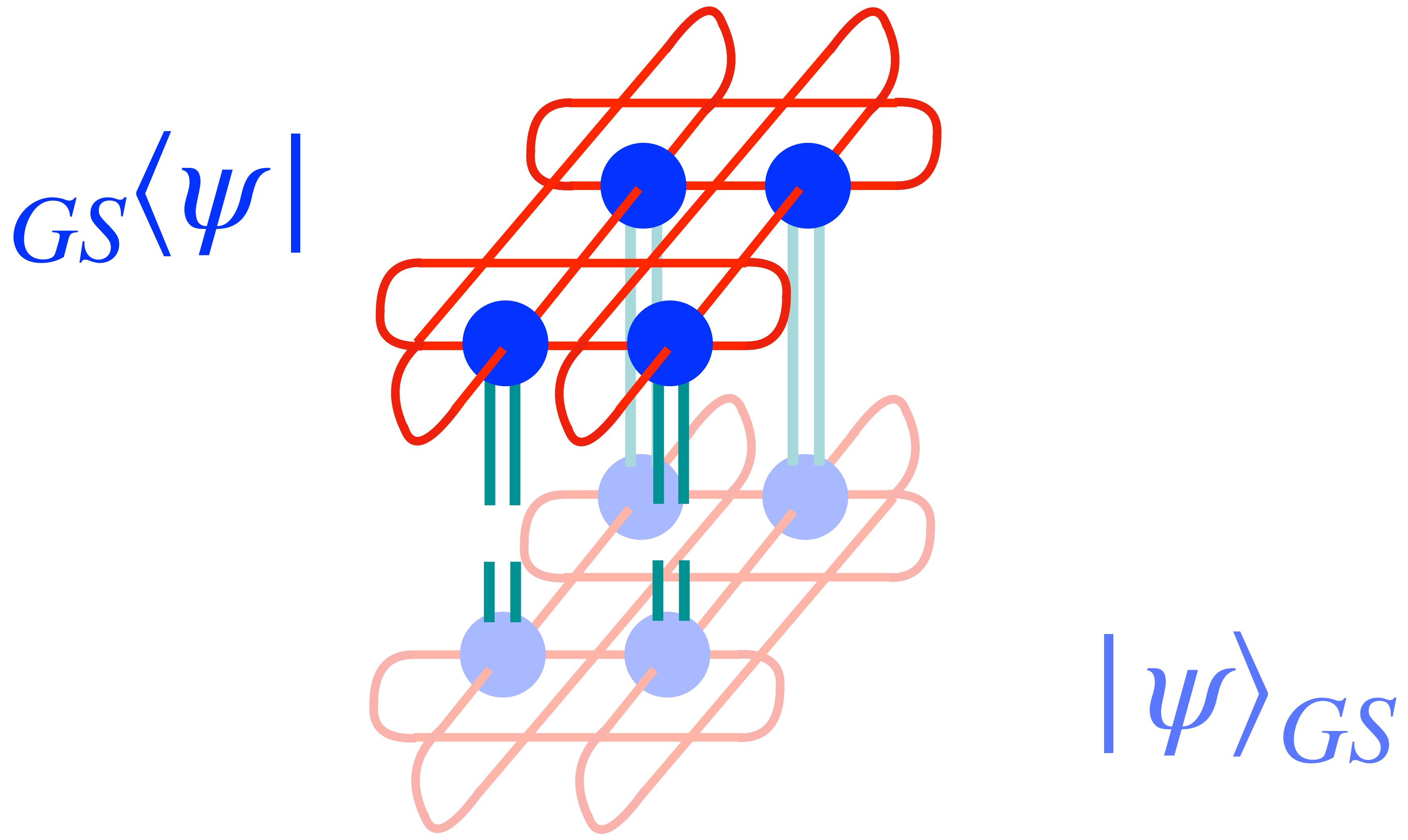
Traceout all virtual legs, and remain only physical legs

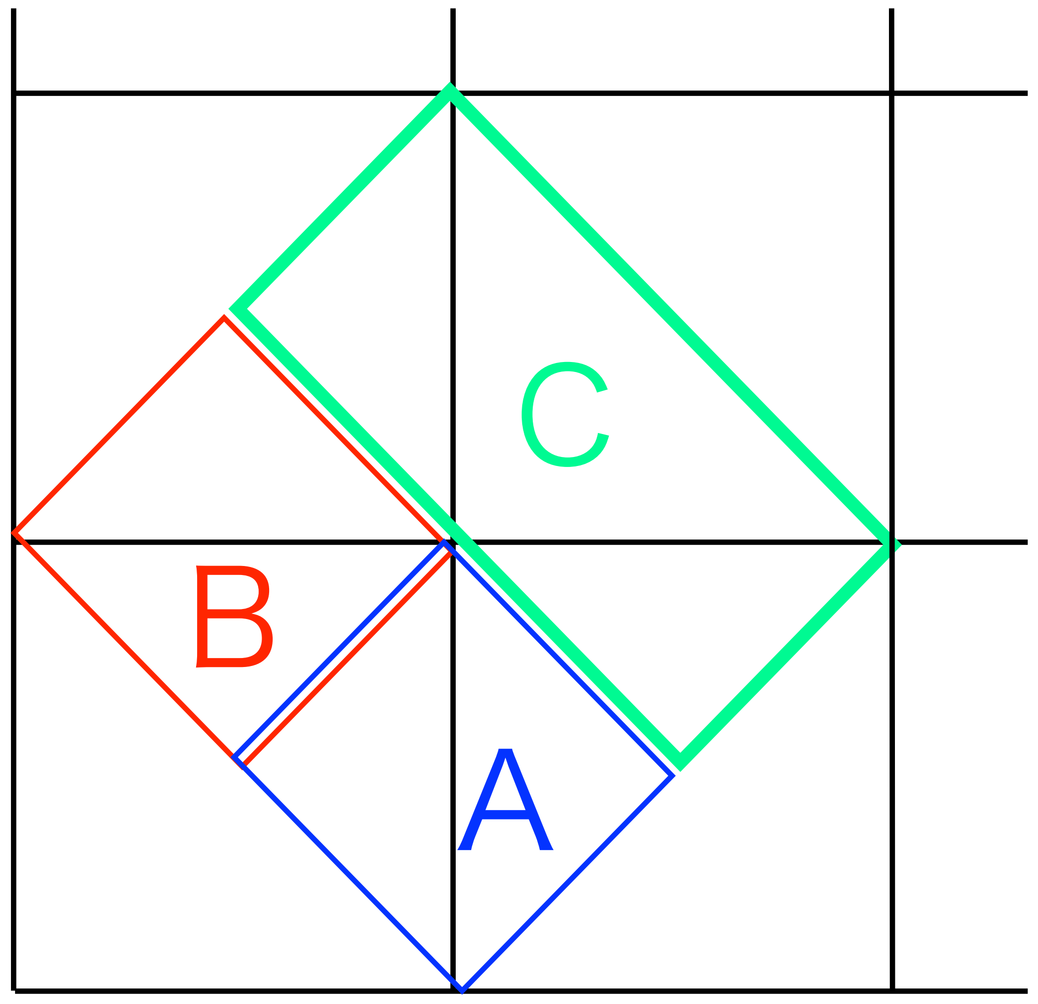
Measure observables (energy, winding loop, etc) $\langle\psi|\,\hat{\mathcal{O}}\,|\psi\rangle$



To generate the ground state,
we measure <H> using trial state and
minimize <H> by tuning the variational
parameters in tensor $A(x)$

Calculation of EE (reduced density matrix)





- We can also calculate ρ_A by not contracting the physical legs in subsystem $\langle\psi|\hat{\rho}_A|\psi\rangle_{ij}$

$$\downarrow$$

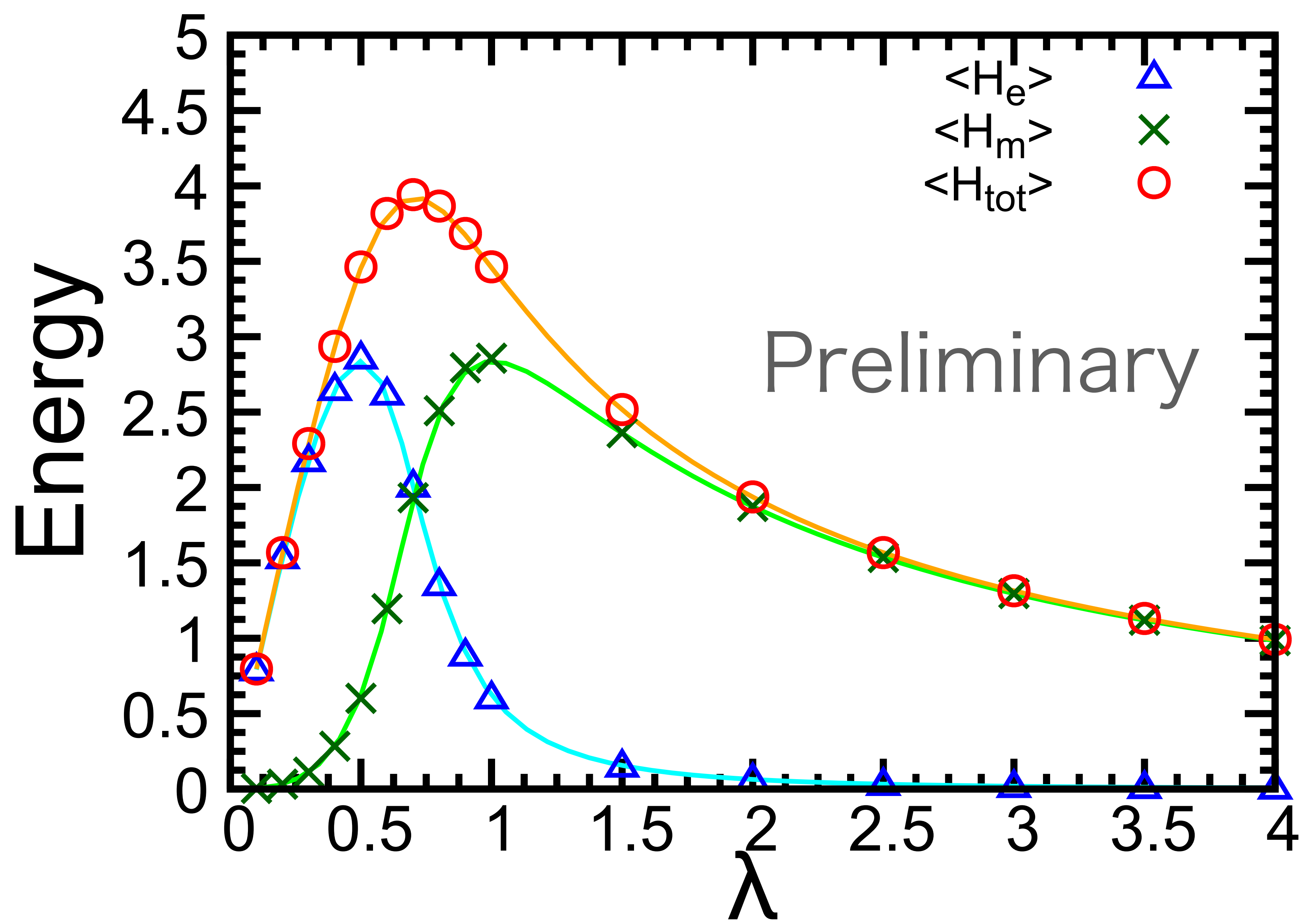
To obtain EE, we evaluate eigenvalues (λ_i) of reduced density matrix $\langle\rho_A\rangle_{ij}$

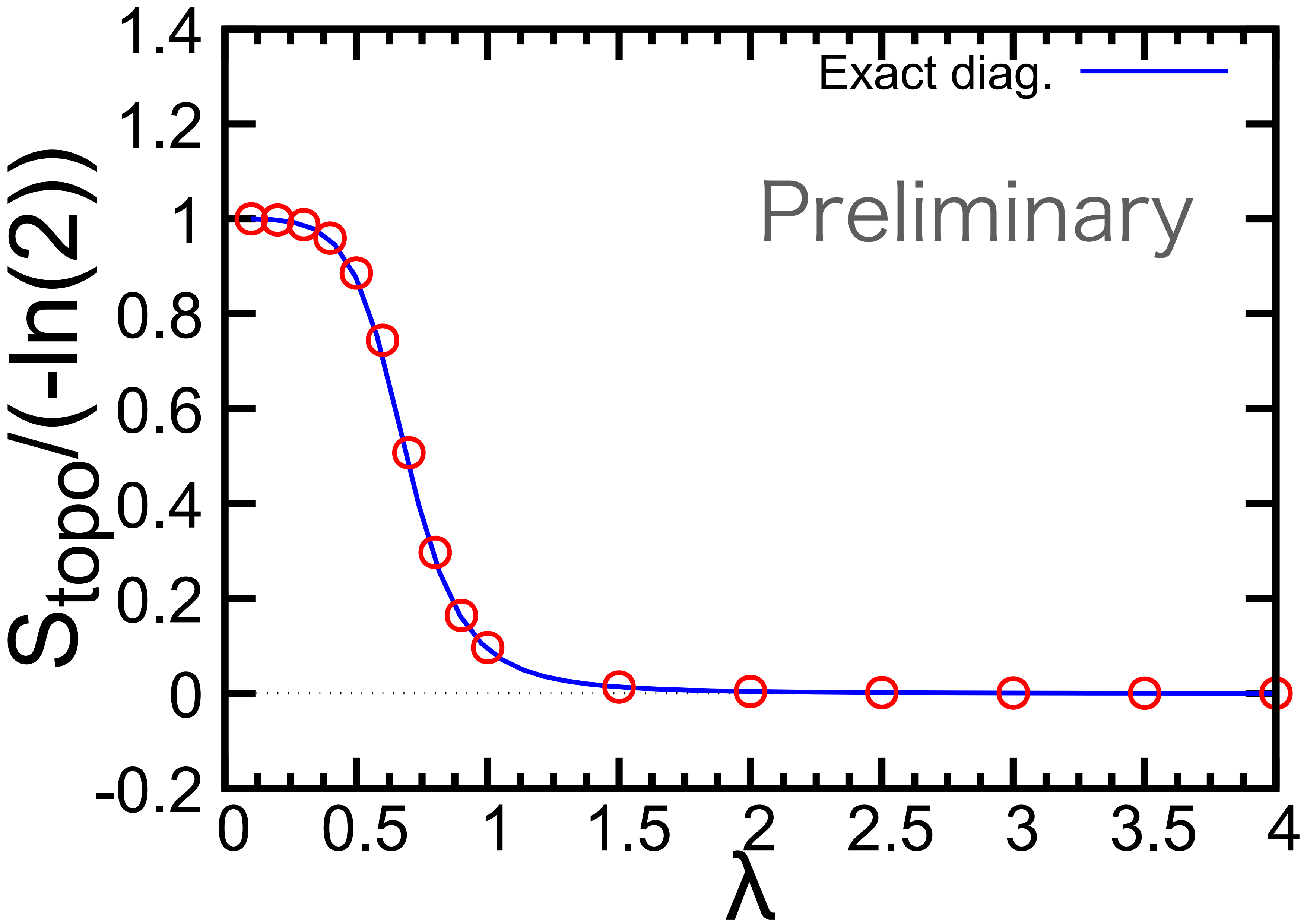
$$S_A = -\sum_i \lambda_i \ln \lambda_i$$

- We take the Levin-Wen layout for topological EE:

$$S_{topo} = S_A + S_B + S_C - S_{AB} - S_{BC} - S_{AC} + S_{ABC}$$

<H> and Topological EE: L = 2 x 2(exact contraction)

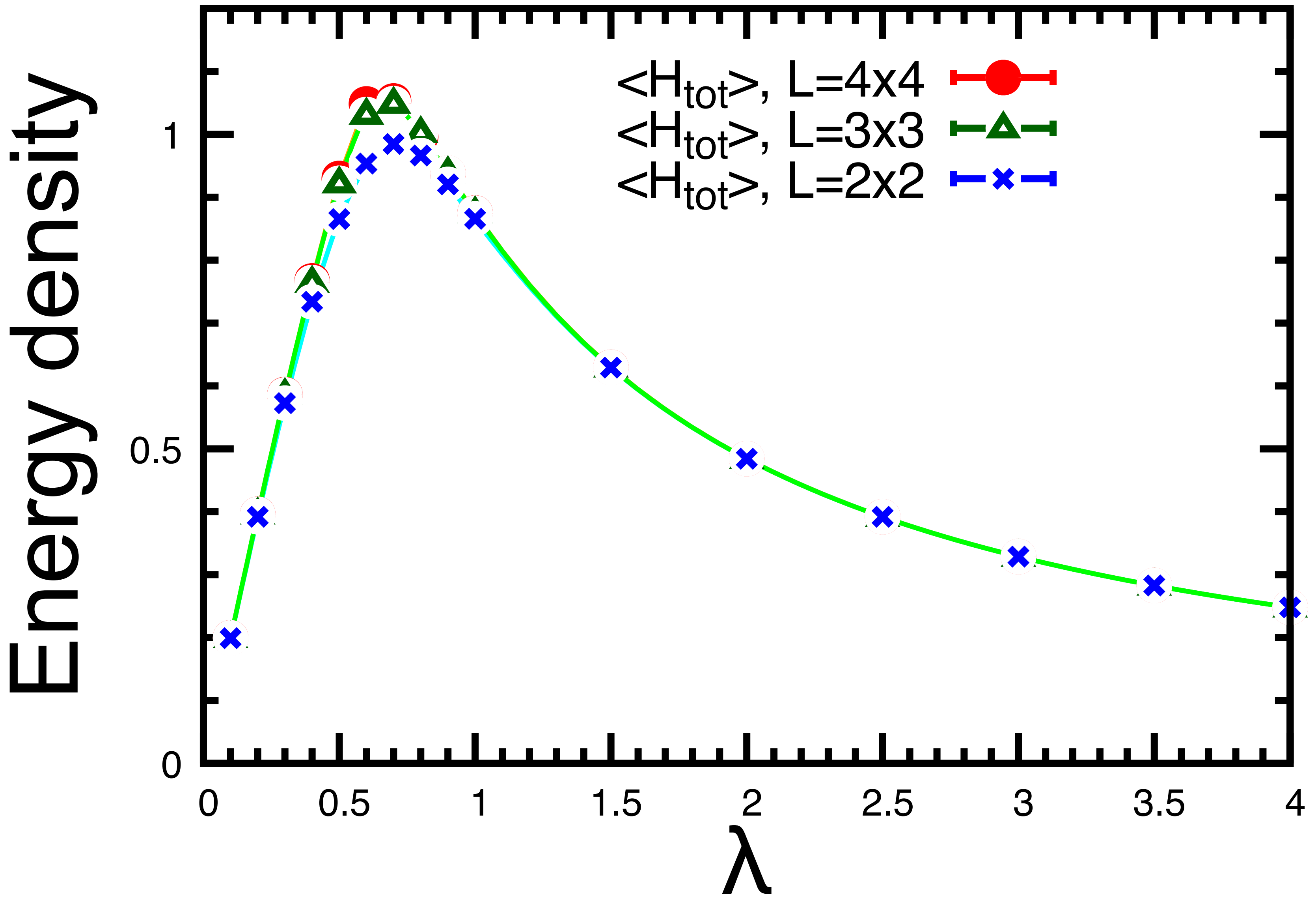




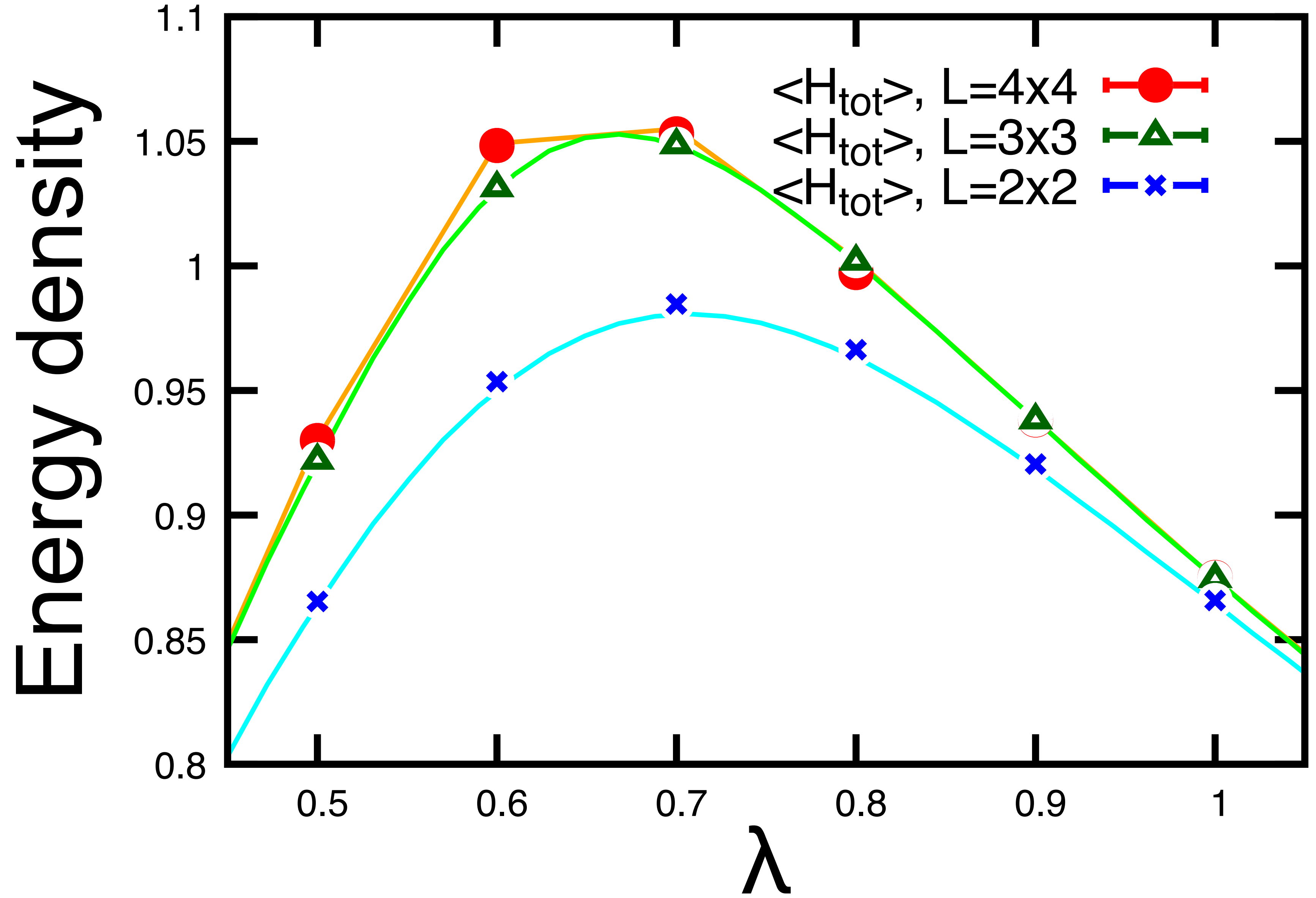
- total Energy
  magnetic Energy
  electric Energy
  In comparison with ED results
  This is F=2 ansatz result (8 variational params.)
  F=1 ansatz doesn't give good results
  especially for $\lambda \approx 0.7$

- Topological EE
  at $\lambda = 0$, the data reproduce S_{topo}= -ln(2)
  deconfined phase: S_{topo} >0
  confined phase : $S_{topo} \approx 0$
  cf.) QC calc. K. J. Satzinger et al., Science (2021)
  R.-Y. Sun et al., PRB(2023)

Volume dependence



Enlarged plot around λ_c



- L=4x4 (w/ HOTRG)
  L=3x3 (Exact contraction)
  L=2x2 (Exact contraction)
  In comparison with ED results

What is efficiently representation for gauge field Hilbert space?

- (general) Kogut Susskind Hamiltonian

$$H = g^2 H_E - \frac{1}{g^2} H_B \ , \quad \text{here } H_E = \sum_n \hat{E}^2_{n,\hat{x}} + \hat{E}^2_{n,\hat{y}}, \ H_B = \sum_n (\hat{U}_n + \hat{U}^\dagger_n)$$

electric part   magnetic part

- In general, $[E, U] \neq 0$

strong coupling basis (E-basis) or weak coupling basis (B-basis)

- The two bases are connected through a Fourier transform (U(1), $\mathbb{Z}_N$)

(character expansion for non-abelian gauge)

U(1): $U = e^{iA}, \ \ |A\rangle = \sum_{E_i} e^{iE_i A} |E_i\rangle$, here $A = [0, 2\pi)$, infinite sum of the value of A

$\mathbb{Z}_N$: $|U_k\rangle = (1/\sqrt{N}) \sum_n \omega^{-ikn} |E_n\rangle$, here $E_n \in \mathbb{Z}$, finite but sometimes large⋯

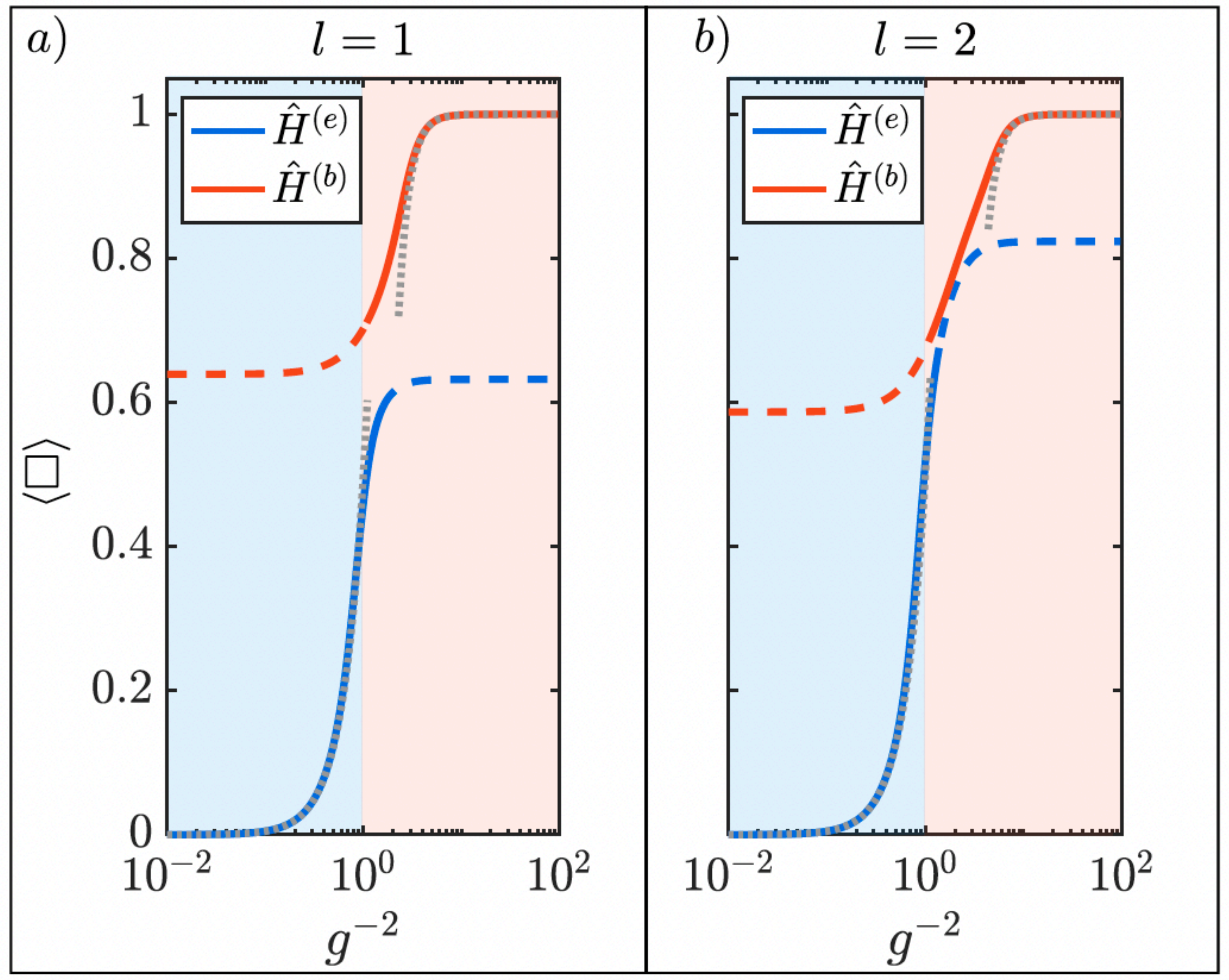
Naive truncation breaks connectivity between the two limits

2+1d $\mathbb{Z}_{2L+1}$ gauge theory w/ reduced Hilbert space ($l < L$)

$|-l\rangle, |-l+1\rangle, \cdots, |0\rangle, \cdots |l\rangle$ in large L (~U(1))

(Calculation method: VQE)

strong coupling



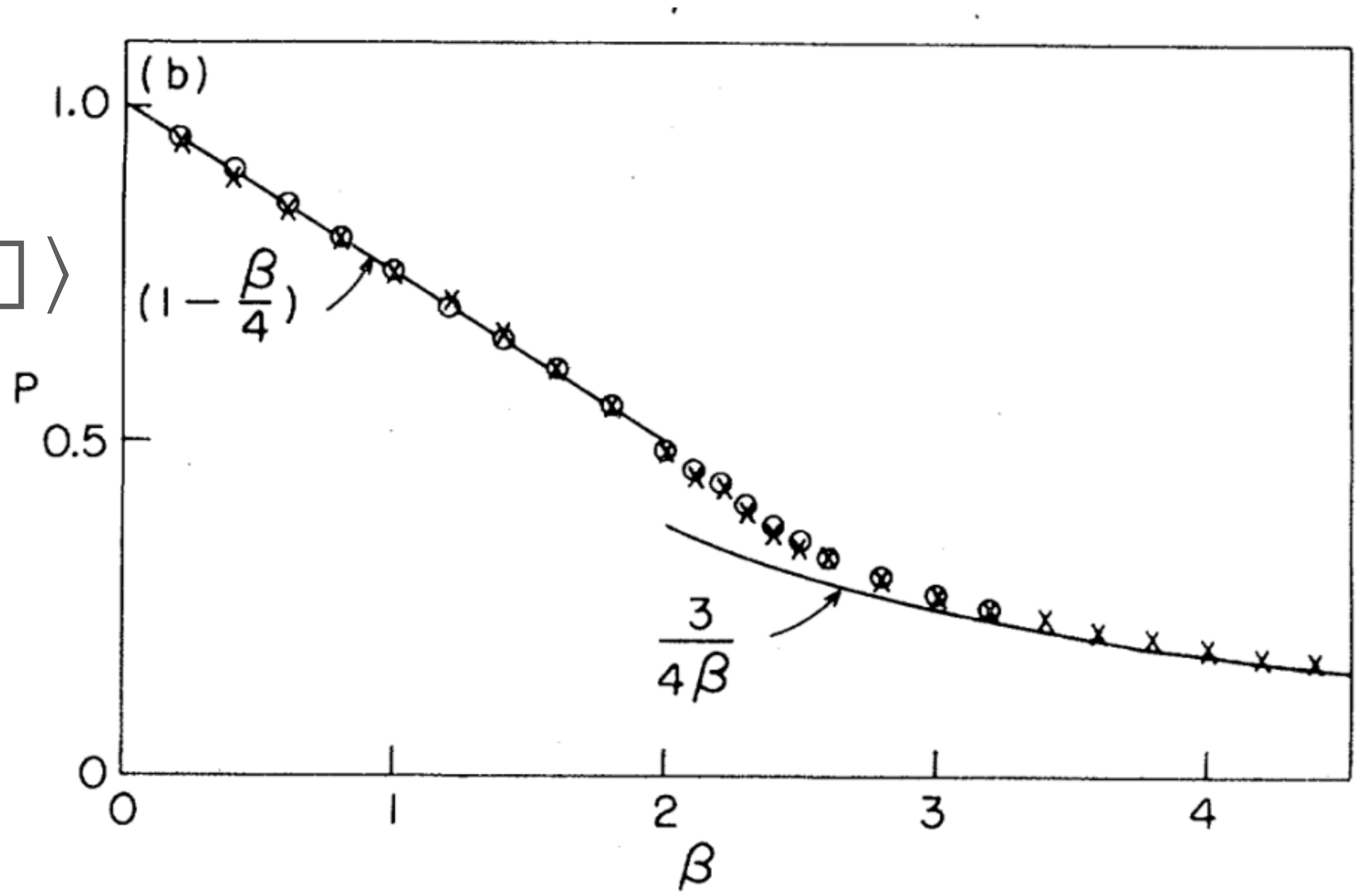
weak coupling

[Paulson et al. (2020)]

4d SU(2) gauge theory on 5^4 lattice

(Calculation method: Monte Carlo)

$1 - \langle \square \rangle$



[M.Creutz, PRL (1979)]

- The results agree with analytical solutions in both limits and their smooth connection allows the theory to take the continuum limit.

Entropic C-fn. in 4d SU(3) Yang-Mills theory

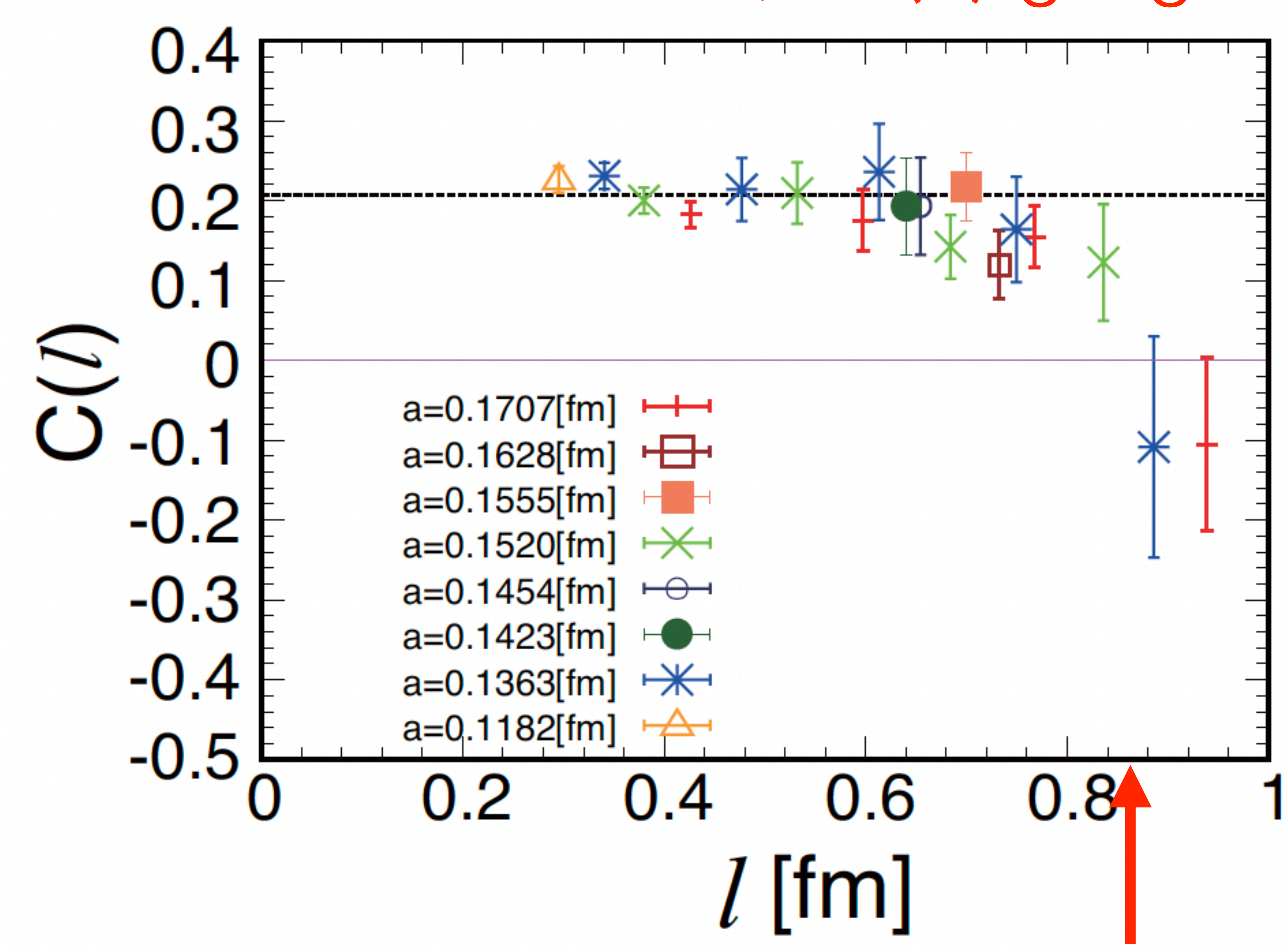
- 4(+0)d SU(N) gauge theory

EI, K.Nagata, Y.Nakagawa, A.Nakamura, V.I.Zakhanov
PTEP 2016 (2016) 6, 061B01

$$S_A(l) = c_0 \frac{\text{Area}}{a^2} - \boxed{c_0' \frac{\text{Area}}{l^2}} + c_1 \log(l/a) + (\text{regular terms})$$

entropic c-fn. $C(l) = l^3 \frac{1}{|\partial A|} \frac{\partial S_A}{\partial l}$

MC method, SU(3) gauge



C~0.2064

$$\boxed{\frac{1}{\Lambda_{\rm QCD}} \left(\frac{1}{T_c}\right) = 0.7 - 0.8[\text{fm}]}$$

✦ entropic c-fn. in short regime correctly counts # of (free) gluons

Ryu and Takayanagi:PRL96(2006)181602
JHEP 0608(2006)045

$C_{\rm gauge} \sim 2c' \cdot 2 \cdot 8 \sim 0.1568$

free real boson $c' \sim 0.0049$

Casini and Huerta:
Phys. Rev. D 93, 105031 (2016)
J. Phys. A42, 504007 (2009)

$C_{\rm gauge} \sim 0.177$

$(c' \sim 0.00553...)$

✦ C(l) decreases around Λ-scale

Quantitative evidence for EE as a probe of confinement!!

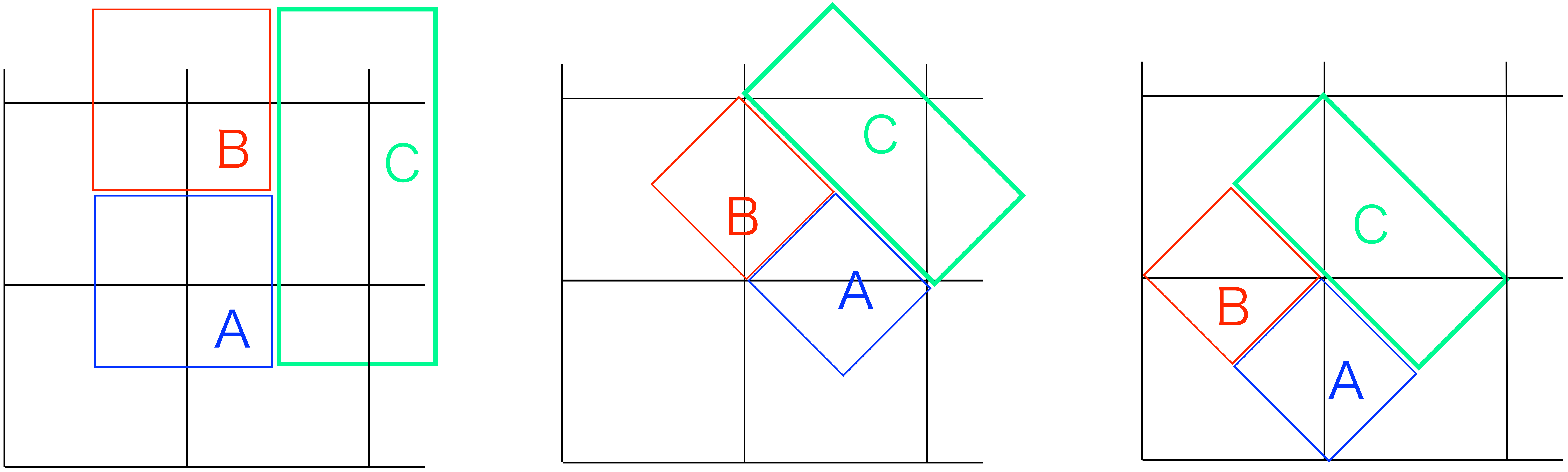
Comment on def. of EE for gauge theories

- If we cut a link, we need to sum over all gauge sectors
  The def. is natural for fermionic systems.

W.Donnelly PRD85 (2012) 085004
S.Ghosh et al., JHEP 09 (2015) 069
S.Aoki et al., JHEP 06 (2015) 187

- Here, we consider a pure gauge theory without fermionic dof on the sites. Then, we take the right def. of subsystems

"cutting a link" def.



Gauged Gaussian fermionic PEPS (GGPEPS) ansatz

- GGPEPS ansatz

Patrick Emonts, Mari Carmen Bañuls, Ignacio Cirac and Erez Zohar, PRD (2020)
Patrick Emonts et al., PRD(2023)
Review paper: Ariel Kelman et al., PRD(2024)
fermionic PEPS: C.V. Kraus, N. Schuch, F. Verstraete, and J. I. Cirac, PRA(2010)

$$|\psi\rangle = \underbrace{\langle\Omega|\prod_{x,i} w^\dagger(x,i)\mathcal{U}_{\mathcal{G}}\prod_{x} A(x)|\Omega\rangle}_{\text{calc. in Q-basis}}\underbrace{|\psi_E\rangle}_{\text{diagonal in P-basis}}$$

- Express a link variable using Gaussian operators of virtual fermions (r, u, l, d)

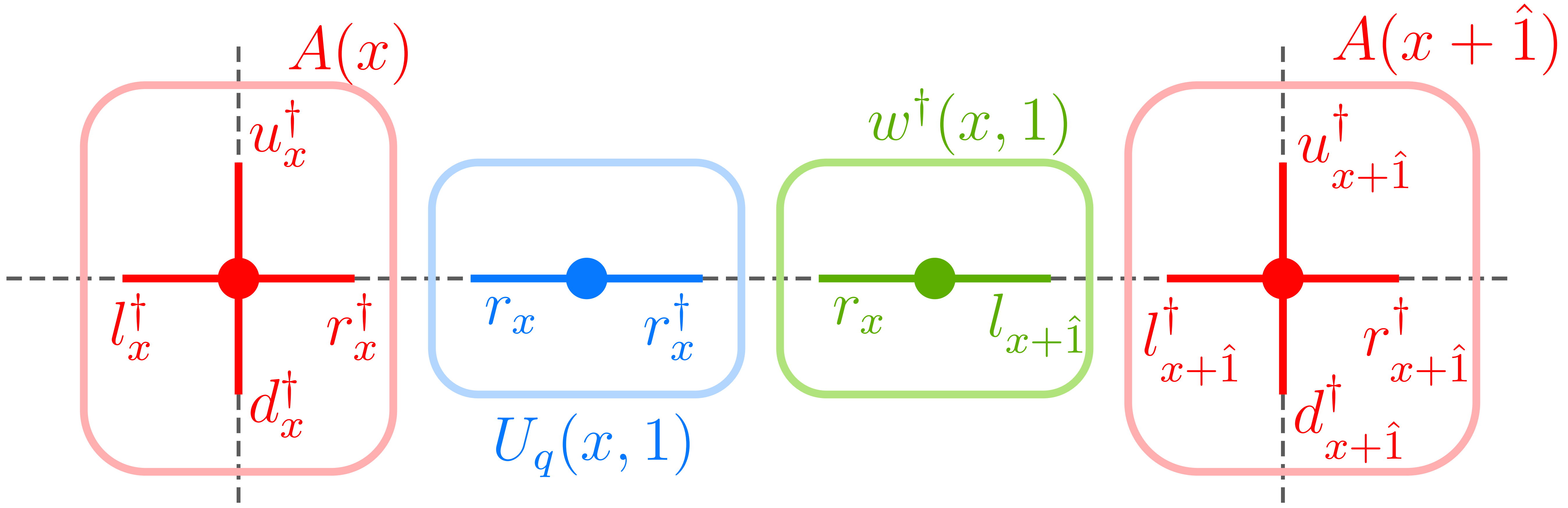
$$A(\mathbf{x}) = \exp\left(T_{\alpha\beta} a^\dagger_\alpha(\mathbf{x})\, a^\dagger_\beta(\mathbf{x})\right)$$

$$a_\alpha = \{r_1, u_1, l_1, d_1, \cdots, r_F, u_F, l_F d_F\}$$

$$w(\mathbf{x},1) = \exp\left(W^1_{\alpha\beta} l^\dagger_\alpha(\mathbf{x}+\hat{\mathbf{e}}_1)\, r^\dagger_\beta(\mathbf{x})\right)$$

$$\mathcal{U}_G(\mathbf{x},i) = \sum_q |q\rangle_{\mathbf{x},i}\langle q|_{\mathbf{x},i} \otimes \mathcal{U}_q(\mathbf{x},i)$$

$$\mathcal{U}_q(\mathbf{x},1) = \exp\left(i\pi q\sum_{\alpha=1}^{F} r^\dagger_\alpha(\mathbf{x})\, r_\alpha(\mathbf{x})\right)$$



- Imposing translational invariance,
  F=1 : 2 complex parameters (minimal ansatz)
  F=2 : 8 complex parameters
  F : dim. of rep. matrix of gauge field
  (# of virtual fermion= 4F)

Advantages of “Gaussian” GPEPS ansatz

- Difficulty of fermionic PEPS (in general): To calc. $\langle\Omega|\hat{a}^\dagger_\alpha(x_i)\cdots\hat{a}_\beta(x_j)\cdots\hat{a}^\dagger_\gamma(x_k)|\Omega\rangle$

  Align these ops. in the order “annihilation → creation” $|\Omega\rangle$

  But, fermionic ops. satisfies $\{\hat{a}^\dagger_i, \hat{a}_j\} = \delta_{ij}$

  Each exchange introduces a factor of (-1). Keeping track of the (-1) factors makes TN calculations complicated.
  -> Using Gaussian PEPS allows the use of the covariance matrix method and/or
  simplifies exchange calculations in (standard) TN approaches.

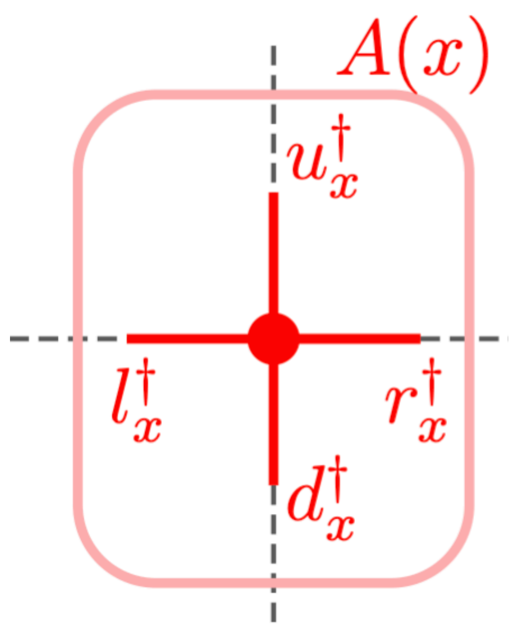
  S. Bravyi, Quantum Inf. and Comp. 5, 216 (2005)

- So far, to calc <O>, MC method has used, but statistical errors in MC make it difficult to optimize the variational parameters

Computational methods for GGPEPS so far

- A(x) has variational params.

$$A\left(\mathbf{x}\right) = \exp\left(T_{\alpha\beta} a_{\alpha}^{\dagger}\left(\mathbf{x}\right) a_{\beta}^{\dagger}\left(\mathbf{x}\right)\right)$$



$$a_\alpha = \{r_1, u_1, l_1, d_1, \cdots, r_F, u_F, l_F d_F\}$$

- The four links from site x are approximated by 4F virtual fermions.
  Imposing translational invariance,
  F=1 : 2 complex parameters (minimal ansatz)
  F=2 : 8 complex parameters

- Calculation strategy
  (1) Find the ground-state PEPS by variationally minimizing ⟨H⟩
  (2) Compute physical observables using the obtained state

- So far, to calc <O>, MC method has used, but statistical errors in MC make it difficult to optimize the variational parameters in (1)

E. Zohar and J. I. Cirac(2018)

Computational methods for GGPEPS so far

- Calculation strategy

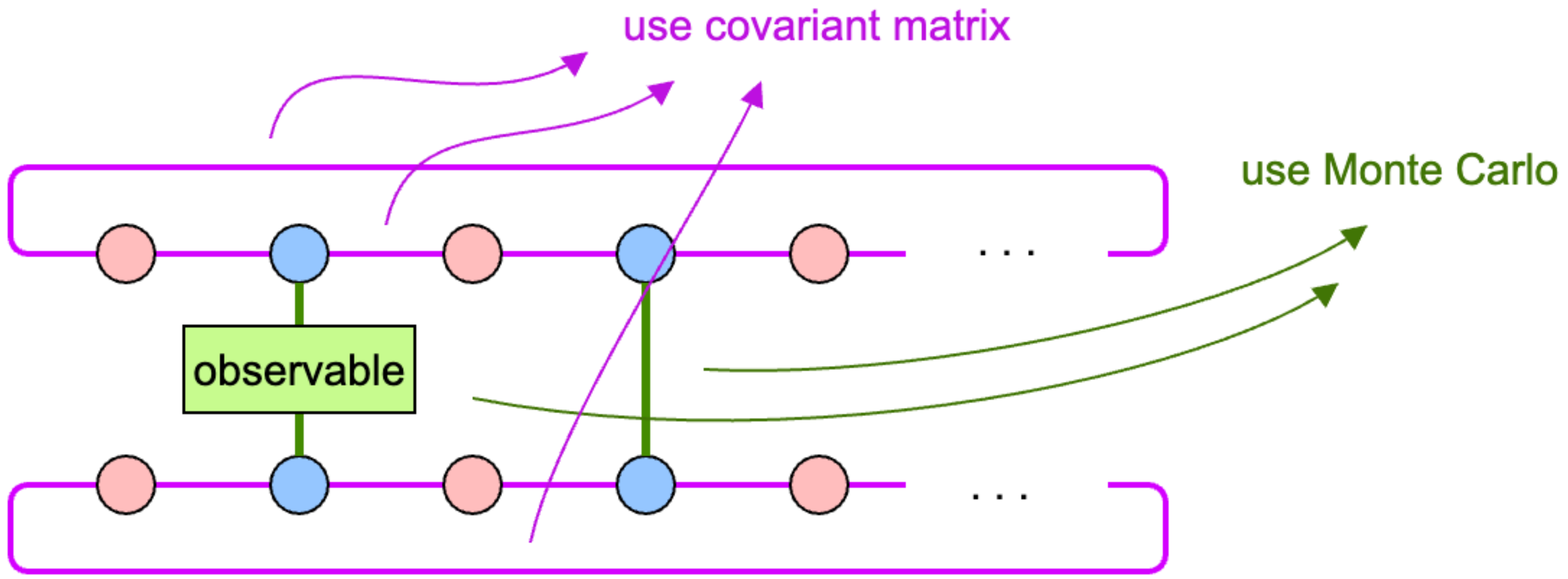
  (1) Find the ground-state PEPS by variationally minimizing ⟨H⟩

  (2) Compute physical observables using the obtained state

- Thanks to the Gaussian PEPS…,

  the use of the covariance matrix and variational MC accelerates the calculation.

E. Zohar and J. I. Cirac(2018)



$$\langle \psi | \mathcal{O} | \psi \rangle = \sum_q \langle q | \mathcal{O} | q \rangle \frac{\langle \psi_F(q) | \psi_F(q) \rangle}{\sum_{q'} \langle \psi_F(q') | \psi_F(q') \rangle}$$

Naive $\sum_q$ needs $\mathcal{O}(\exp(L^2))$ -> $\mathcal{O}(L^2)$ in MC

- However, statistical errors in MC make it difficult to optimize the variational parameters