Tensor network representation for numerical calculation and its application for the lattice QFT

[KN, Kei Suzuki arXiv:2207.14078]
[KN, L. Funcke, K. Jansen et al. arXiv:2107.14220]
[Daisuke Kadoh, KN arXiv:1912.02414]

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2022/10/06@Riken

Photo: Bonn, Germany, 2022

◉ Contents

Theoretical aspects of Lattice QFT

- What is the Lattice QFT?

Classical field theory on the discrete spacetime

$+$

Path integral quantization

$$Z = \int \mathrm{D}\phi e^{-S_{\text{lattice}}}$$

$$\downarrow$$

$$\int \mathrm{d}x \to \sum_x$$

Lattice quantum field theory

(with Monte-Carlo)

◉ Quantum correspondence

◇ Is there Quantum correspondence?

→Tensor network representation

$$\int D\overline{\psi}D\psi \exp\left[-\sum_x \mathcal{L}(\overline{\psi}_x,\psi_x)\right] \Longleftrightarrow \sum_{\sigma_i} \exp\left[-\beta\left(J\sum_i \sigma_i\sigma_{i+1} + h\sum_i \sigma_i\right)\right]$$

$$\{\overline{\psi},\psi\} \Longleftrightarrow \{\sigma_i\}$$

→ Need to consider path integral measure

(Another method: MPS, PEPS… as a Hamiltonian formalism)

◉ Tensor representation of numerical integration

◇ Physically？

1. Generalized transfar matrix (tensor)
2. Spin statistial representation (e.g. Ising model)
3. Hopping term expansion

◇ Advantages and disadvantages

○Sign problem

○Another representation ×High cost (high dim)

○Low cost (low dim) △Systematic error

○Partition function

→Tensor Renormalization group

◉ Examples: Variation of TRG

(Simple) Tensor renormalization group (TRG)

[M.Levin and C. P. Nave arXiv:cond-mat/0611687]

Higher-Order TRG (HOTRG)

[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

Triad TRG

[Daisuke Kadoh, KN arXiv:1912.02414]

◉ Examples: Variation of TRG

Simple TRG,
Anisotropic TRG,
Bond-weighted TRG,
Core TRG,
CTMRG,
GIRT,
HOTRG,
Randomized TRG,
SRG,
TNR,
Loop-TNR,
Triad TRG,…

…and these combinations.

◉ Examples: Variation of TRG

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◉ (Simple) Tensor renormalization group (TRG)

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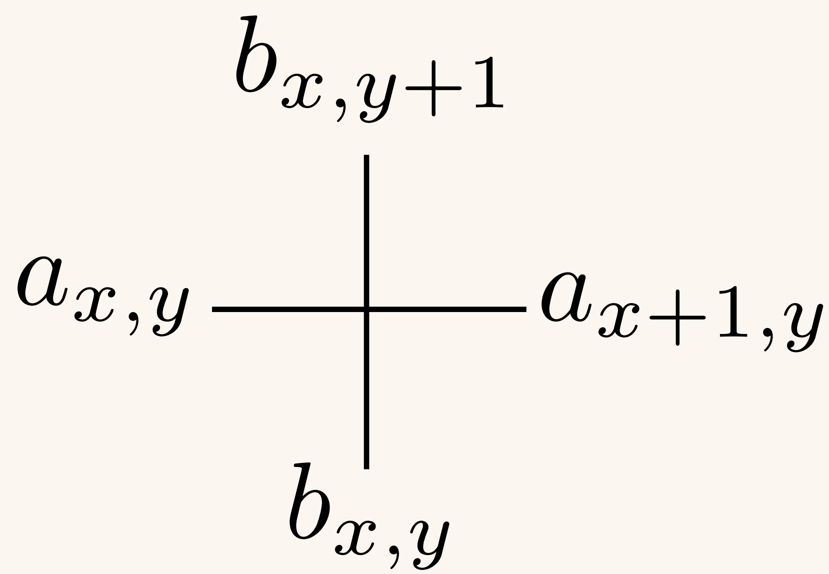
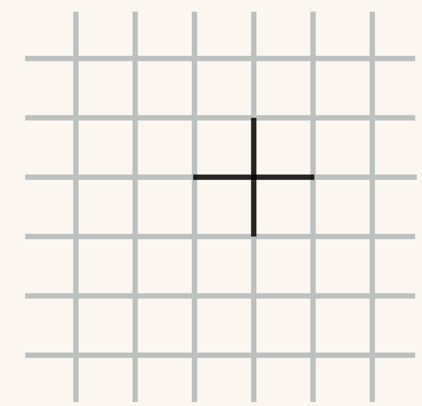
◇ Starting point: network representation

$$Z = \sum_{a,b} \prod_{x,y} T_{a_{x,y}, a_{x+1,y}, b_{x,y}, b_{x,y+1}}$$

$$T_{a_{x,y}, a_{x+1,y}, b_{x,y}, b_{x,y+1}} =$$



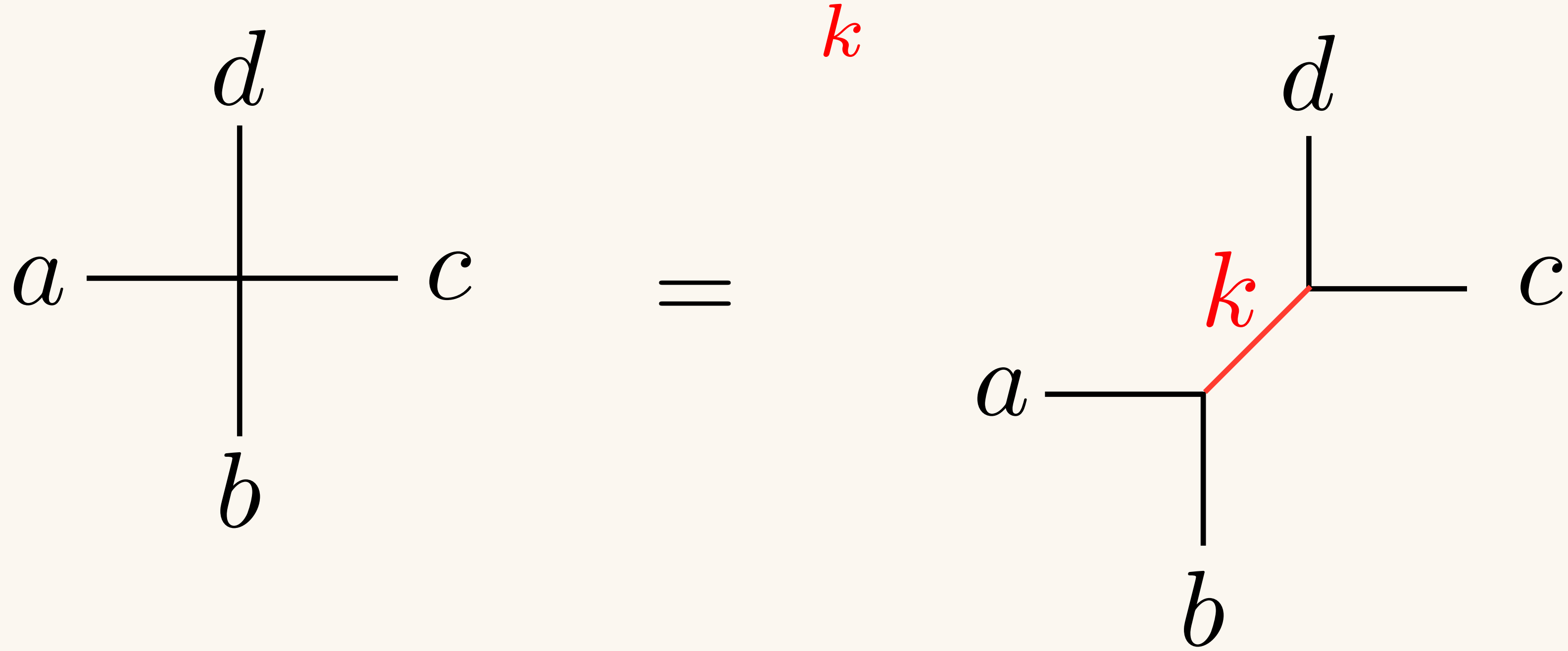


Naive contraction costs $\propto \{\mathrm{dim}(a)\mathrm{dim}(b)\}^{\mathrm{Volume}}$

→ How can we calculate (approximate) this contractions?

Singular Value Decomposition (SVD)

$$T_{abcd} = \sum_{k}^{D} A_{ab}{}^{k} \lambda^{k} B_{cd}{}^{k}$$



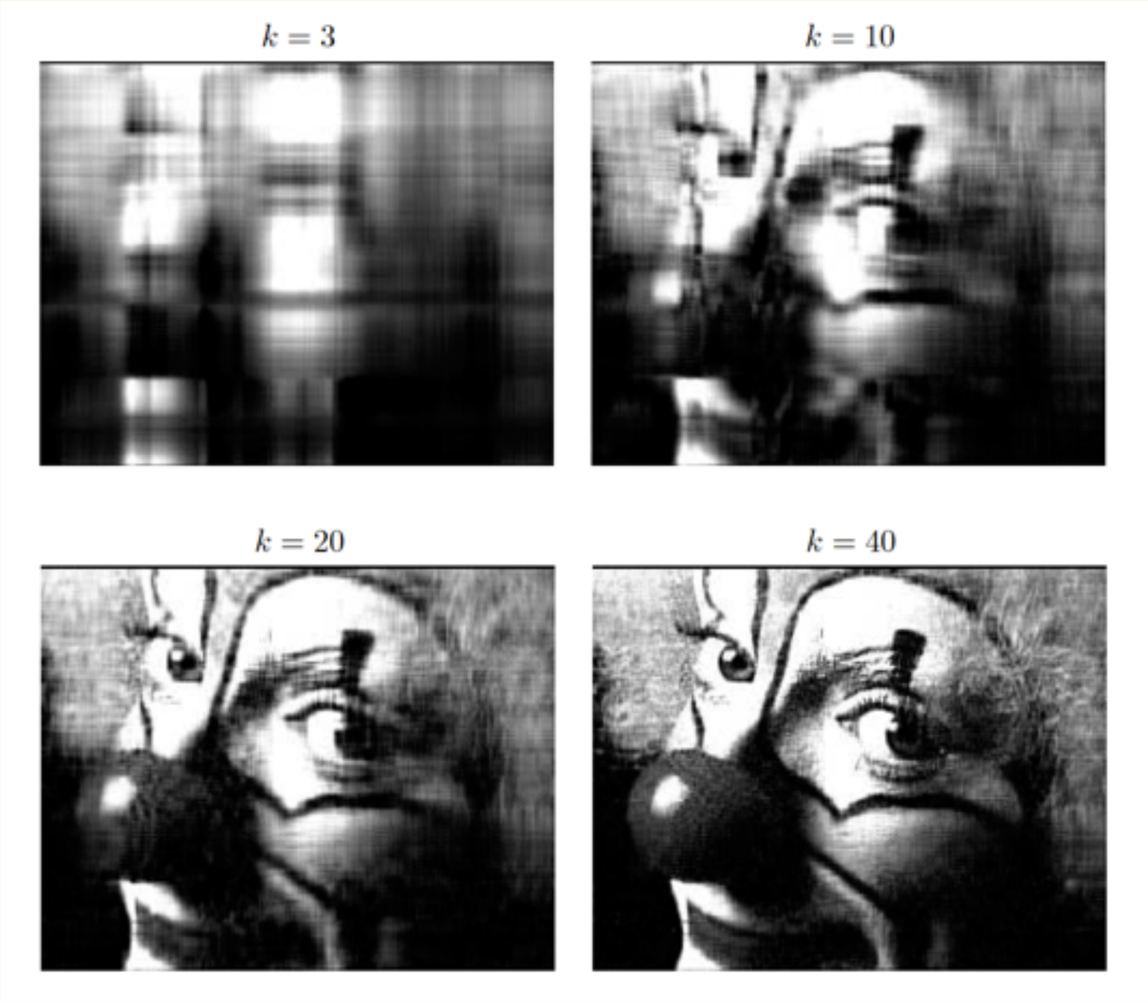
◇ Larger singular values λ have much "information" of T

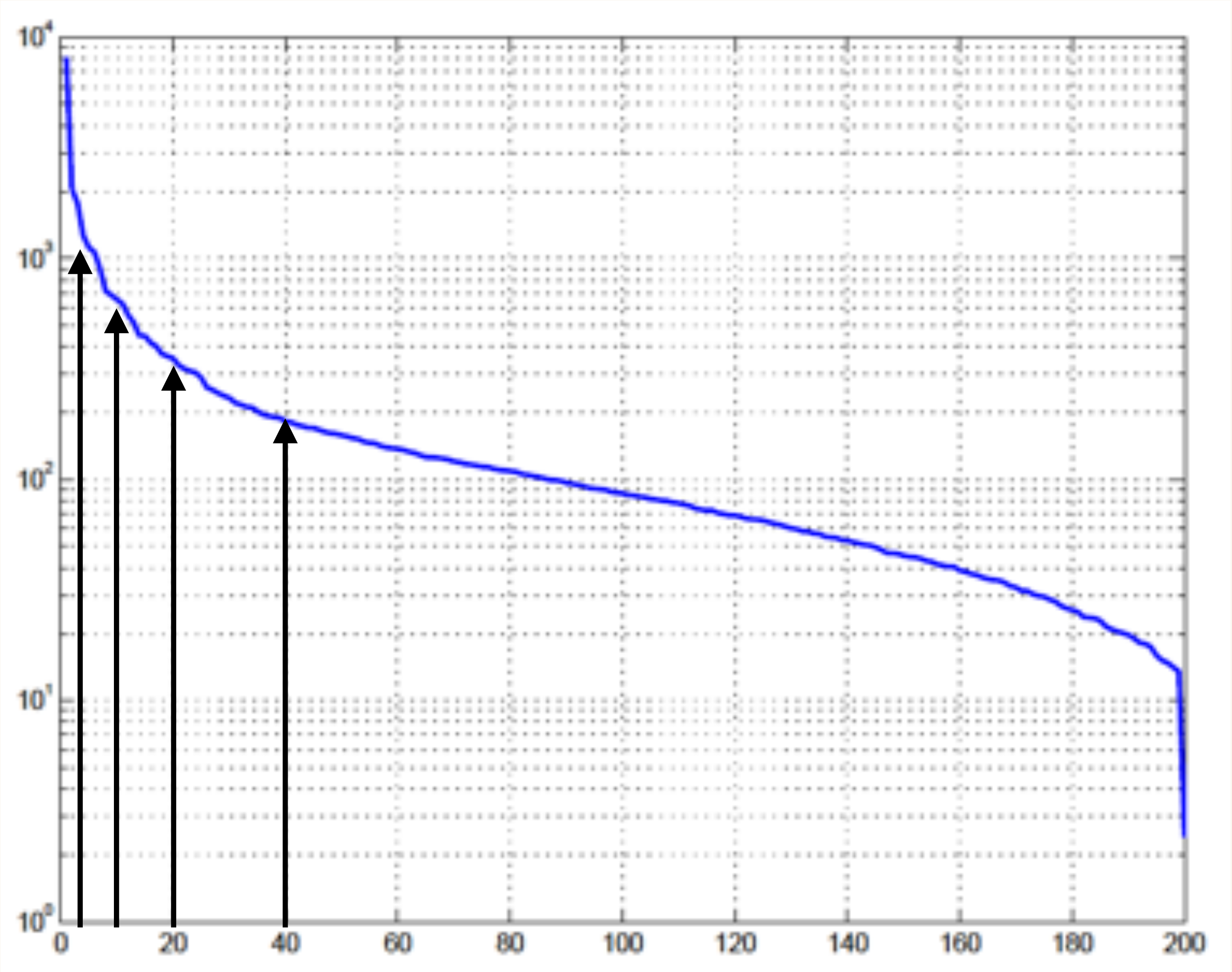
→ (Frobenius norm)

→ We can approximate the matrix by the cutoff of index k

$$\dim(k) = \dim(a)\dim(b) \to D$$

◉ SVD for a coarse graining (e.g. Image)

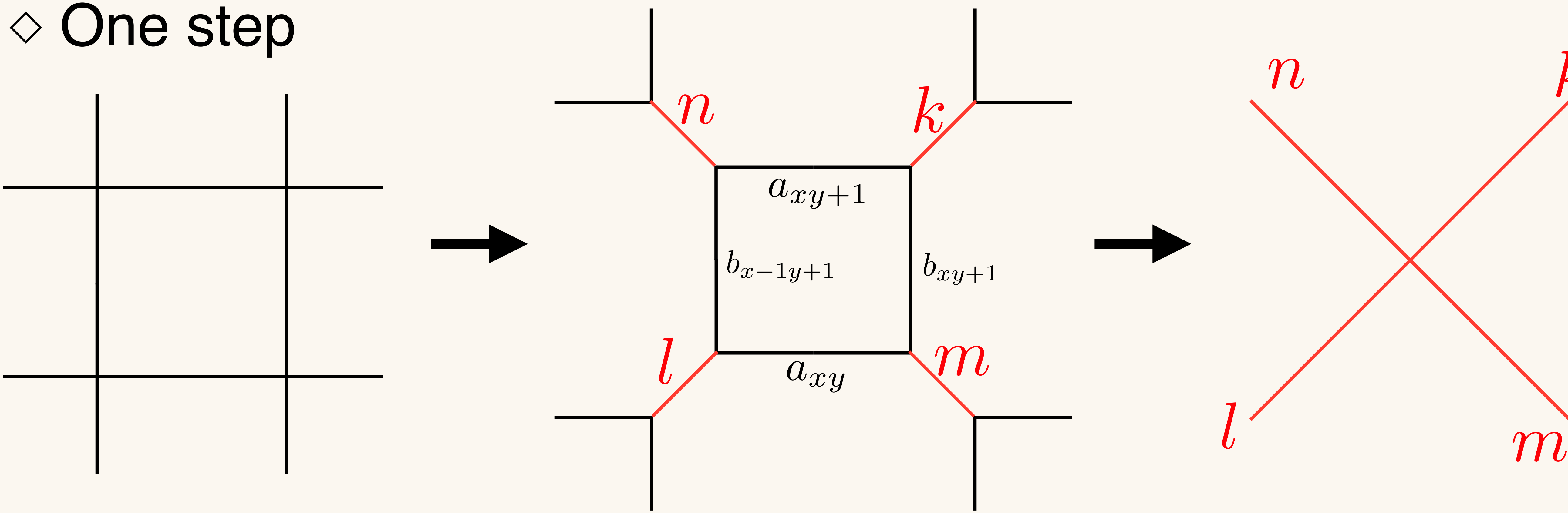




[http://www.na.scitec.kobe-u.ac.jp/~yamamoto/lectures/cse-introduction2009/cse-introduction090512.PPT]

◉ SVD for a coarse graining (e.g. Ising)

◇ One step



$$T_{abcd} = \sum_k A^k_{ac} B^k_{bd}$$

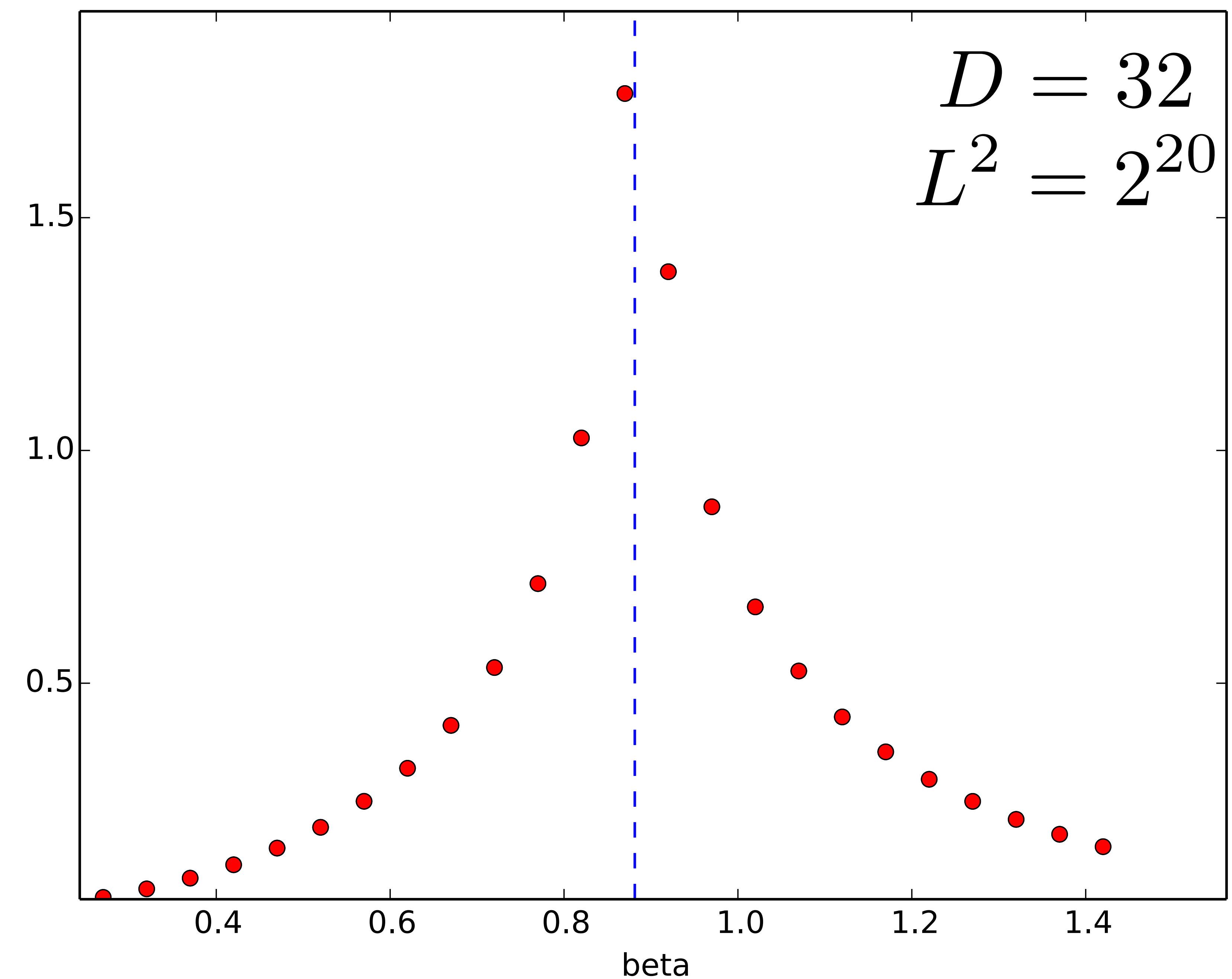
$$T_{abcd} = \sum_k C^k_{ad} D^k_{bc}$$

$$T^{(n+1)}_{klmn} = \sum_{a,b} A^k_{a_{xy+1} b_{xy+1}} B^l_{a_{xy} b_{x-1y+1}} C^m_{a_{xy} b_{xy+1}} D^n_{a_{xy+1} b_{x-1y+1}}$$

→ Exponential Volume reduction $V \to \dfrac{V}{2}$

◉ SVD for a coarse graining (e.g. Ising)

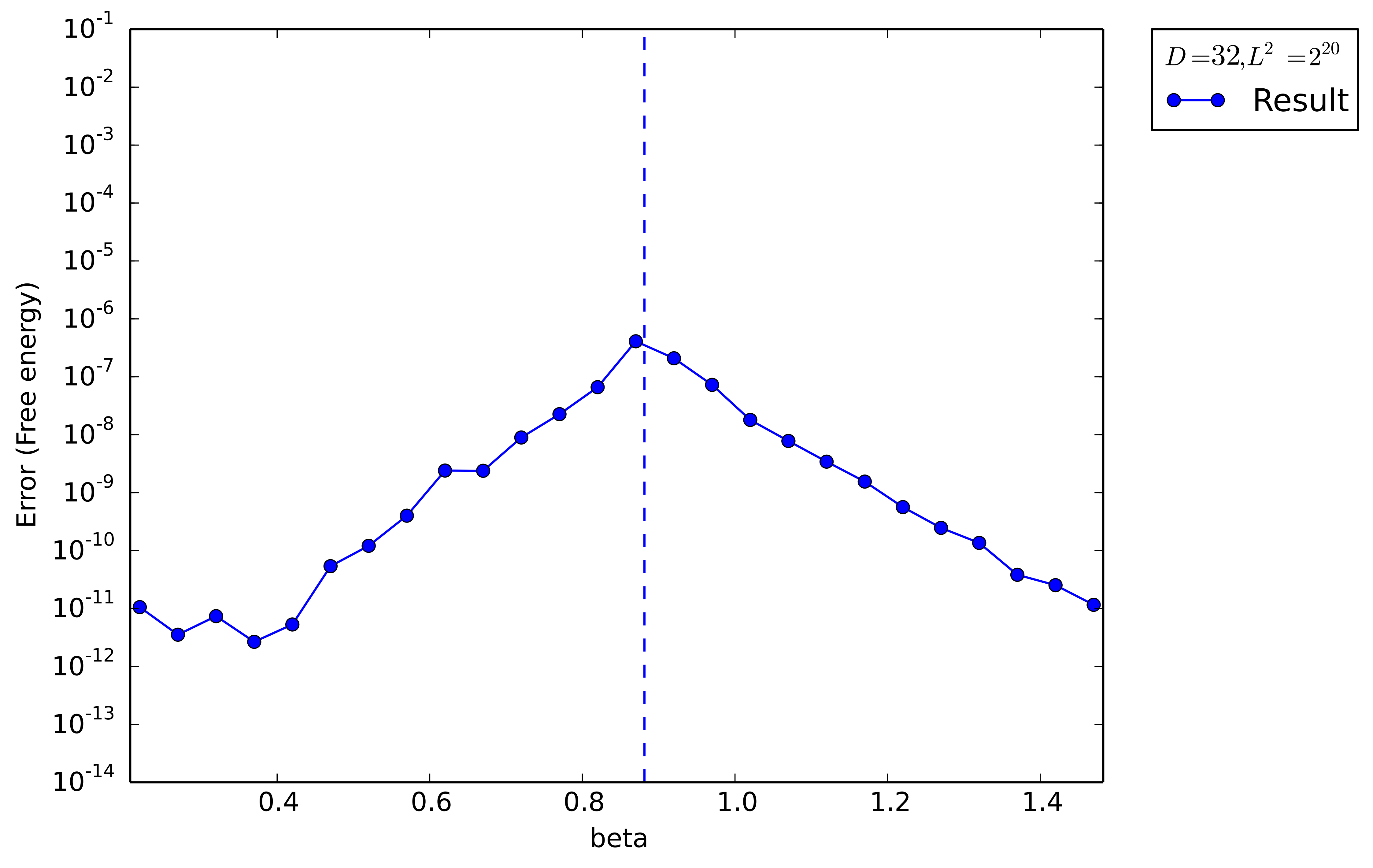
◇ Critical behaviour (Specific heat)



75[s], by truncated SVD

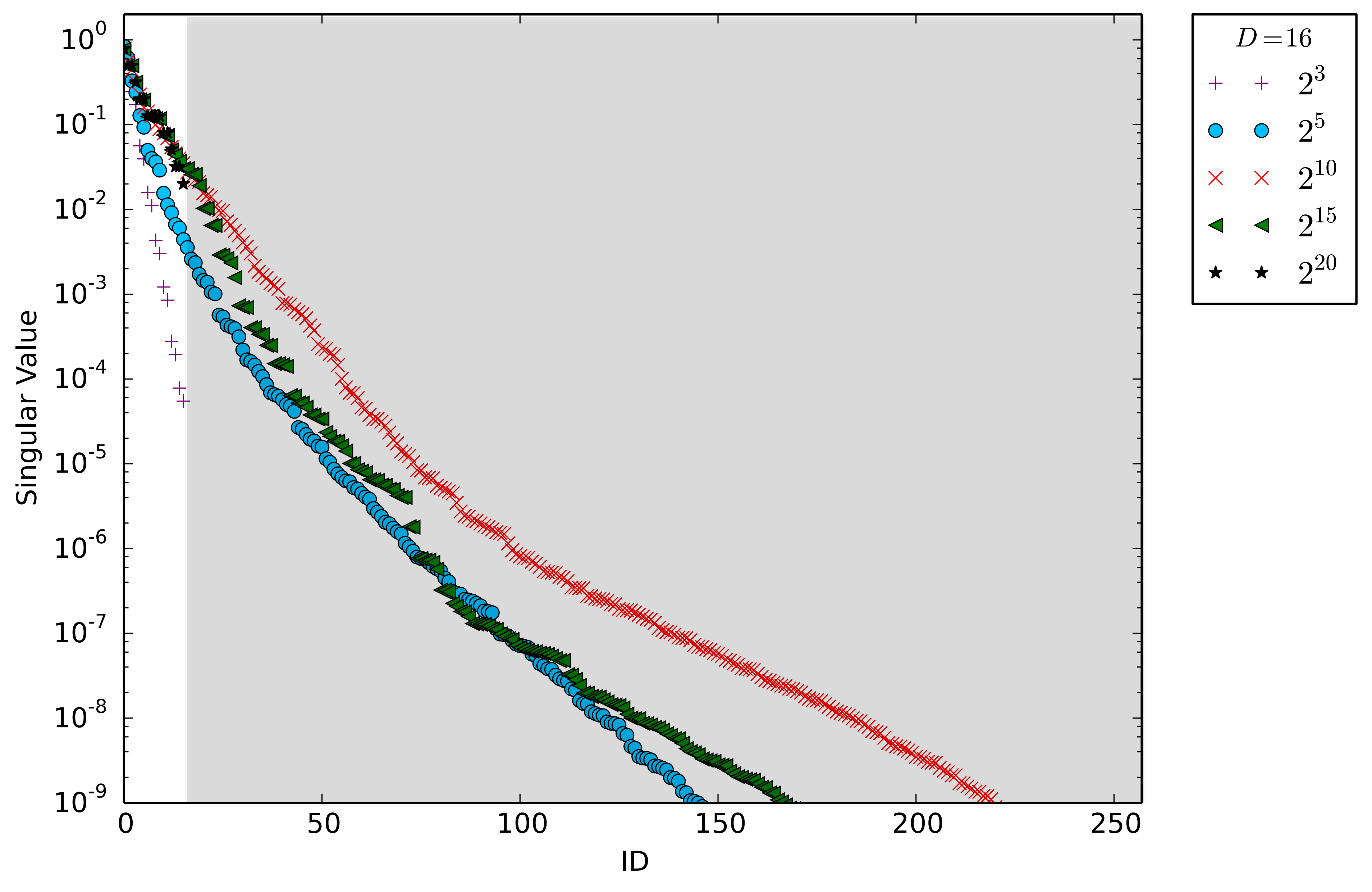
◉ SVD for a coarse graining (e.g. Ising)

◇ Difference from exact result (Free energy)



◉ Exponential damping of singular value

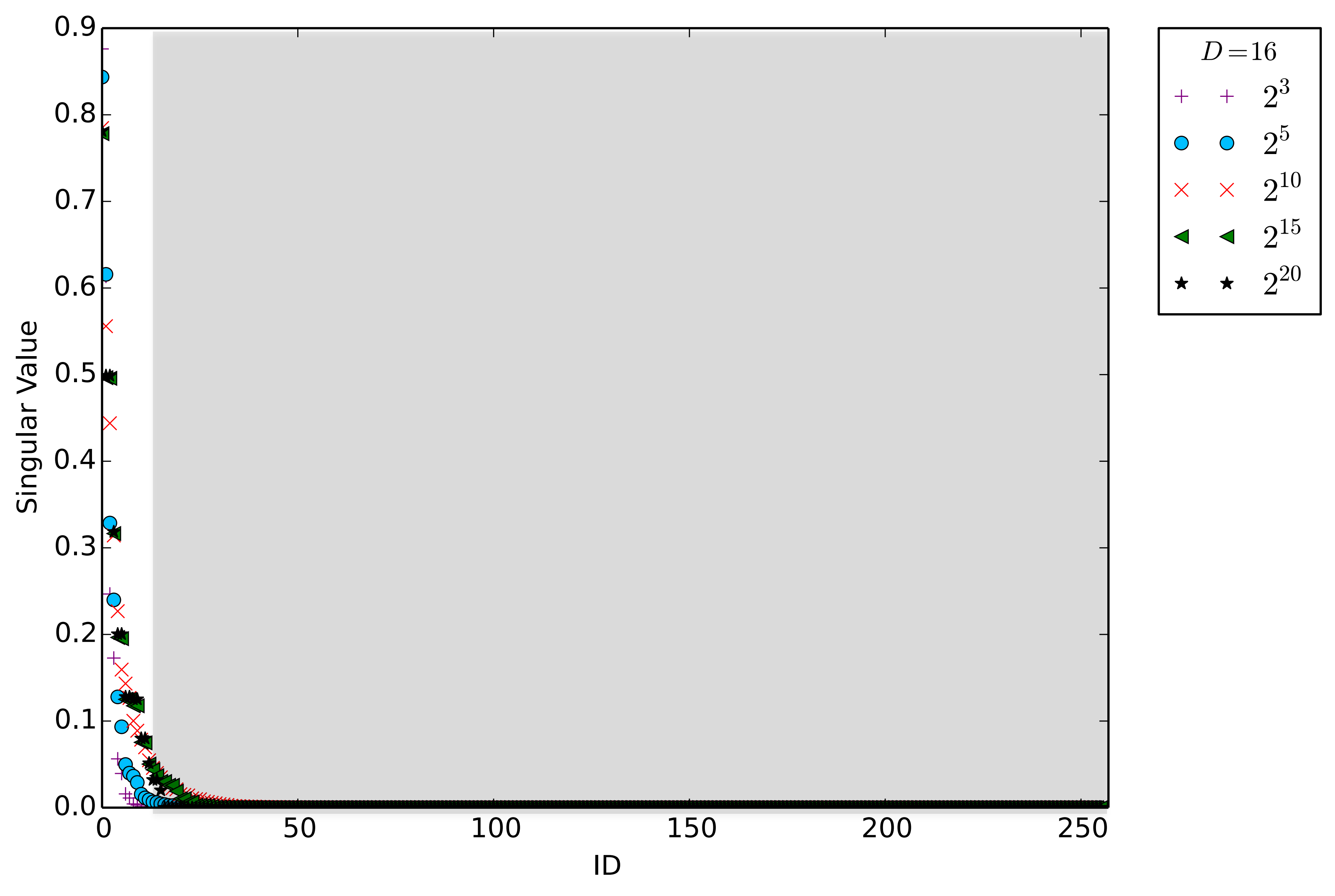
◇ Why this truncation is so good?



→ Exponential damping helps the approximation

Exponential damping of singular value

◇ Why this truncation is so good?



→ Exponential damping helps the approximation

◉ Numerical costs for simple TRG

◇ How fast?

SVD: $$T_{abcd} = \sum_k A^k_{ac} B^k_{bd}$$ $O(D^6)$

Contraction: $$T^{(n+1)}_{klmn} = \sum_{a,b} A^k_{a_{xy+1} b_{xy+1}} B^l_{a_{xy} b_{x-1y+1}} C^m_{a_{xy} b_{xy+1}} D^n_{a_{xy+1} b_{x-1y+1}}$$ $O(D^6)$

$$2^{2V} \to O((\log V) \times D^6)$$

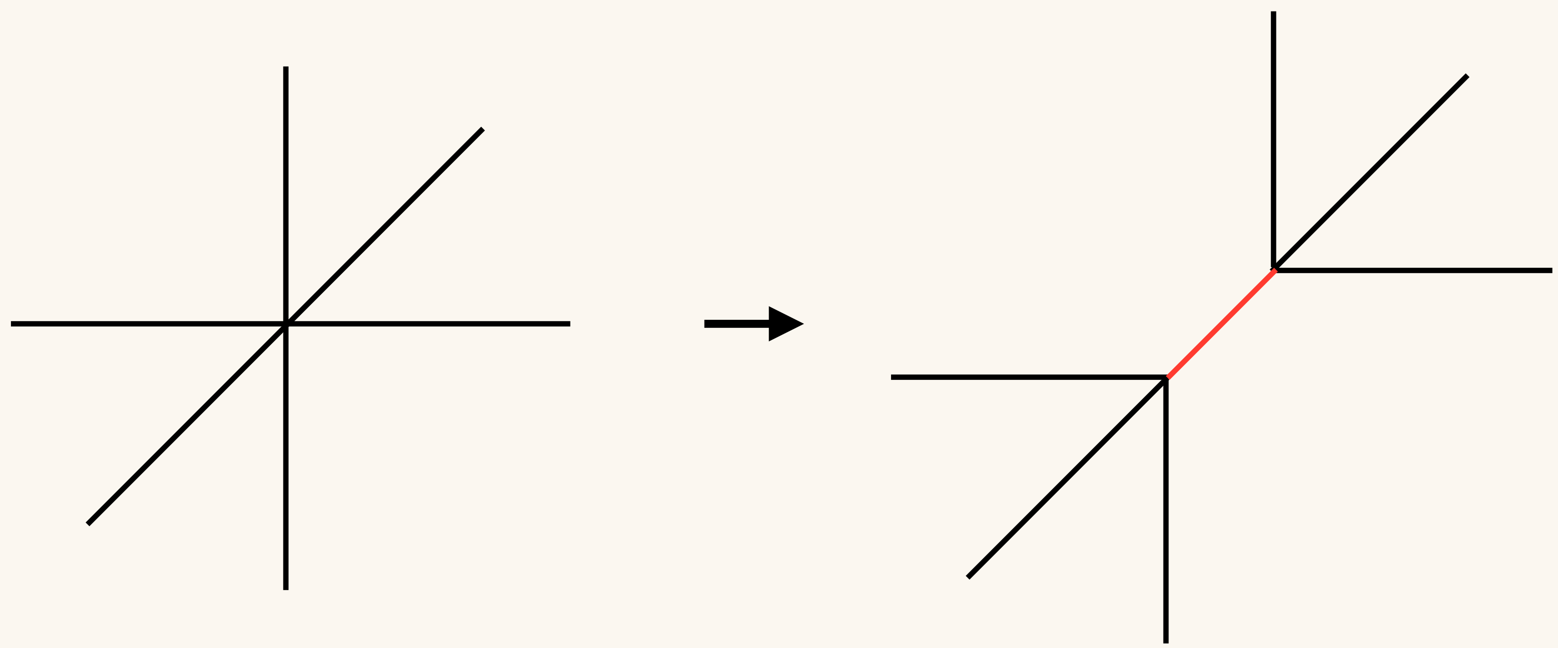
◇ Large D is still difficult.
(Higher dimension, complicated system…)

→ We need more sophisticated algorithm.

◉ Cost for Higher-dimensional system

◇ Can we generalize (simple) TRG for higher dimension?

→ Formally we can, but bad approximation (and Cost)



Cutoff:	$D^3 \to D$
Cost:	$O(D^{12})$

We need more faster method (for more interesting system)

◉ Examples: Variation of TRG

(Simple) Tensor renormalization group (TRG)

[M.Levin and C. P. Nave arXiv:cond-mat/0611687]

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[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

Triad TRG

[Daisuke Kadoh, KN arXiv:1912.02414]

◉ Higher-Order TRG (HOTRG)

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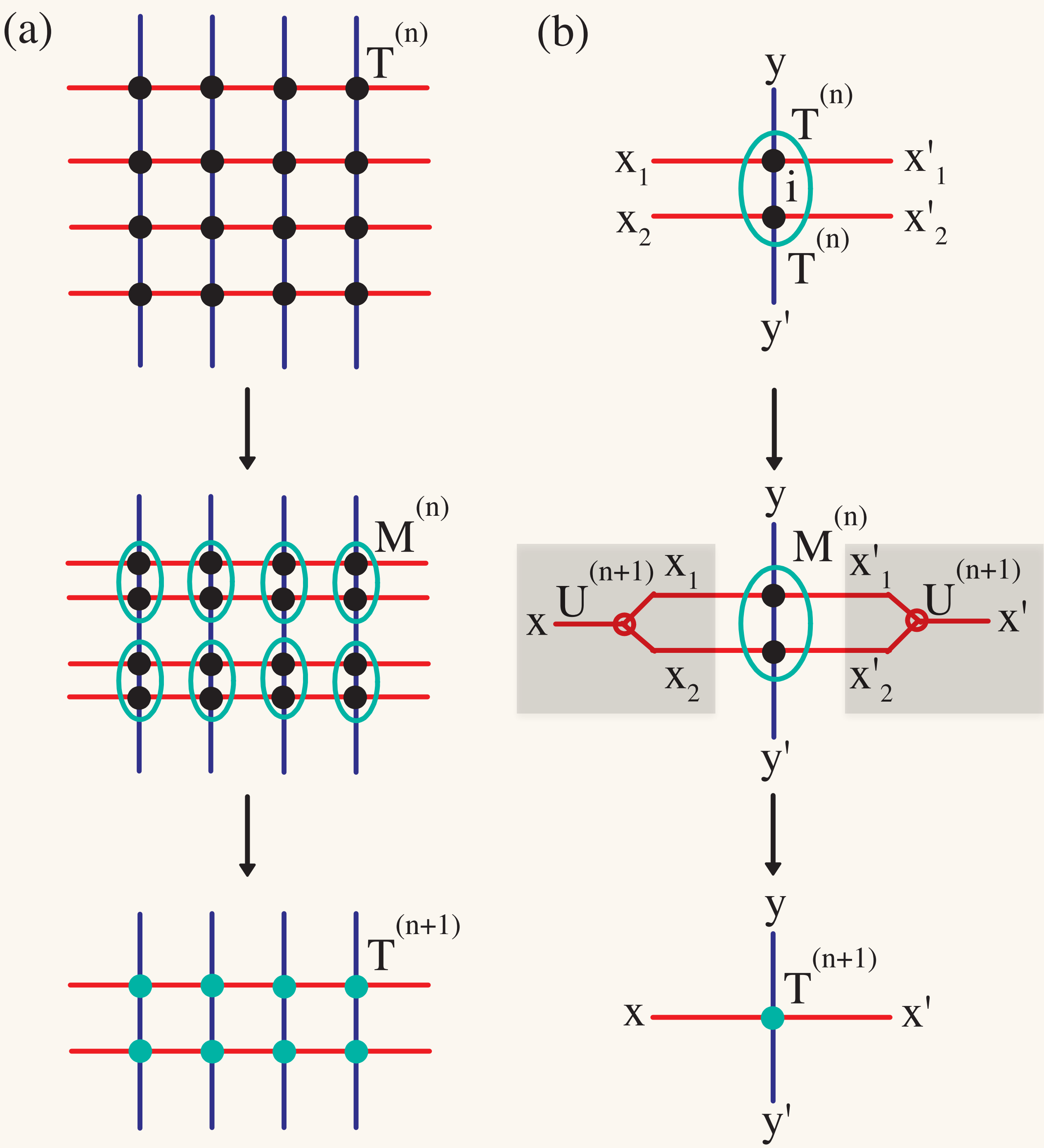
◇ Contraction by projection operator U



→ U is made by SVD

$$M_{x_1x_2x'_1x'_2yy'} \equiv \sum_k T_{x_1x'_1yk}T_{x_2x'_2ky'}$$

$$[M^tM]_{[x_1x_2][\chi_2\chi_2]} \equiv \sum_{abcd} M^t_{[x_1x_2][abcd]}M_{[abcd][\chi_1\chi_2]}$$

SVD Cutoff: $D^2 \to D$
Cost: $O(D^6)$

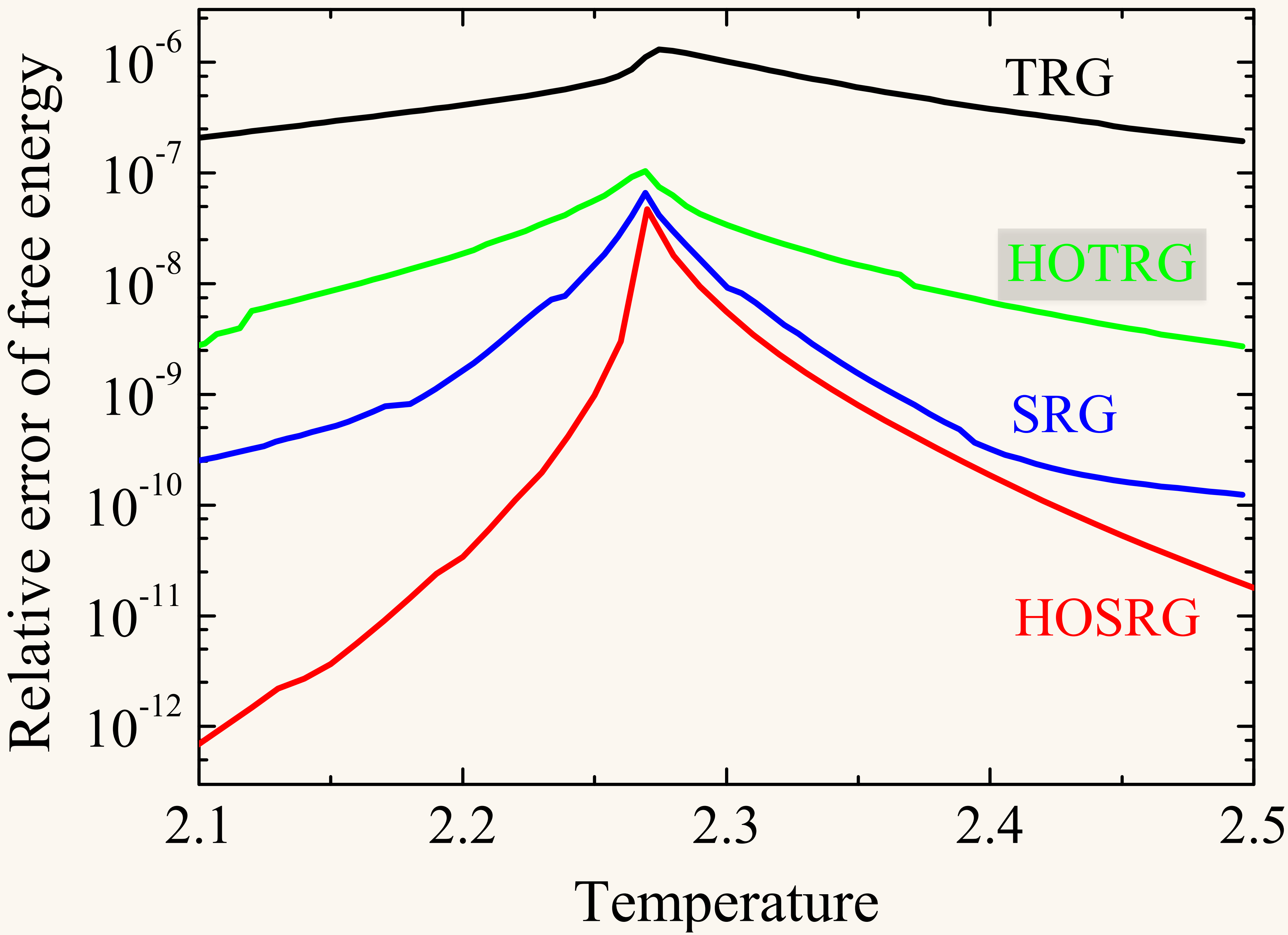
$$[M^tM]_{[x_1x_2][\chi_2\chi_2]} = \sum_k U^k_{[x_1x_2]}\lambda^k U^k_{[\chi_1\chi_2]}$$

Contraction Cost: $O(D^7)$

◉ Higher-Order TRG (HOTRG)

[Z.Y. Xie, J. Chen, et al. arXiv:1201.1144]

◇ Critical behaviour

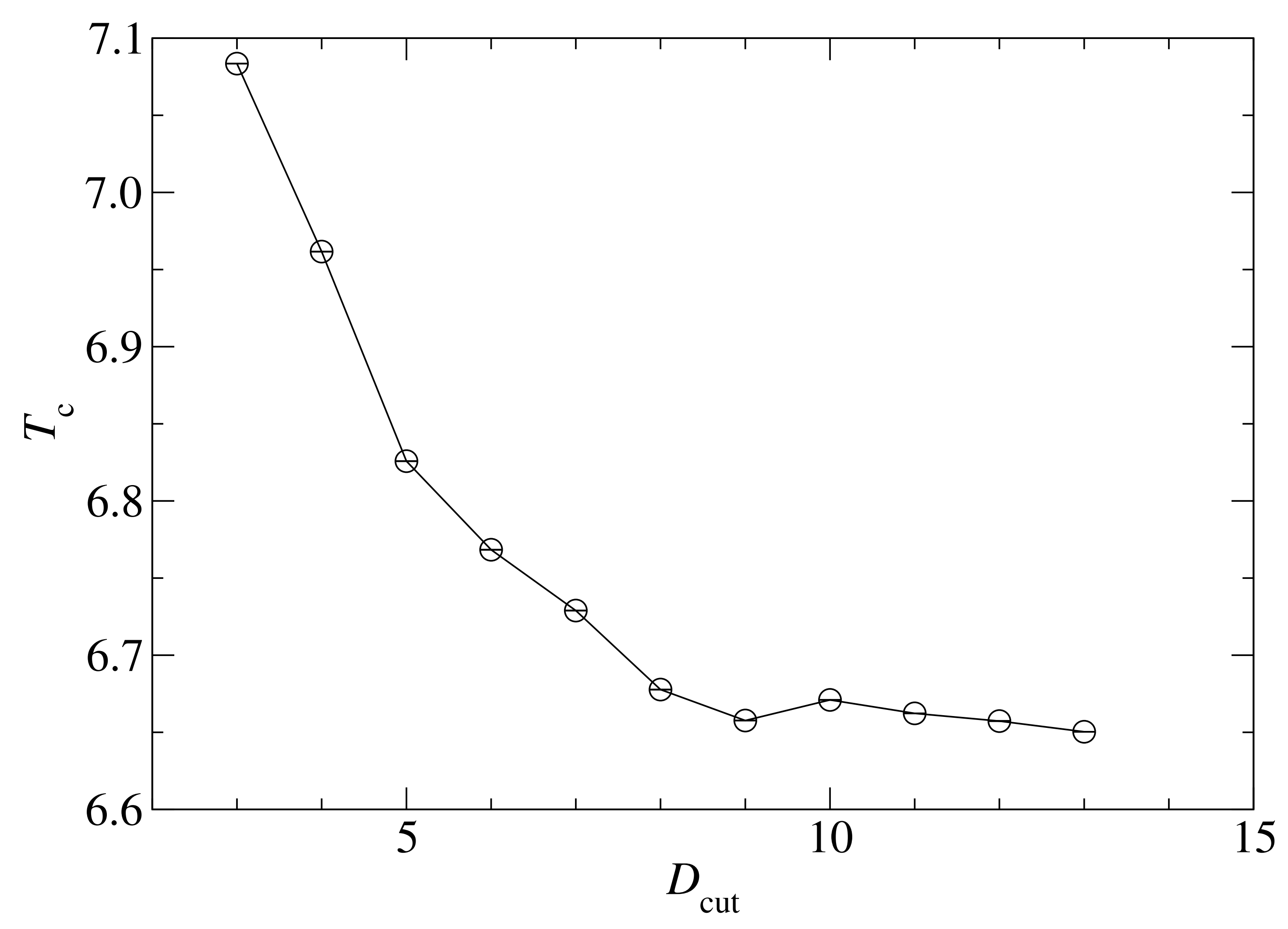


◉ Numerical costs for HOTRG

◇ More higher dimension? → still difficult.

Cost: $O(D^{4\mathrm{dim}-1})$

◇ 4-dim Ising $O(D^{15})$ [S.Akiyama, Y.Kuramashi et al. arXiv:1906.06060]



$D = 13$ @Oakforest-PACS

$$L^4 \leq 1024^4$$

$$T_c(D = 13) = 6.650365(5)$$

Monte-Carlo

$$L^4 \leq 80^4 \qquad (200)$$

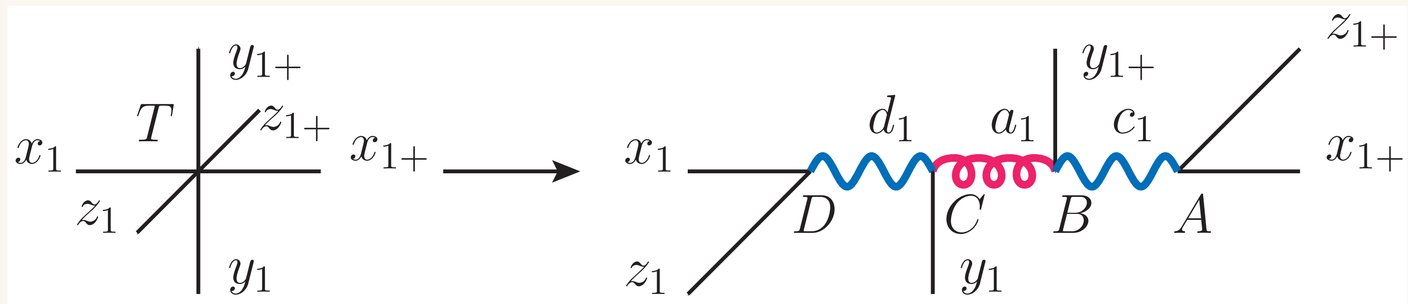
$$T_c = 6.68026(2)$$

[P.H. Lundow and K. Markstrom arXiv:1202.3031]

◉ Triad RG

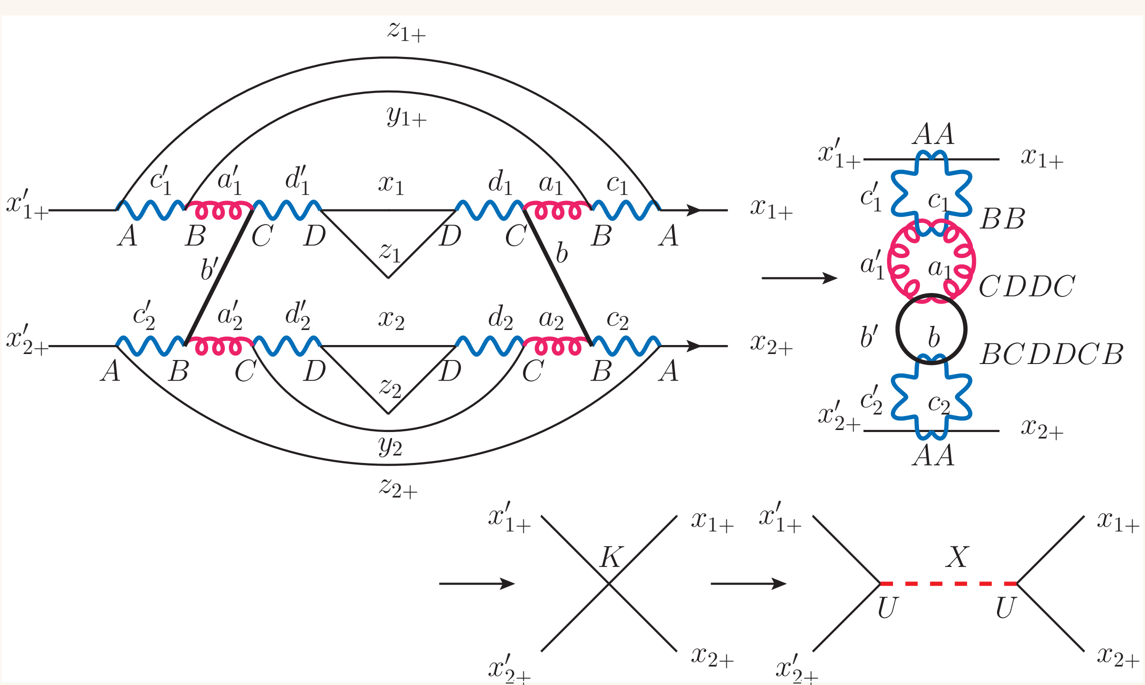
[Daisuke Kadoh, KN arXiv:1912.02414]

◇ Using the Triad (Rank-3) tensor as a fundamental tensor

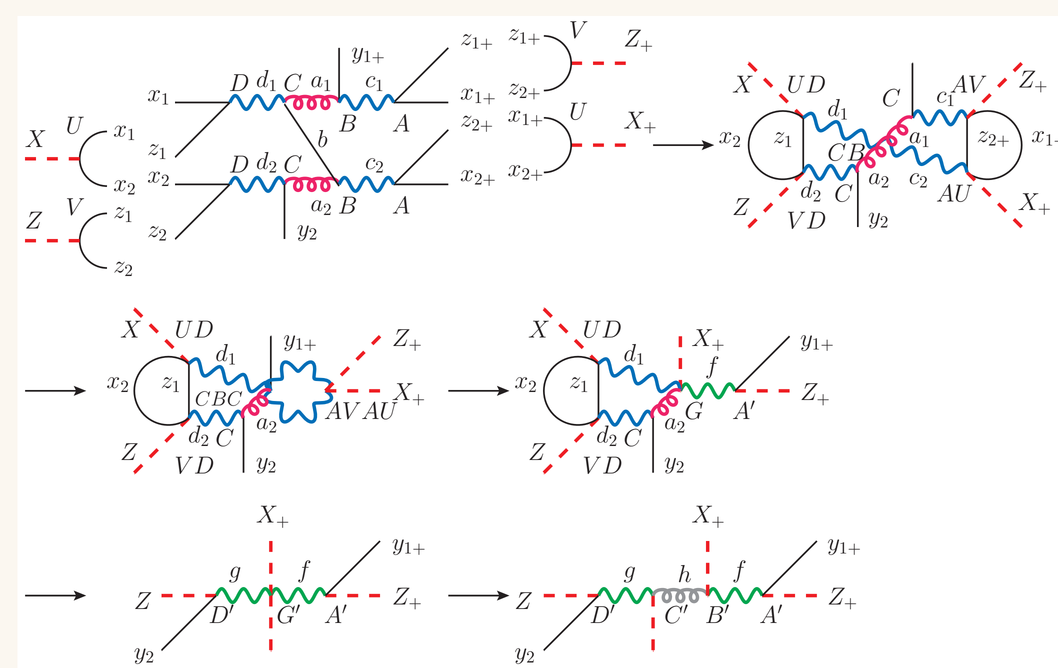


→ We apply HOTRG-like procedure to Triad tensor rep.

◇ projection operator U



◇ contraction part



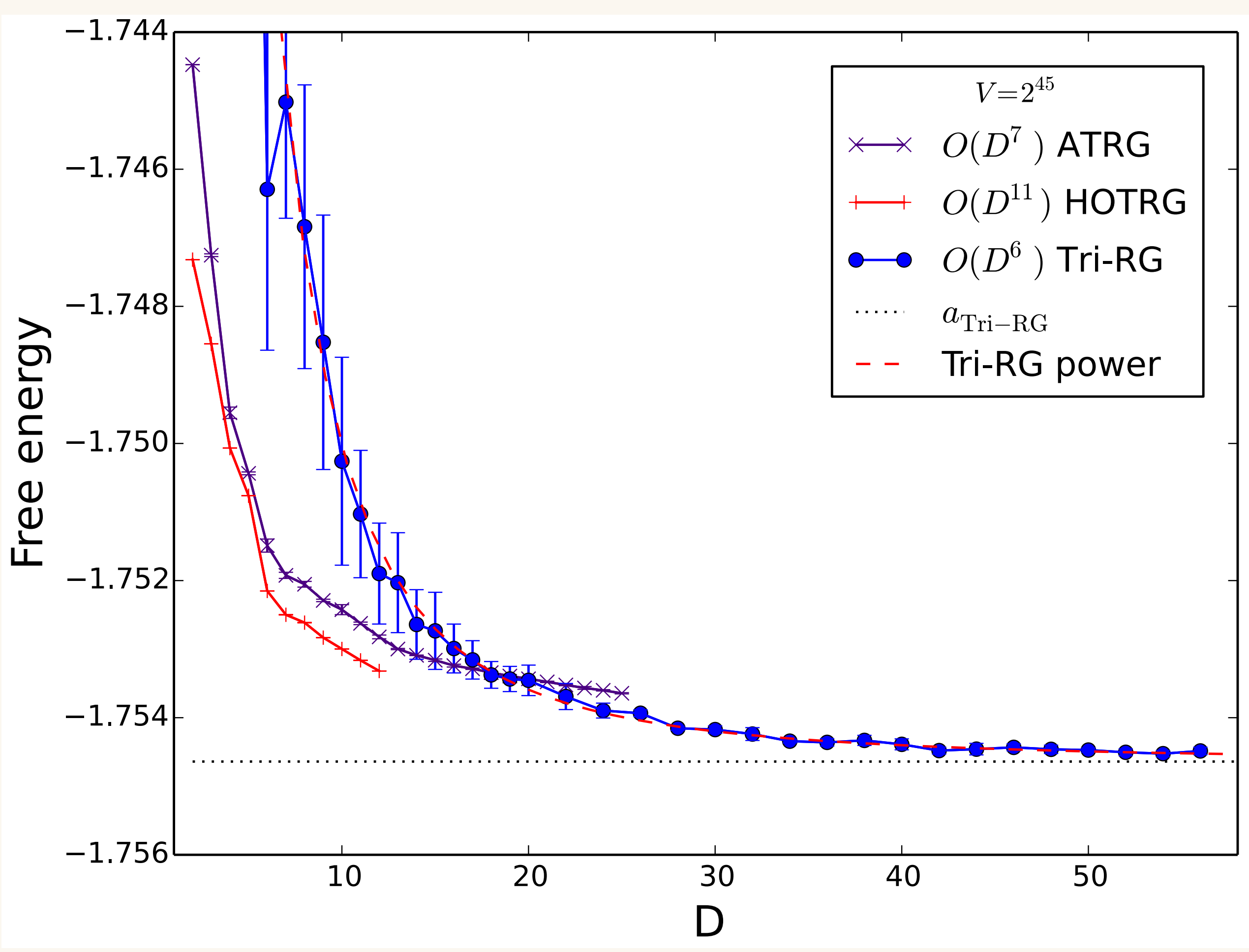
Triad RG

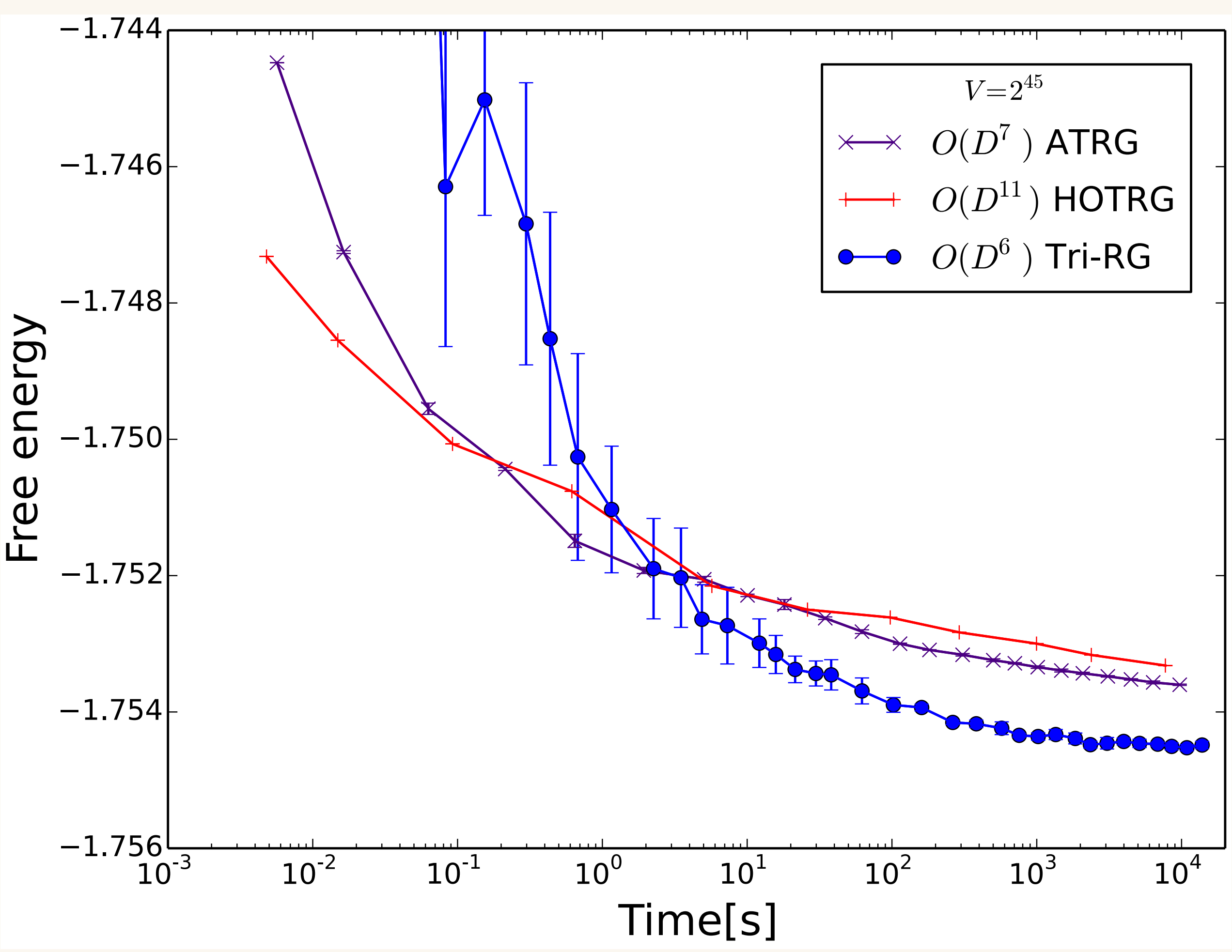
[Daisuke Kadoh, KN arXiv:1912.02414]

◇ Triad rep. reduces the cost.

$$O(D^{4\mathrm{dim}-1}) \to O(D^{\mathrm{dim}+3})$$

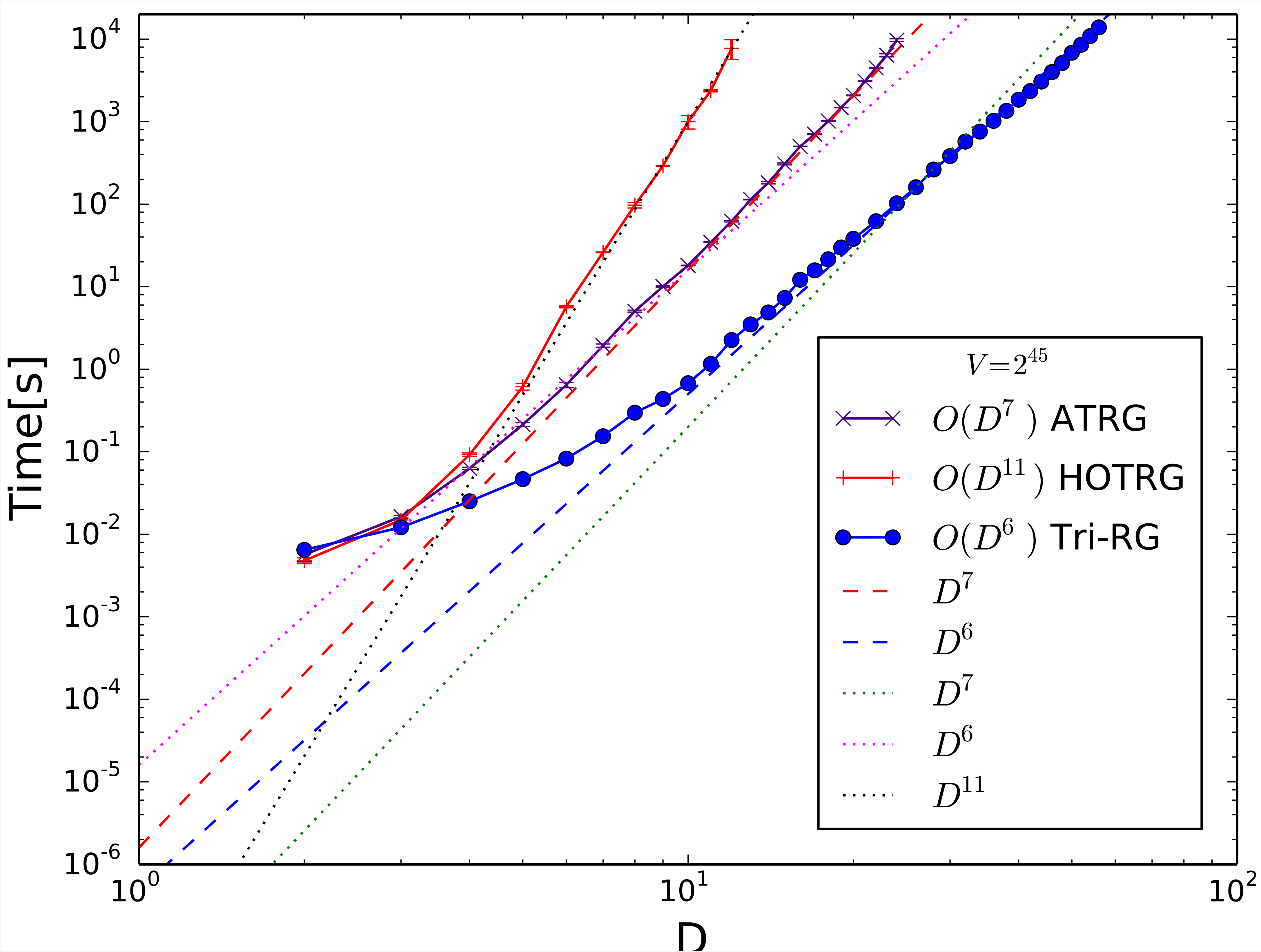
◇ 3-dim Ising



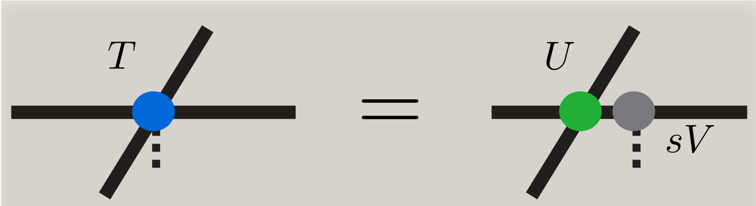


◉ Triad RG

[Daisuke Kadoh, KN arXiv:1912.02414]



◉ PEPS and TRG (low order approximation)

◇ PEPS cost reduction: 

→Partial SVD for low order approximation could reduce the cost of PEPS.

$$O(D^{7\sim9}) \to O(D^5)$$

(2012)

[Wei Li, et al. arXiv:1209.2387 (2012)]

◇ Anisotropic TRG (ATRG: TRG cost reduction by low order)

◇ Triad TRG (HOTRG cost reduction by low order)

$$O(D^{4\mathrm{dim}-1}) \to O(D^{2\mathrm{dim}+1}), O(D^{\mathrm{dim}+3})$$

(2019)

→Low order approximation could reduce the cost,

+ extension to higher dimension.

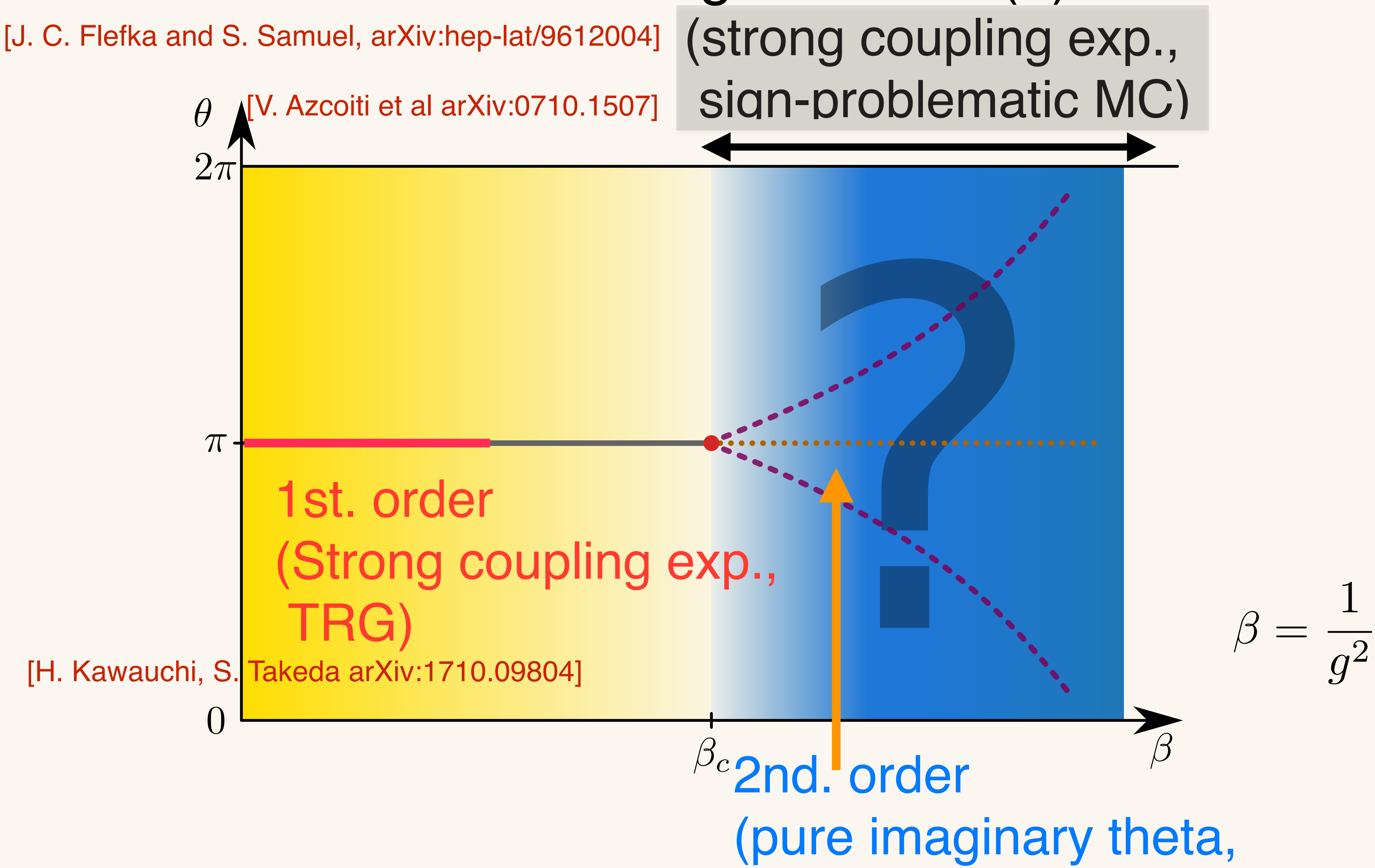
[D Adachi, et al. arXiv:1906.02007 (2019)]

[D Kadoh, KN. arXiv:1912.02414 (2019)]

→We need to know understandings in both formalisms.

◉ Contents

● Motivation: Phase diagram of CP(1) model



→ Large beta region is not strongly confirmed.

From Lagrangian to the tensor

$$e^{-S_{\theta=0}} = \exp\left[-2\beta \sum_{x,\mu} \left[z_x^* z_{x+\hat{\mu}} U_\mu + z_x z_{x+\hat{\mu}}^* U_\mu^\dagger\right]\right]$$

z : complex scaler field
U_μ: link variable

◇ Using expansion by orthogonal function $f_{l,m}$

$$\int dz f_{l,m}(z', z) f^*_{l',m'}(z'', z) = \frac{1}{d_{l,m}} \delta_{l,l'} \delta_{m,m'} f_{l,m}(z', z)$$

$l + m \leq k_{\max}$

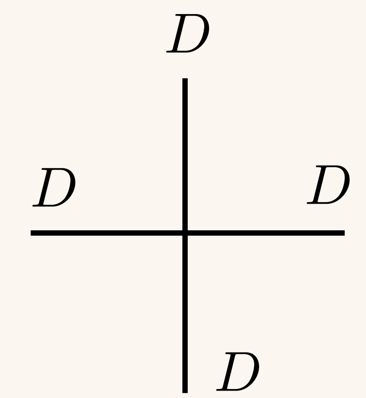
$I_n(x)$: Modified Bessel

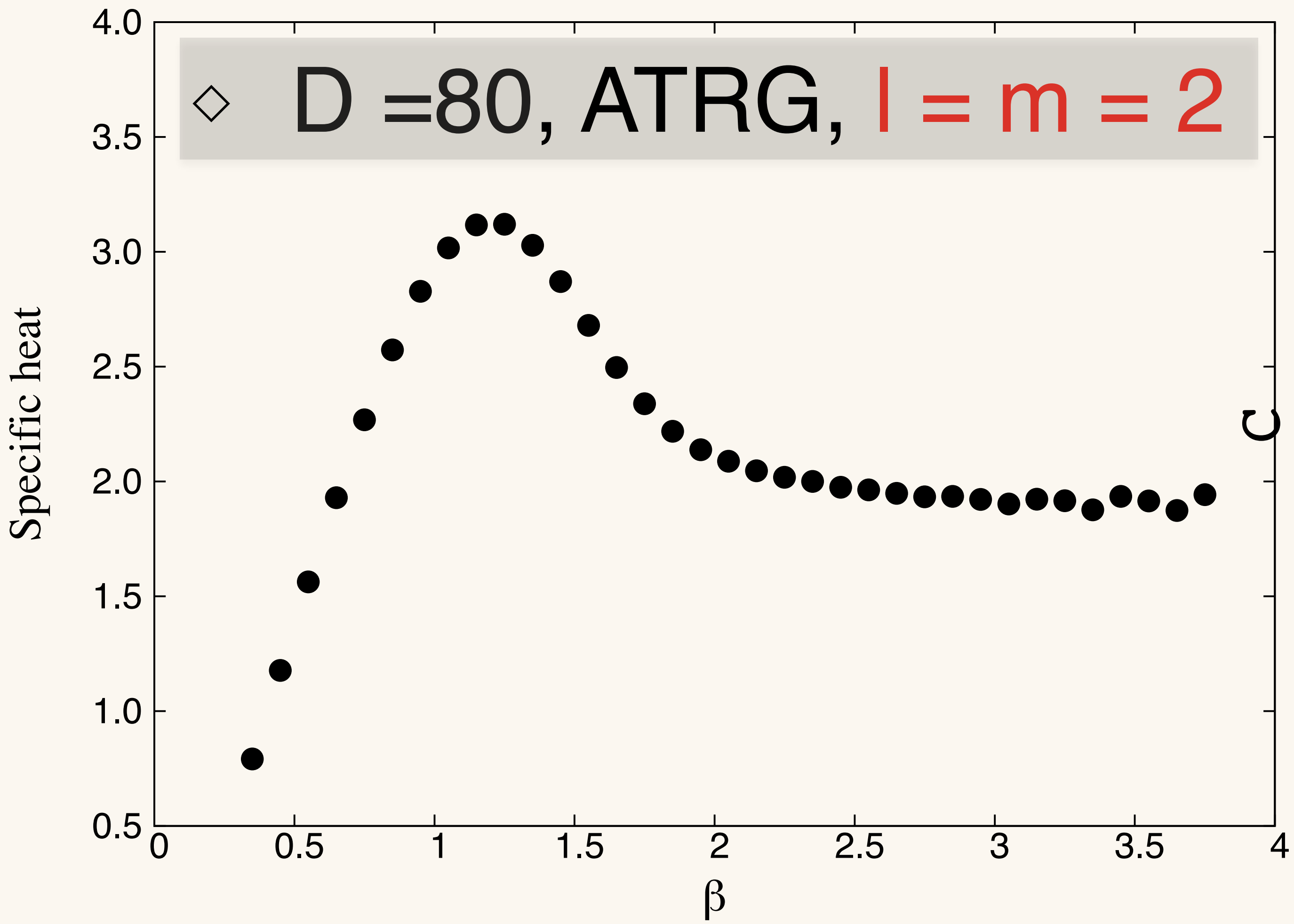
$$e^{-S_{\theta=0}} = \prod_{x,\mu} \frac{1}{2\beta} \sum_{l,m=0}^{\infty} I_{l+m+1}(4\beta) d_{l,m} f_{l,m}(z_x, z_{z+\hat{\mu}})$$

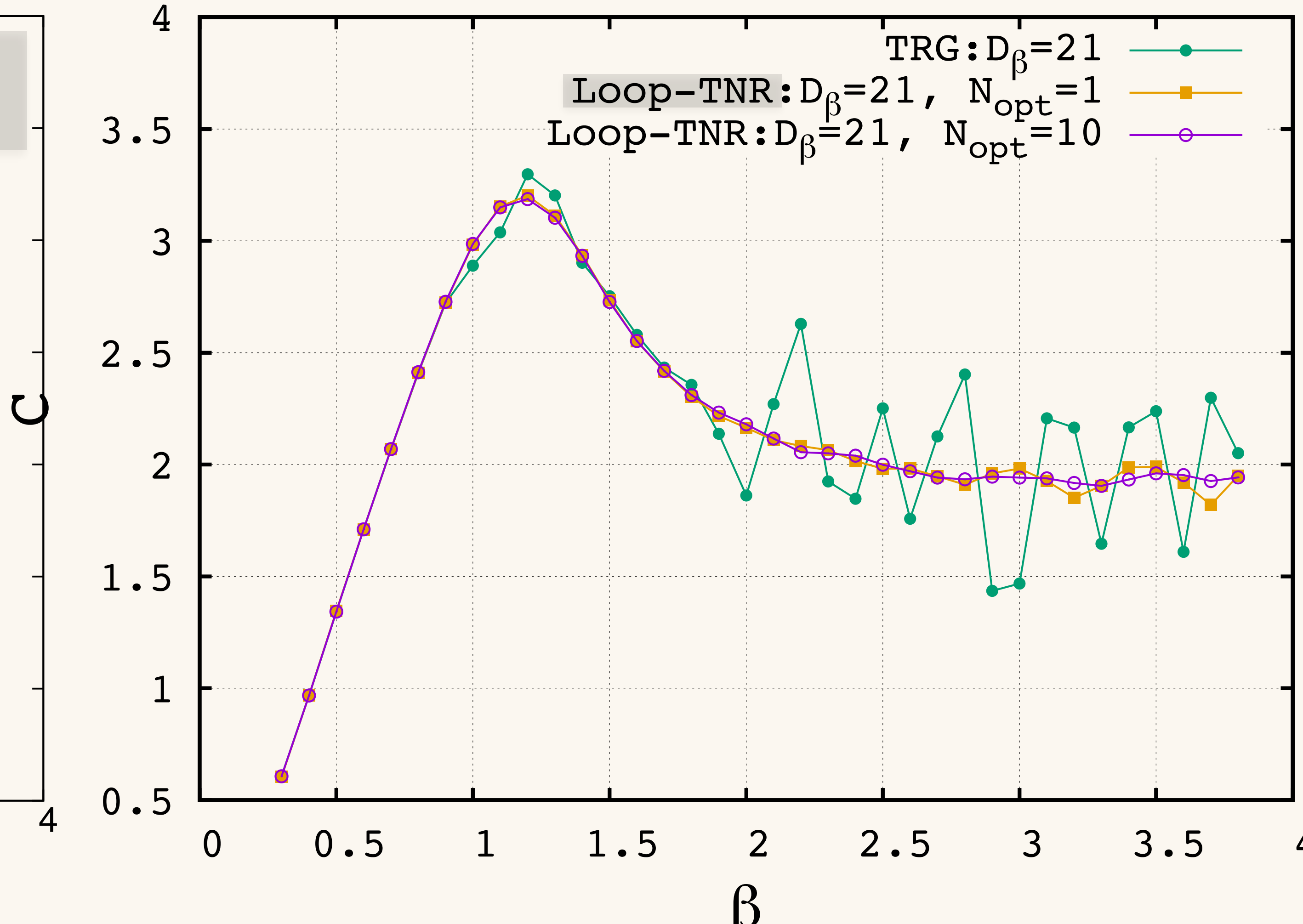
→We need to truncate the index l, m.

Specific heat of CP(1) model with $\theta = 0$.

$$\frac{\beta^2}{V}\frac{\partial^2}{\partial \beta^2}\ln Z$$







[H. Kawauchi, S. Takeda arXiv:1710.09804]

[ATRG: D. Adachi et al 1906.02007]

→ Sufficiently large bond size D produces reliable results.

◉ Character expansion of the theta term

◇ Theta term is also character expanded.

$$e^{i\frac{\theta}{2\pi}q_p} = \sum_{n_p\in\mathbb{Z}} e^{in_p q_p} \frac{2\sin(\pi n_p + \theta/2)}{\theta + 2\pi n_p}$$

$$q_p = A_{x,1} - A_{x+\hat{1}-\hat{2},2} - A_{x-\hat{2},1} + A_{x-\hat{2},2} \mod 2\pi$$

↓

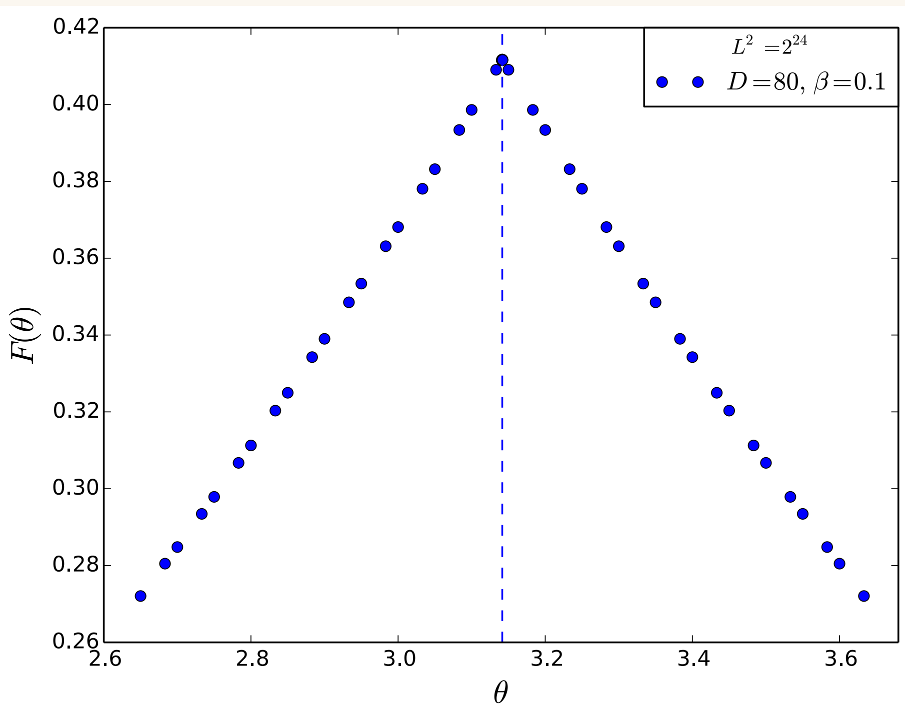
We need to truncate the index n_p.

→ The order of the truncation error is $O(1/n_p)$.

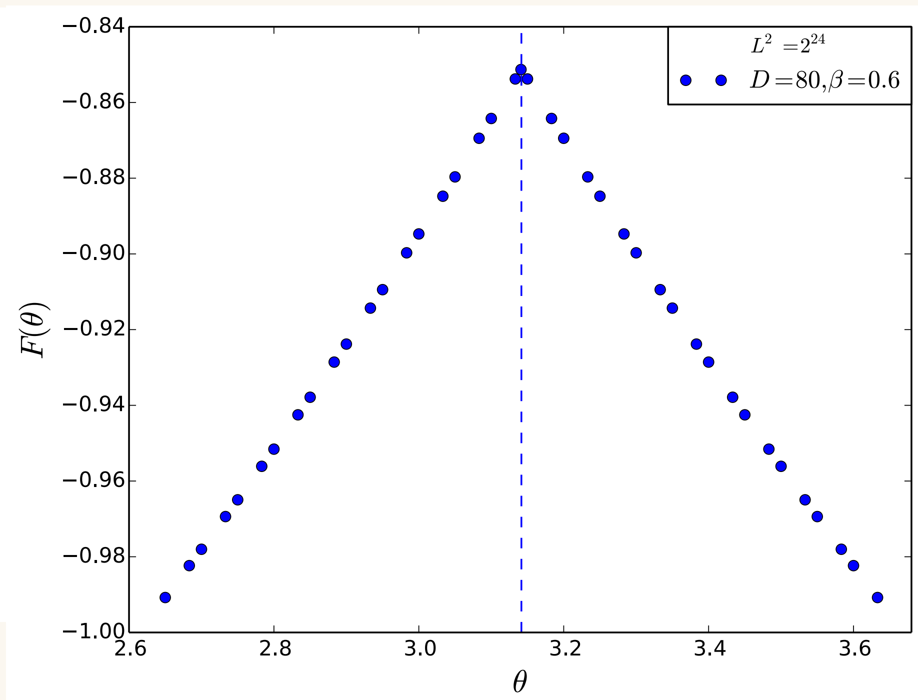
Free energy with theta term

$$D = 80$$
$$l + m \leq 2$$
$$\# n_\theta = 2$$
$$V = 2^{24}$$

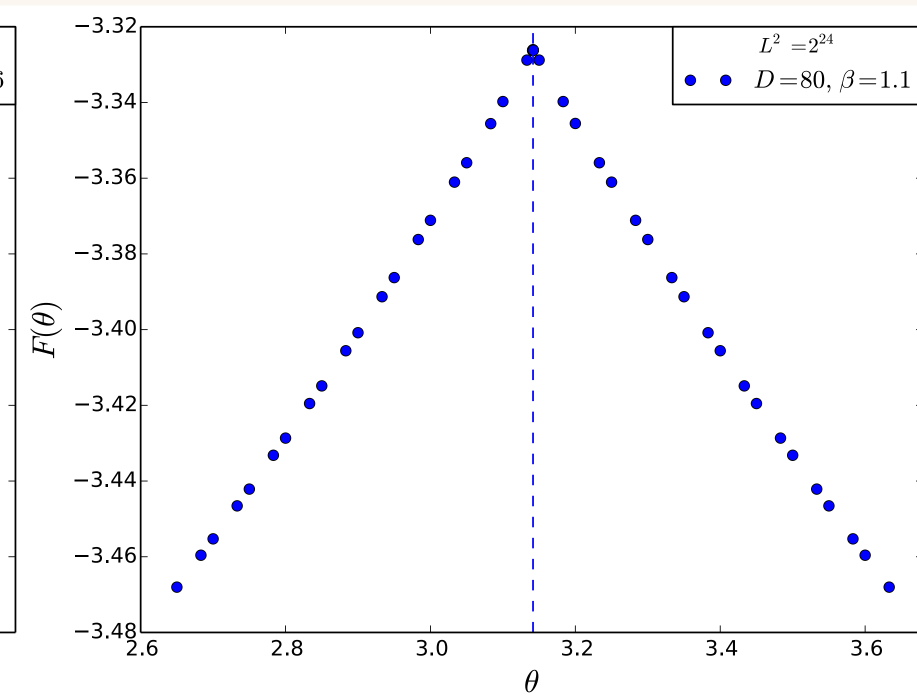
◇ beta = 0.1



◇ beta = 0.6



◇ beta = 1.1

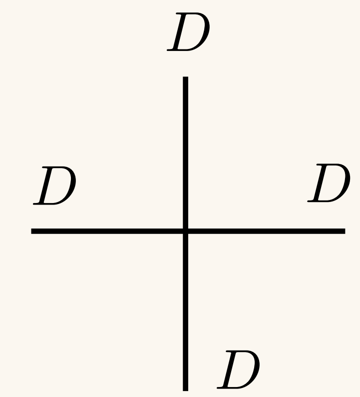


→ Clear kink structure imply the first-order transition

◇ We should estimate the systematic error.

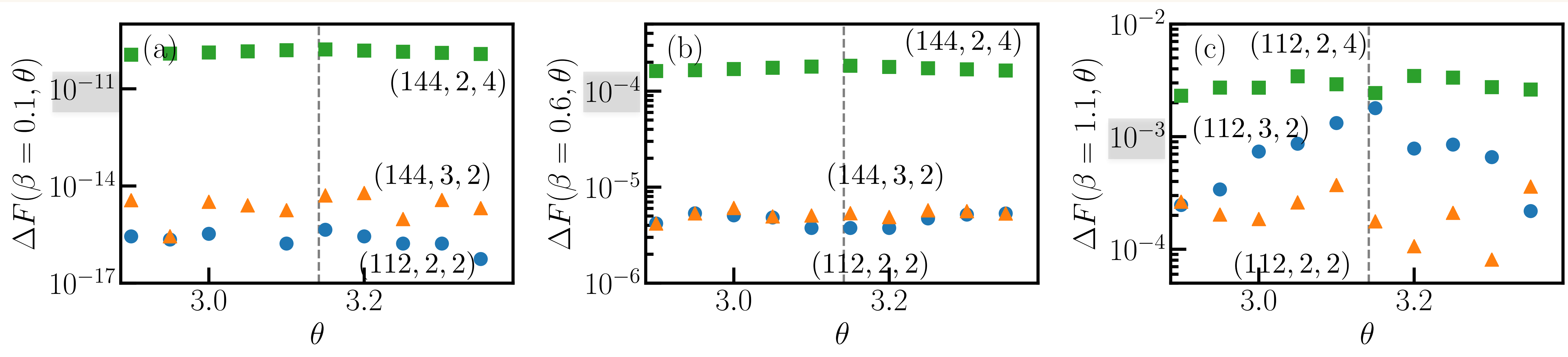
◉ Systematic error

$$l + m \leq k_{\max}$$



$$\Delta F(\beta,\theta) = |F(\beta,\theta)_{(D,k_{\max},\#n_\theta)} - F(\beta,\theta)_{(80,2,2)}|$$

◇ beta = 0.1 ◇ beta = 0.6 ◇ beta = 1.1

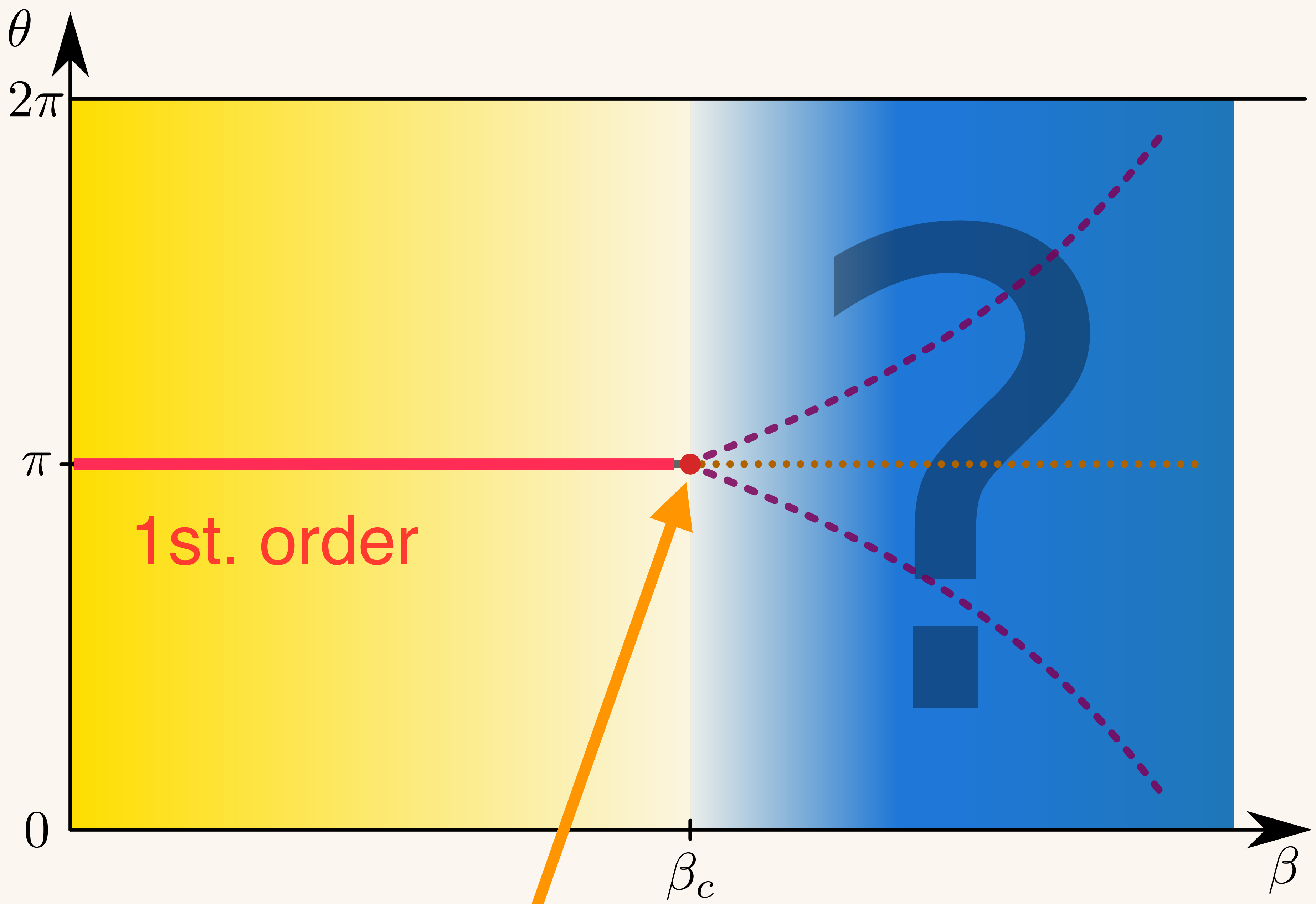


◇ SVD bond size truncation: $|F(\beta,\theta)_{(112,2,2)} - F(\beta,\theta)_{(80,2,2)}|$

◇ #Charactor expansion term: $|F(\beta,\theta)_{(144,3,2)} - F(\beta,\theta)_{(80,2,2)}|$

◇ #topological term, $\#n_\theta$: $|F(\beta,\theta)_{(144,2,4)} - F(\beta,\theta)_{(80,2,2)}|$

◉ Motivation: Phase diagram of CP(1) model



→ In our analysis, $1.1 \leq \beta_c$ is strongly favored.

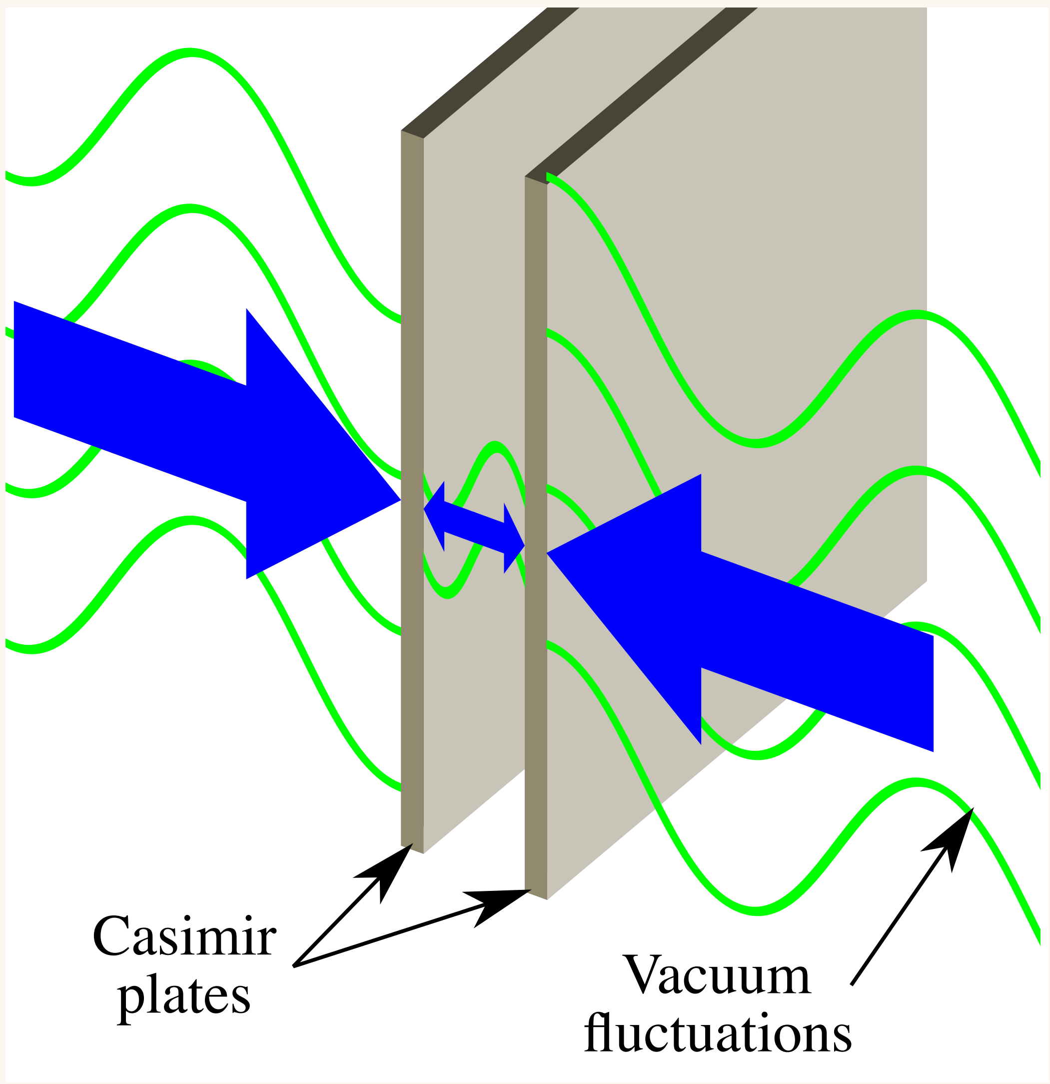
◉ Contents

◉ Casimir energy (theory and experiment)

$$E_{\mathrm{Cas}}(L) \equiv E_{\mathrm{vac}}(L) - E_{\mathrm{vac}}(\infty)$$

$$E_{\mathrm{vac}}(\infty) \propto \int d^3k \sqrt{\mathbf{k}^2 + m^2}$$

◇ Vacuum energy shift from the energy in infinite volume.



◇ It is originally suggested for photon field in 1948.

[H.B.G. Casimir, Proc. K. Ned. Acad. Wet. 51, 793 (1948)]

◇ An experiment confirmed in 1996.

[S. K. Lamoreaux, PRL78 (1997), 5]

[T. Ishikawa, K.N., and K. Suzuki, arXiv:2005.10758]

◉ Casimir energy and regularization

$$E_{\mathrm{Cas}}(L) \equiv E_{\mathrm{vac}}(L) - E_{\mathrm{vac}}(\infty)$$

◇ Vacuum energy shift from the energy in infinite volume.

◇ Regularization is needed.

$$E_{\mathrm{vac}}(\infty) \propto \int d^3k \sqrt{\mathbf{k}^2 + m^2} \qquad \to \infty$$

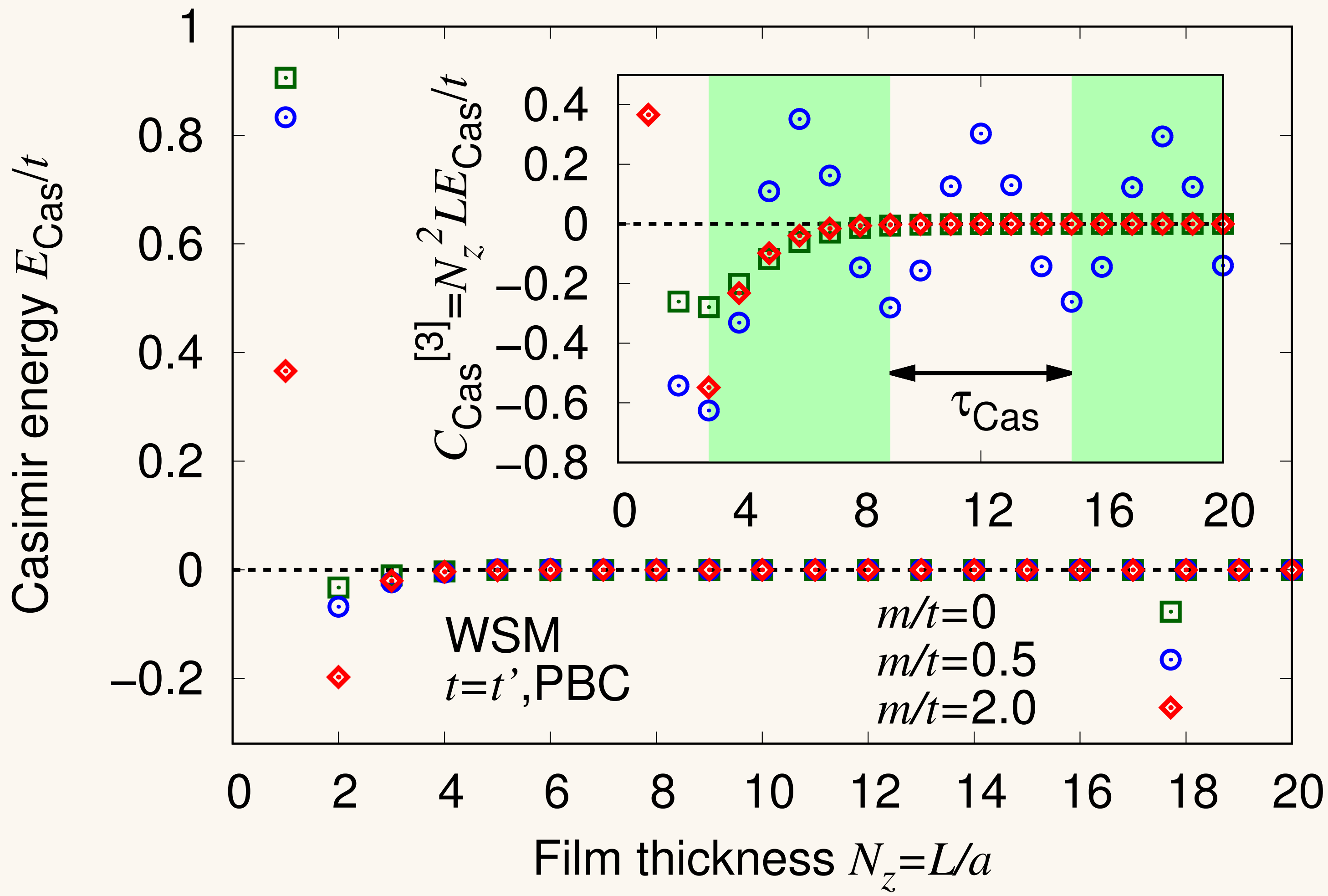
$$E_{\mathrm{vac}}(L) \propto \int d^2k \sum_{n=0}^{\infty} \sqrt{k_1^2 + k_2^2 + \left(\frac{2n\pi}{L}\right)^2 + m^2} \qquad \to \infty$$

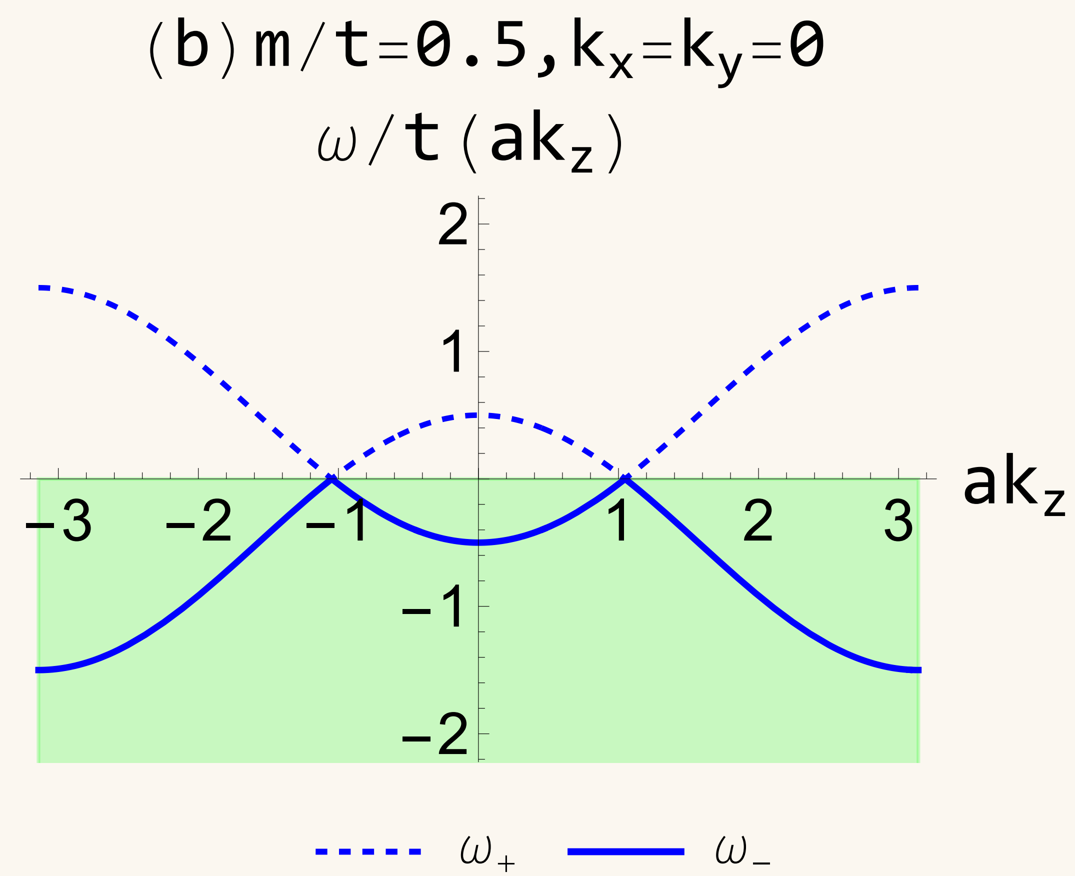
◇ Zeta-function, Abel-Plana formula…etc.

→ We apply the lattice regularization.

[K.N., and K. Suzuki, arXiv:2207.14078]

Oscillating Casimir effect



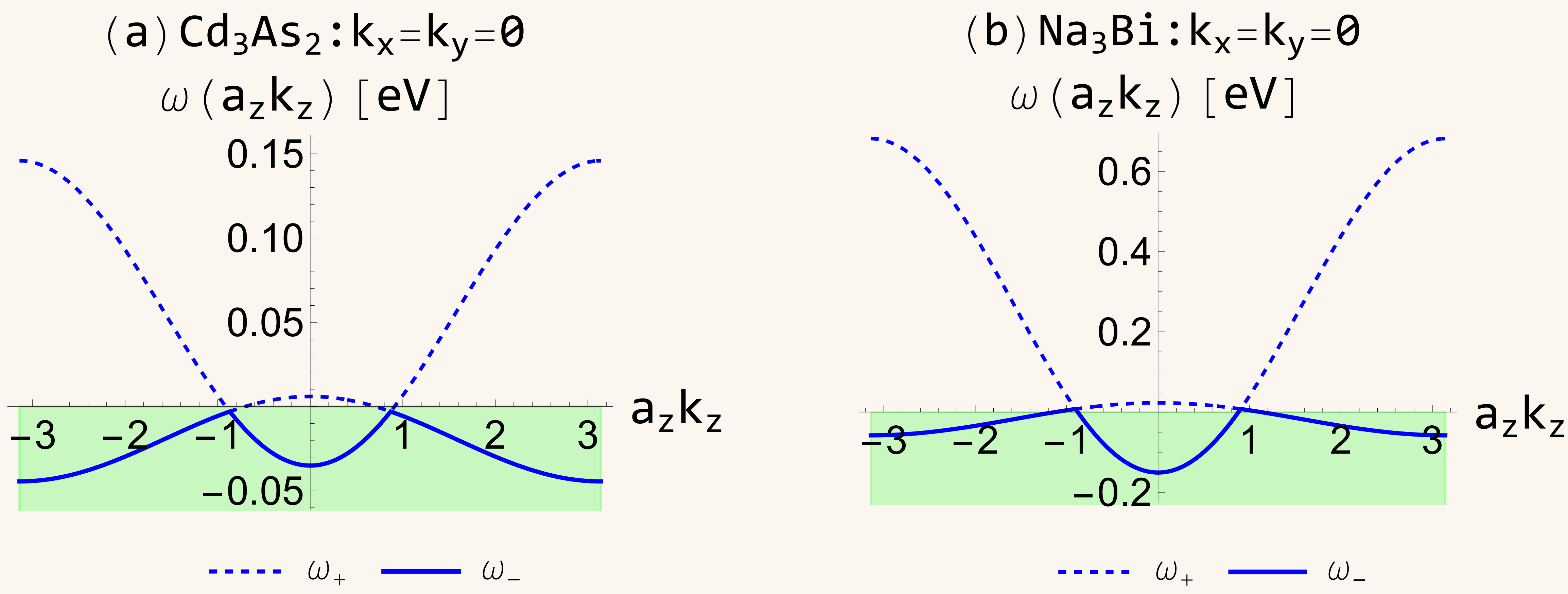


→ We find an oscillation with a period $\tau_{\mathrm{Cas}} = 6$.

→ Dirac/Weyl points are at $\frac{\pi}{3}$.

$$\tau_{\mathrm{Cas}} = \frac{2\pi}{a_z k_{\mathrm{WP/DP}}}$$

◉ Dispersion relation of Cd3As2 and Na3Bi

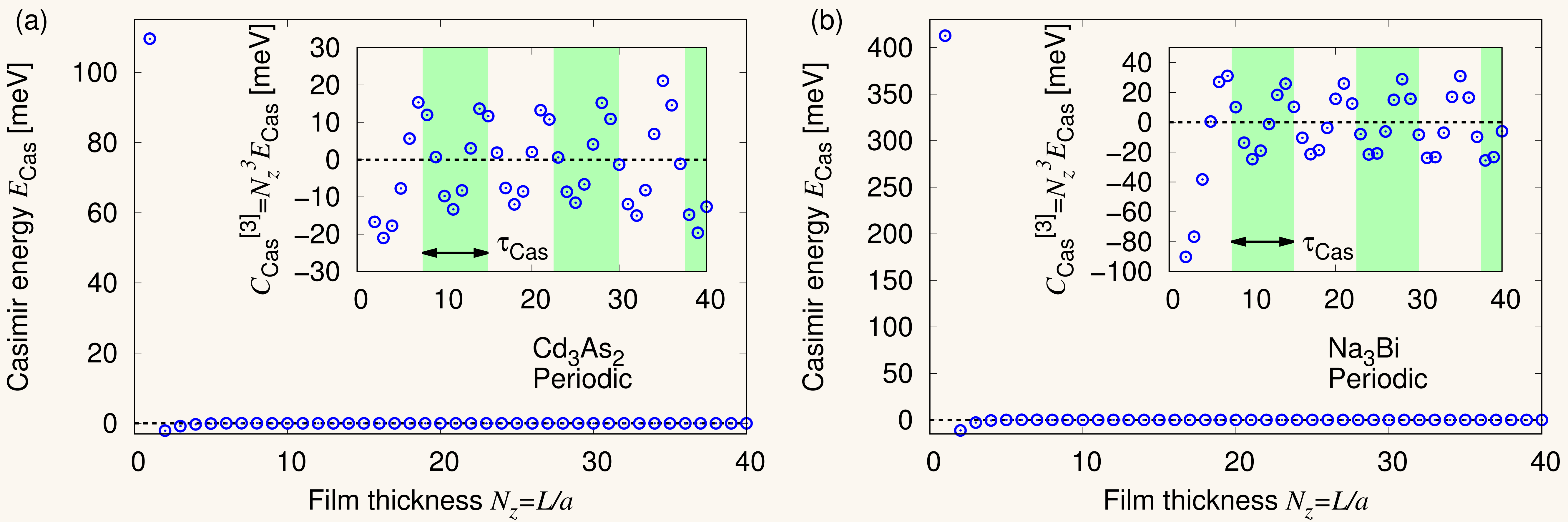


◇ Dirac points are at $\simeq \dfrac{\pi}{3.6}$

→ Periods are expected as $\tau_{\mathrm{Cas}} \simeq 7.2$

$$\tau_{\mathrm{Cas}} = \frac{2\pi}{a_z k_{\mathrm{WP/DP}}}$$

◉ Cd3As2 and Na3Bi



◇ We find oscillation periods, as expected.

→ The oscillation is a general behaviour in realistic DSMs.

◉ Summary

- Self-Introduction. Tensor network, lattice QFT with fermion formulations (including the model of the condensed-matter).

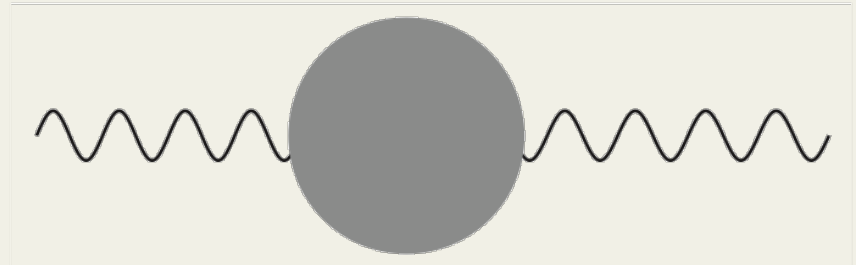
- SVD can produce locally optimal approximation, and take the truncated contractions.

- Traid TRG introduce triad (3-order) tensor to reduce the cost.

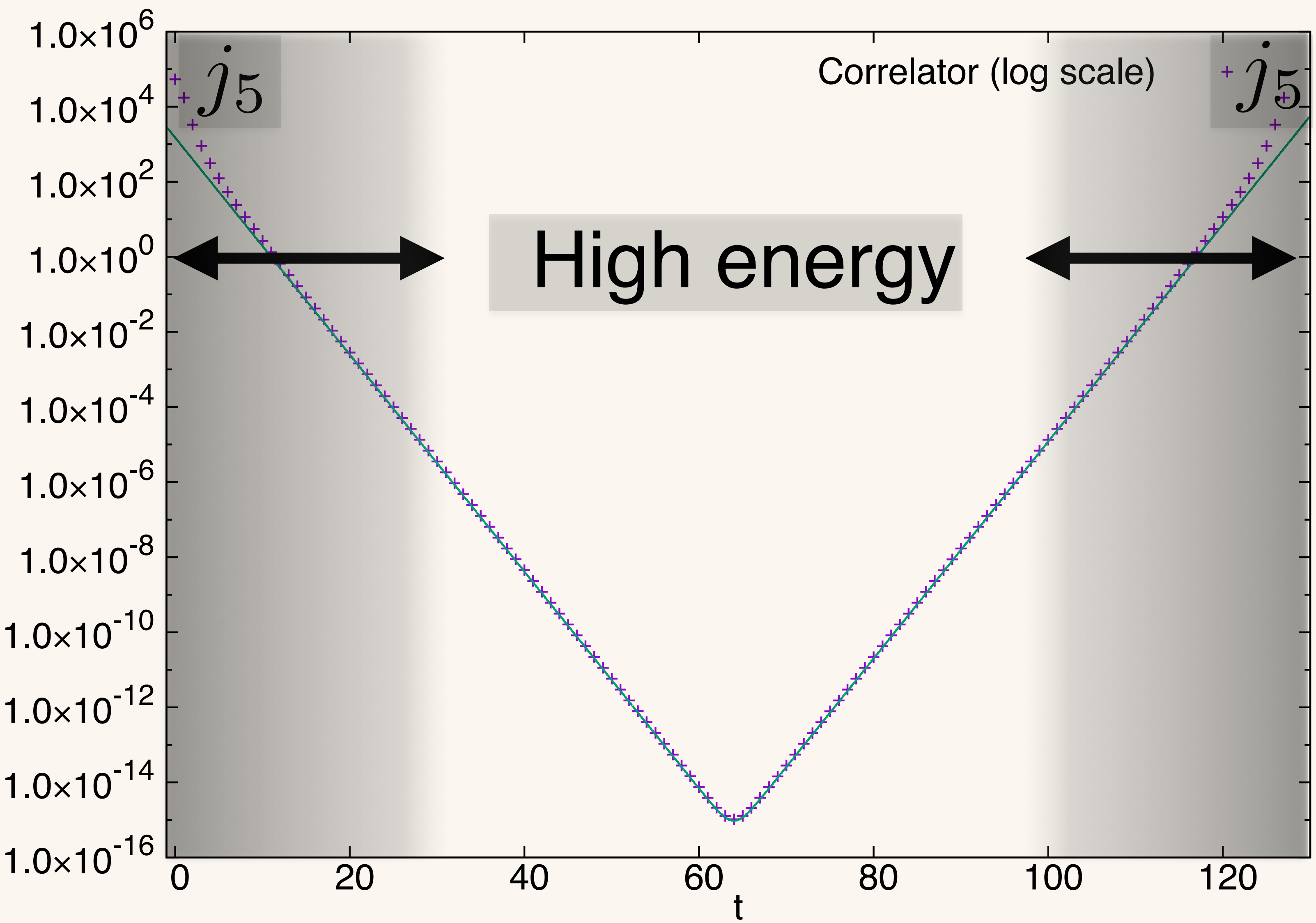
- In CP(1) model, we use sophisticated algorithm to produce reliable result.

- I also mention that the lattice condensed matter systems with Casimir energy as a future application of TRG.

Current correlator



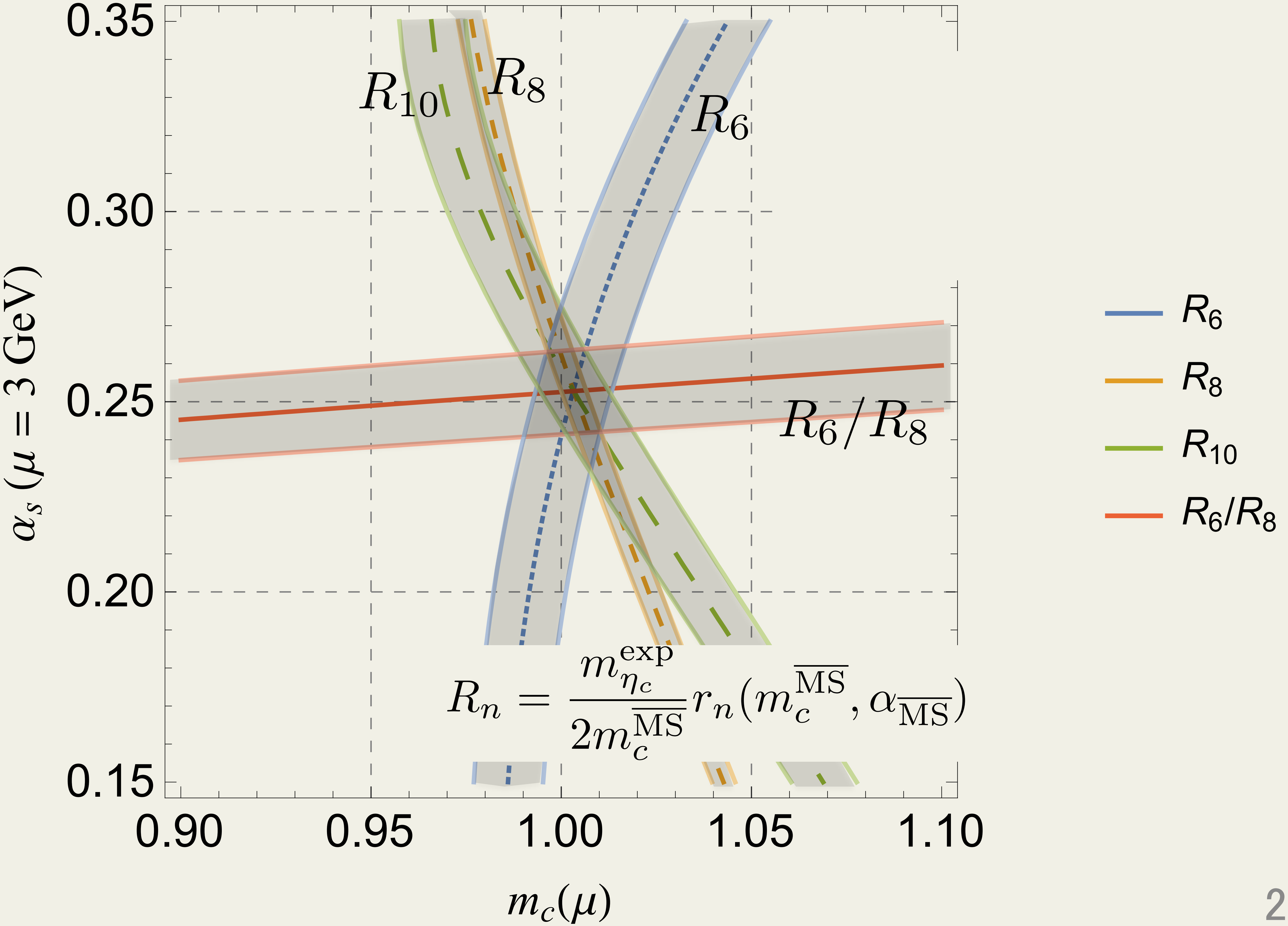
$$G(t) = a^6 \sum_{\mathbf{x}} (am_{0c})^2 \langle j_5(x) j_5(0) \rangle$$



◇ Moment (→Differential)

$$g_{2n} = \frac{1}{n!}\left(\frac{\partial}{\partial q^2}\right)^n (q^2 \Pi(q^2))_{q^2=0}$$

$$G_n = \sum_t \left(\frac{t}{a}\right)^n G(t)$$


0.35
0.30
0.25
0.20
0.15
0.90
0.95
1.00
1.05
1.10
$\alpha_s\,(\mu = 3\ \mathrm{GeV})$
$m_c(\mu)$
R_{10}
R_8
R_6
R_6/R_8
$R_n = \frac{m_{\eta_c}^{\exp}}{2m_c^{\overline{\mathrm{MS}}}} r_n(m_c^{\overline{\mathrm{MS}}}, \alpha_{\overline{\mathrm{MS}}})$
R_6
R_8
R_{10}
R_6/R_8