



Application of
machine learning and quantum computation
in high energy physics

Shuzhe Shi
Tsinghua University



施舒哲
清华大学

“first principle” microscopic theory: quantum field theory $L \leftrightarrow H$

non-perturbative lattice QFT: thermodynamics, transport

fermion field

$$\prod_{\vec{x}} \left(\prod_{\text{spin, charge}} \otimes \left\{ \begin{array}{l} \text{occupied} \\ \text{unoccupied} \end{array} \right\} \right)_{(\vec{x})} \text{color, flavor}$$

gauge field

$$\prod_{(\vec{x}, \vec{x}+d\vec{x})} \left(\prod_{\text{spin}} \otimes \left\{ \begin{array}{c} \vdots \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \vdots \end{array} \right\} \right)_{(\vec{x}, \vec{x}+d\vec{x})}^{N_c^2-1}$$

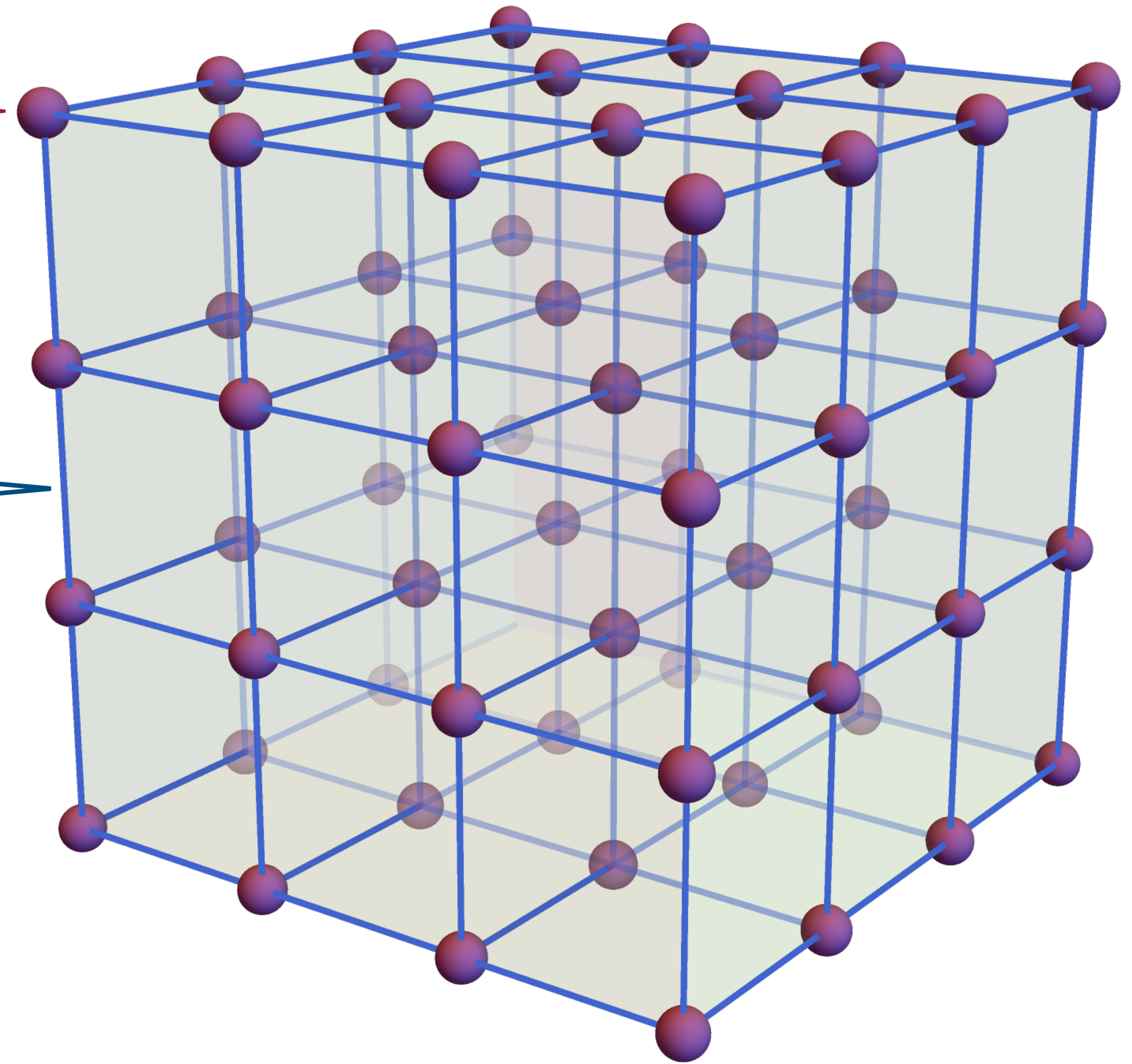
field operators

$$\{\hat{\psi}_n^\dagger, \hat{\psi}_m\} = \delta_{n,m}, \quad \{\hat{\psi}_n, \hat{\psi}_m\} = \{\hat{\psi}_n^\dagger, \hat{\psi}_m^\dagger\} = 0,$$

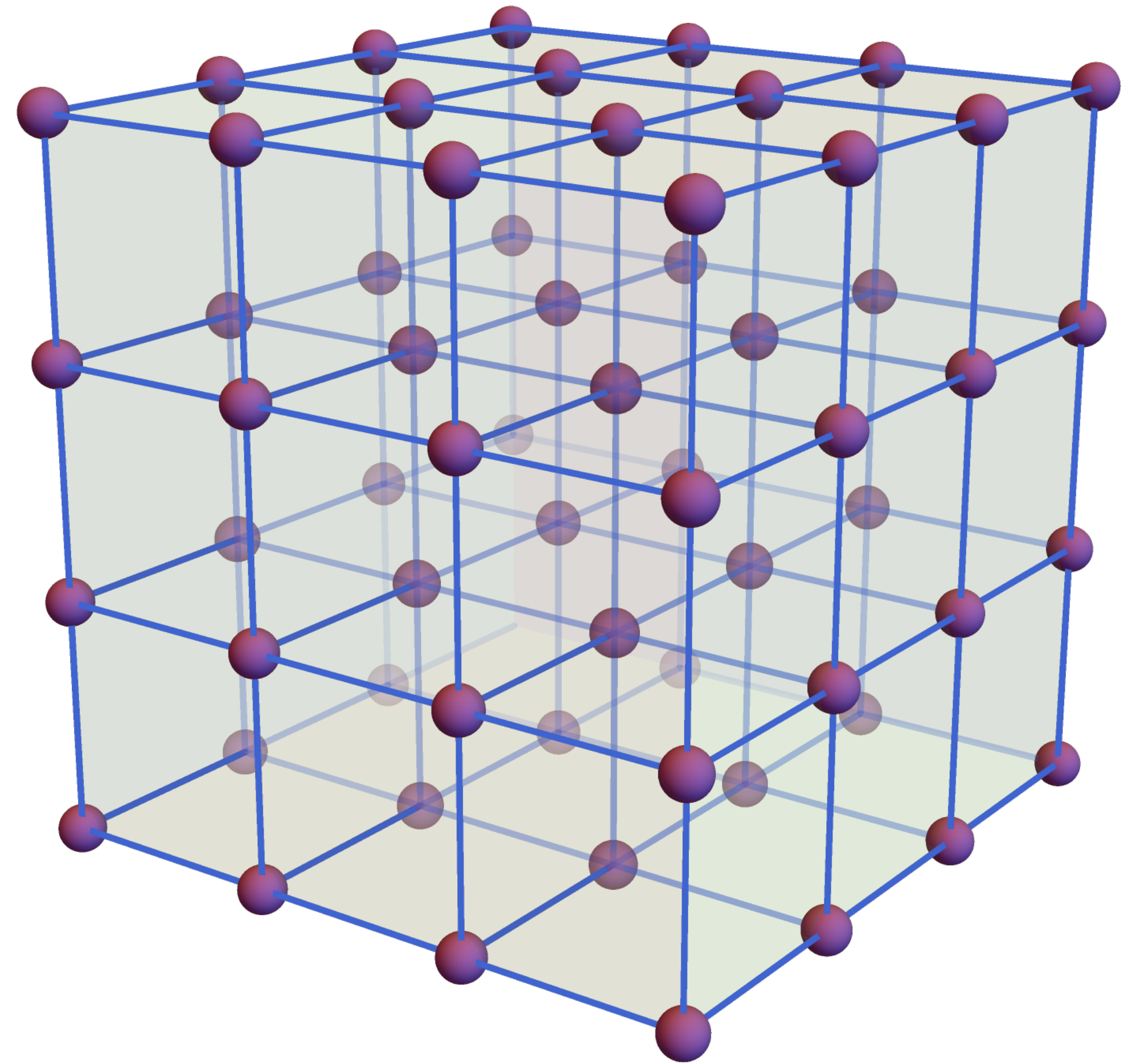
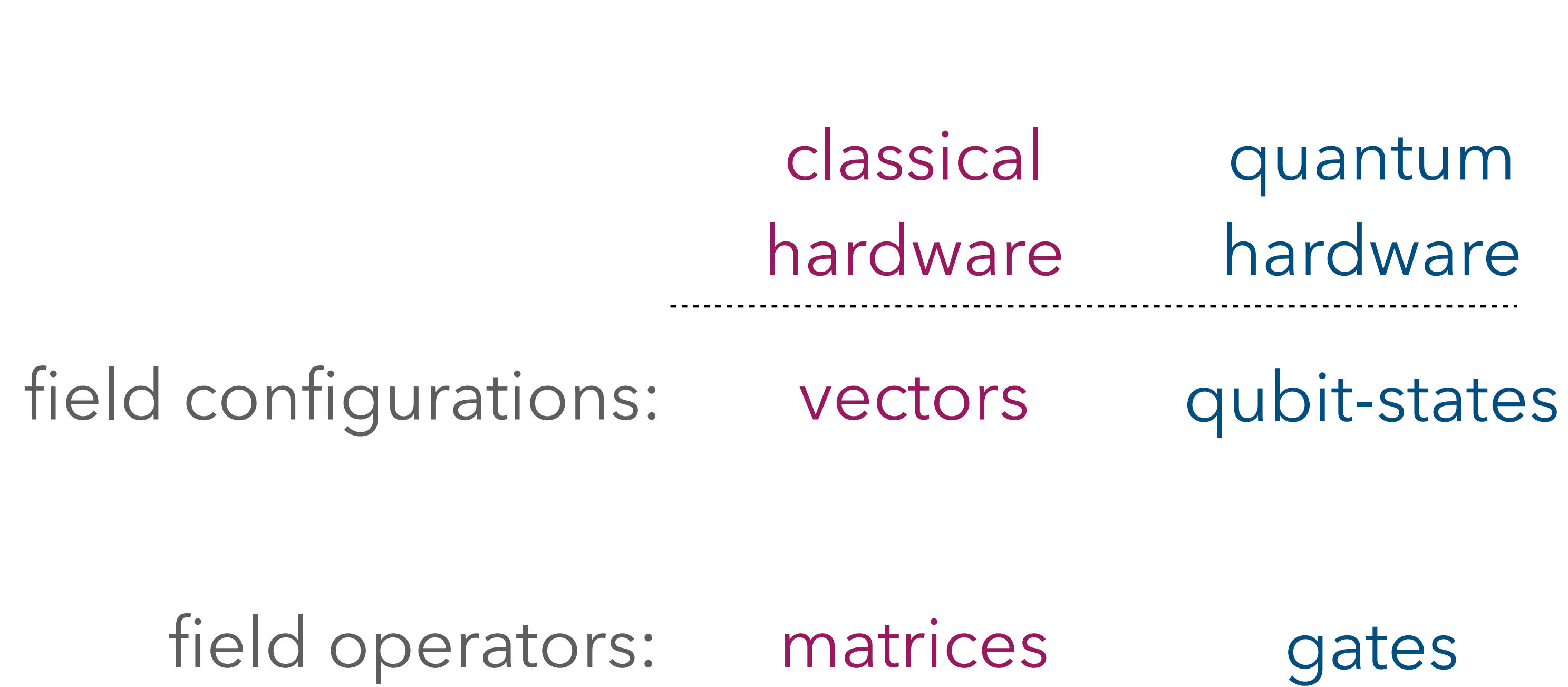
$$[\hat{\Pi}_n, \hat{A}_m] = \delta_{n,m}, \quad [\hat{\Pi}_n, \hat{\Pi}_m] = [\hat{A}_n, \hat{A}_m] = 0.$$

indices: spin, charge, color, flavor, \vec{x} , ...

[Shaw, Lougovski, Stryker, Wieber, Quantum 4, 306]



[Jordan, Wigner, Z.Phys.47,631(1928)]



hadron structure

$$\hat{H} |\Psi_{\text{vac}}\rangle = E_{\text{gnd}} |\Psi_{\text{vac}}\rangle$$

$$\hat{H} |\Psi_{\text{meson}}\rangle = E_{1\text{st}} |\Psi_{\text{meson}}\rangle$$

Reviews:

[C. W. Bauer et al., PRX Quantum 4, 027001 (2023)]

[Bauer, Davoudi, Klco, Savage, Nature Rev. Phys. 5, 420 (2023)]

[Li, Guo, Lai, Liu, Wang, Xing, Zhang, Zhu (QuNu Collaboration), PRD.105.L111502, PRD.109.036025, Sci.ChinaPhys.Mech.Astron.66,281011]

thermal properties

$$\langle O \rangle = \text{tr}(\hat{O} e^{-\beta(\hat{H}-\mu\hat{Q})}) / Z$$

[Hidaka, Yamamoto, 2409.17349]

[Hayata, Hidaka, JHEP09(2023)126, JHEP07(2024)106]

[Ebner, Muller, Schafer, Seidl, Yao, PRD.109.014504]

[Yao, PRD.108.L031504]

[Czajka, Kang, Ma, Zhao, JHEP08,209]

[Ikeda, Kharzeev, Meyer, **SS**, PRD.108.L091501]

real-time evolution

$$\partial_t |\Psi(t)\rangle = -i \hat{H} |\Psi(t)\rangle$$

$$\partial_t \hat{\rho}(t) = -i [\hat{H}, \hat{\rho}(t)]$$

$$O(t) = \text{tr}(\hat{O} \hat{\rho}(t))$$

[de Jong, Lee, Mulligan, Ploskon, Ringer, Yao, PRD.106.054508]

[Farrell, Illa, Ciavarella, Savage, PRX Quantum.5.020315; PRD.109.114501]

[Florio, PRD.109.L071501] [Ikeda, Kang, Kharzeev, Qian, Zhao, JHEP10(2024)031]

[Shile Chen, **SS**, Li Yan, 2412.00662] [Lee, Mulligan, Ringer, Yao, PRD.108.094518]

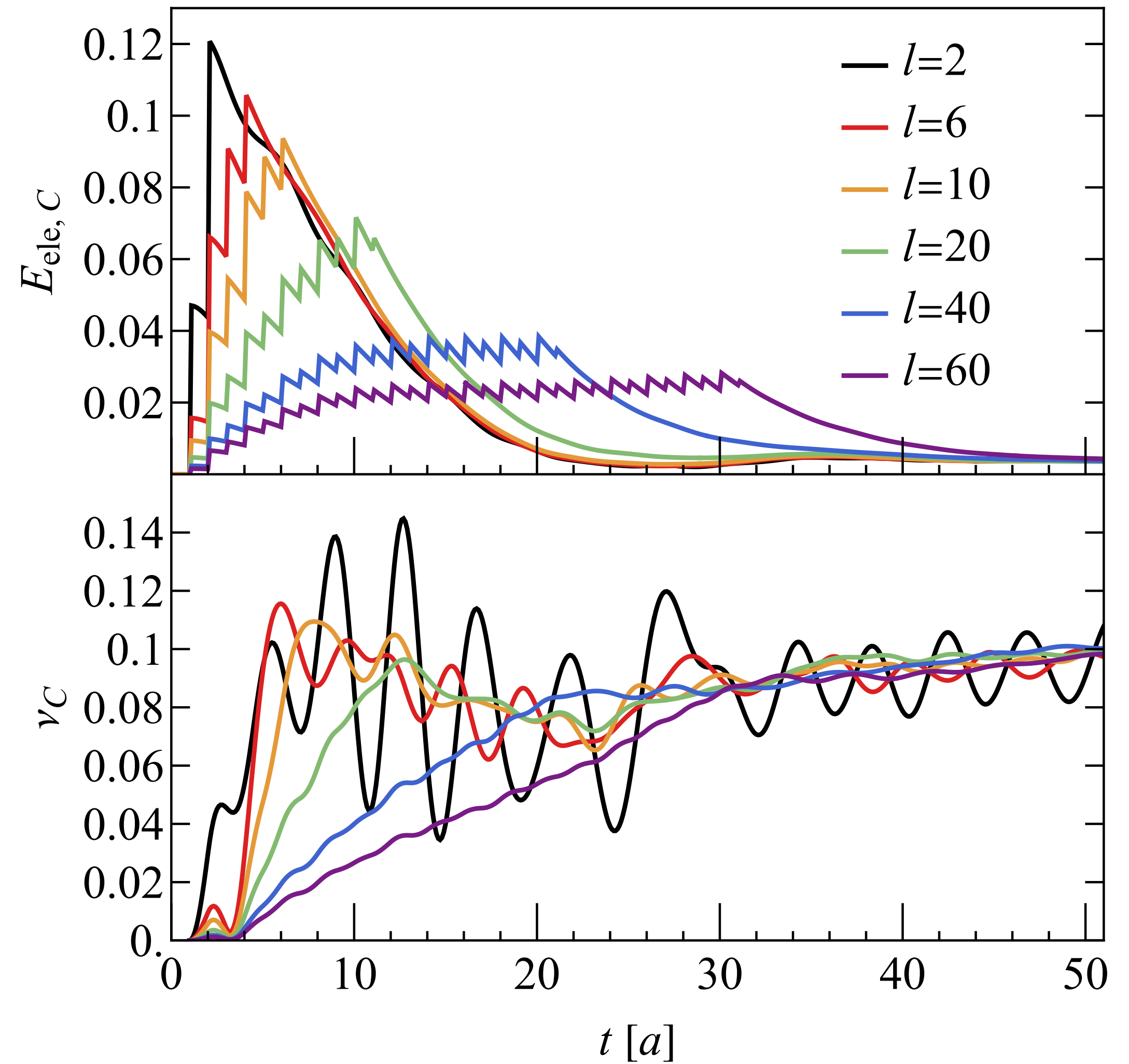
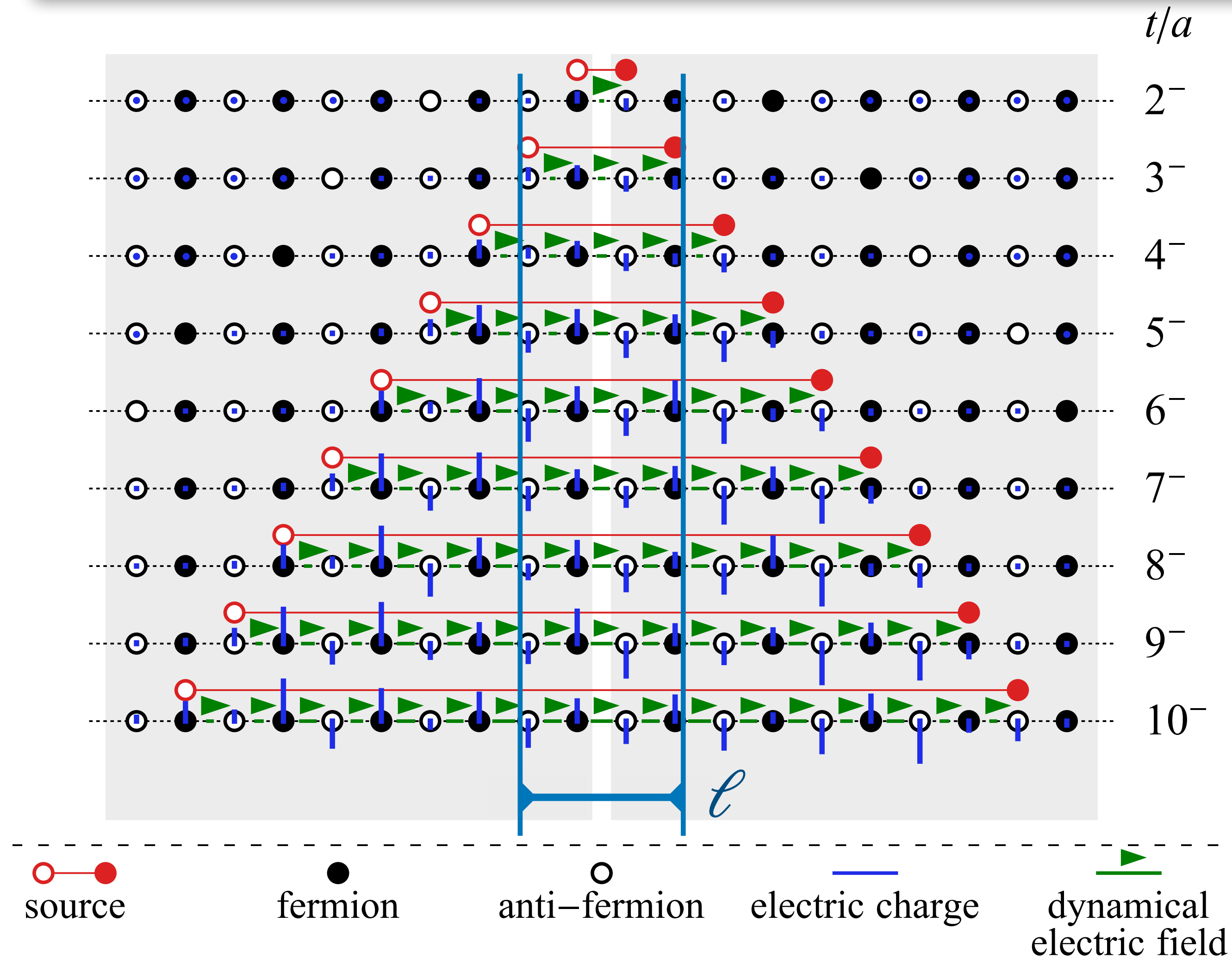
[Ikeda, Kharzeev, **SS**, PRD.108.074001] [Wu, Du, Zhao, Vary, PRD.110.056044]

[Ikeda, Kharzeev, Kikuchi, PRD.103.L071502] [Kharzeev, Kikuchi, PRes.023342]

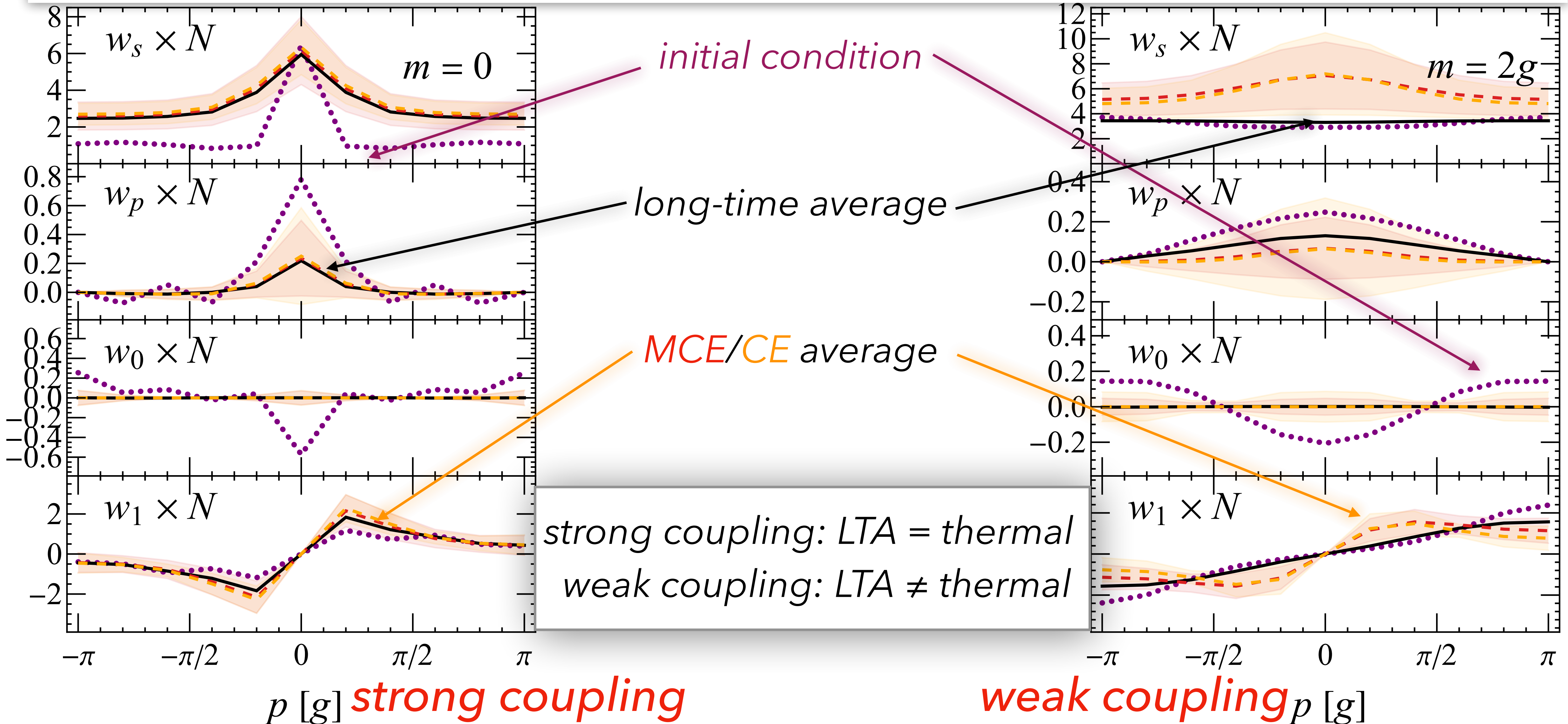
[Florio, Frenklakh, Ikeda, Kharzeev, Korepin, **SS**, Yu, PRL.131.021902; PRD.110.094029]

Schwinger model:
w/ source

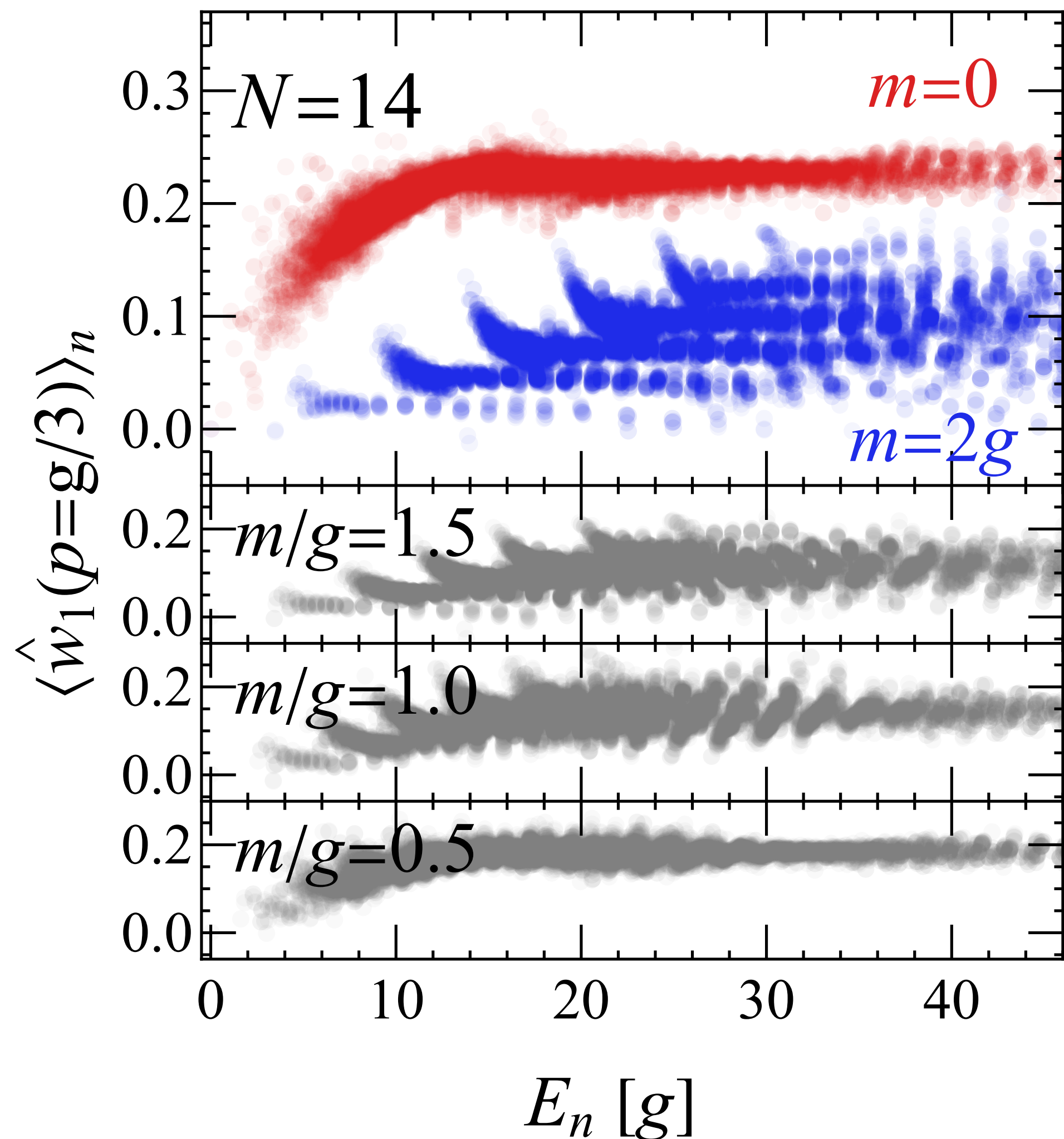
$$H(t) = \int \left(\frac{E^2}{2} - \bar{\psi}(i\gamma^1 \partial_x - g\gamma^1 A - m)\psi - j_{\text{ext}}^1(t)A \right) dx.$$



Schwinger model: $H(t) = \int \left(\frac{E^2}{2} - \bar{\psi}(i\gamma^1 \partial_x - g\gamma^1 A - m)\psi \right) dx.$ $\hat{W}_{\alpha\beta}(t, z, p) = \int \bar{\psi}_\alpha(z_+) U(z_+, z_-) \psi_\beta(z_-) e^{i\frac{py}{\hbar}} dy$



Schwinger model: $H(t) = \int \left(\frac{E^2}{2} - \bar{\psi}(i\gamma^1 \partial_x - g\gamma^1 A - m)\psi \right) dx.$ $\hat{W}_{\alpha\beta}(t, z, p) = \int \bar{\psi}_\alpha(z_+) U(z_+, z_-) \psi_\beta(z_-) e^{i\frac{py}{\hbar}} dy$



eigenstate thermalization hypothesis

$\langle n | \hat{O} | n \rangle \approx f_O(E_n)$

$\sum_n p_n \langle n | \hat{O} | n \rangle \approx f_O(\sum_n p_n E_n)$

general pure state

thermal

$|c_n|^2$

$e^{-\beta E_n} / Z$

$\langle O \rangle_{PS}$

\approx

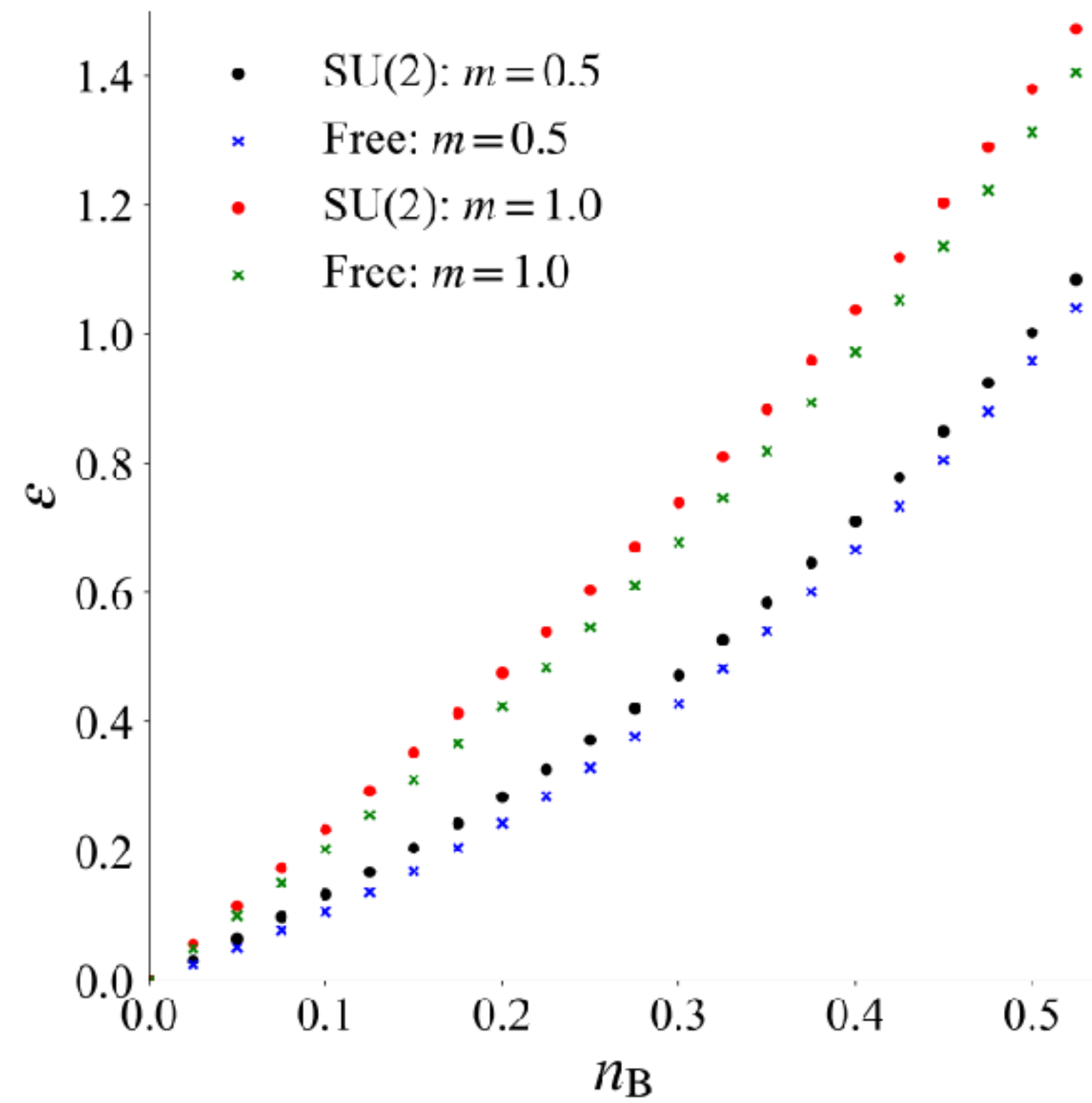
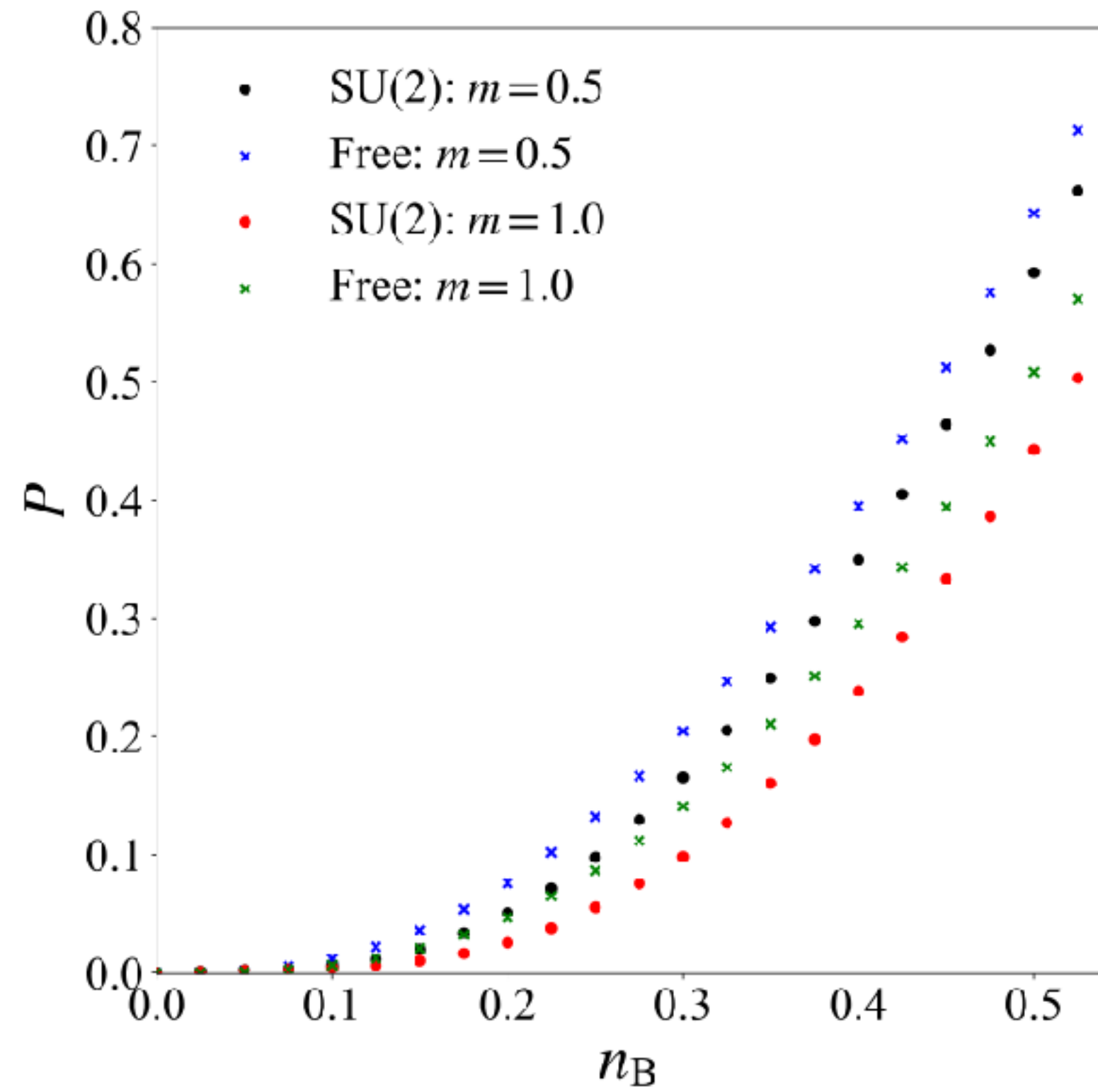
$\langle O \rangle_{th}$

if $\langle E \rangle_{PS}$

$=$

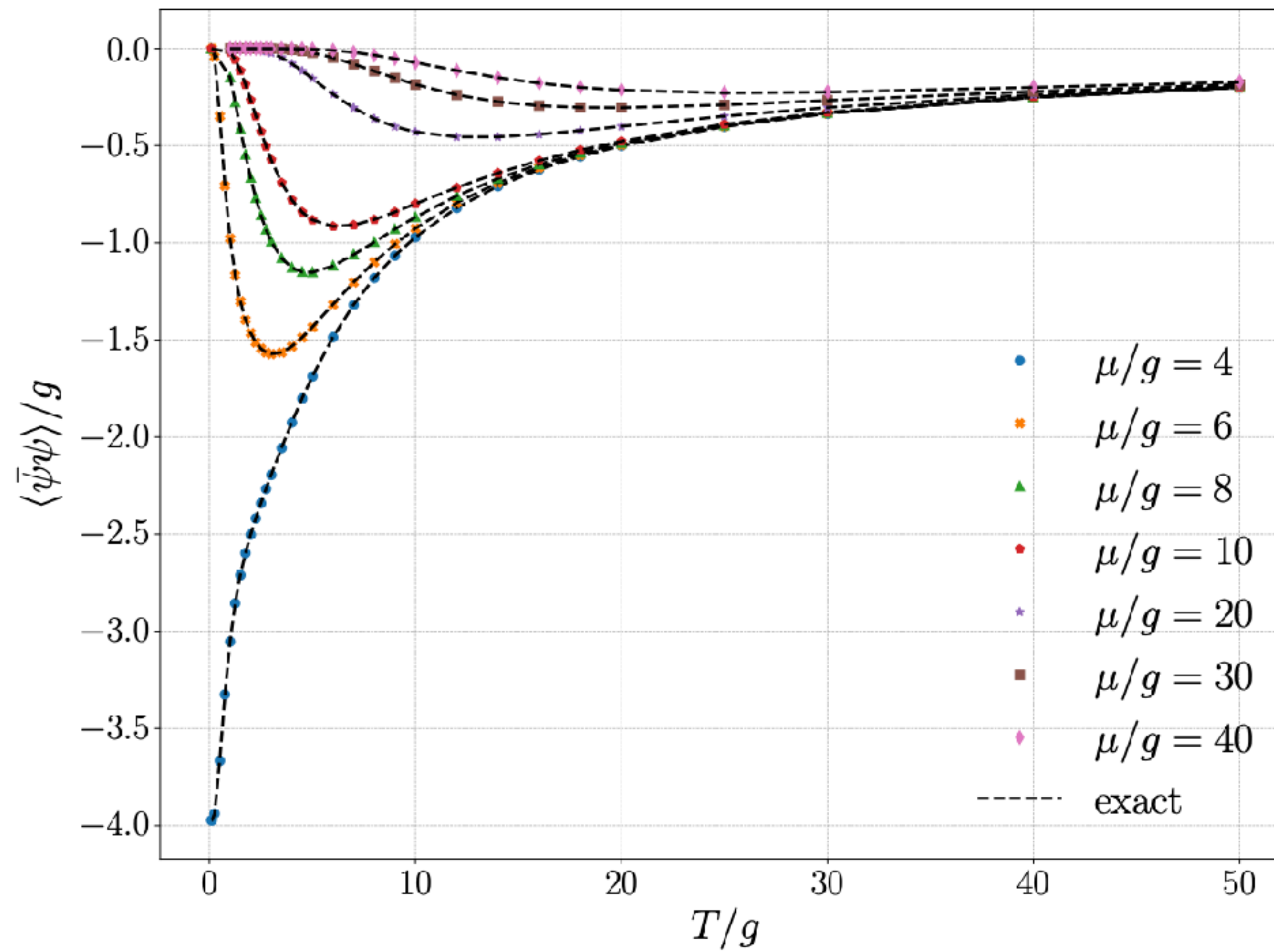
$\langle E \rangle_{th}$

SU(2) non-Abelian gauge theory in 1+1D

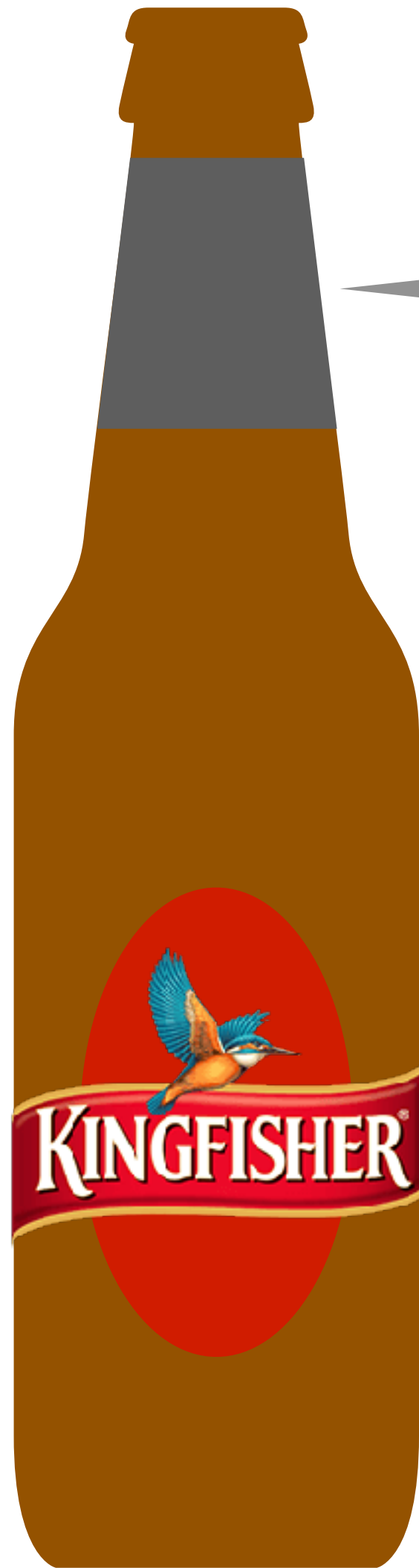


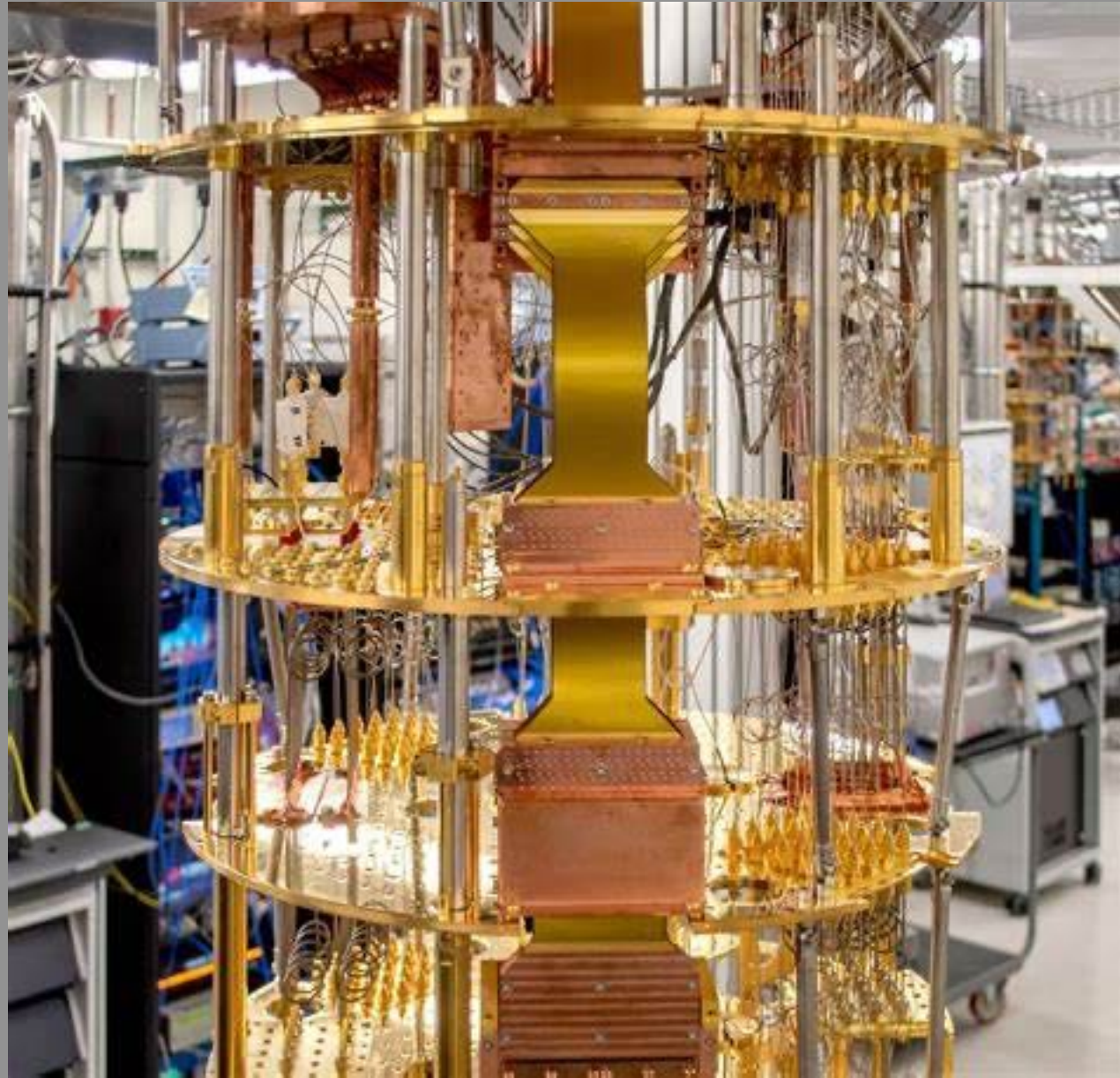
No first-order phase transition? b/c 1+1D?

SU(2) non-Abelian gauge theory in 1+1D




*Chiral condensate at finite T, μ
using real Quantum Computers!*





Noise in QCs!



hadron structure

$$\hat{H}|\Psi_{\text{vac}}\rangle = E_{\text{gnd}}|\Psi_{\text{vac}}\rangle$$

$$\hat{H}|\Psi_{\text{meson}}\rangle = E_{\text{1st}}|\Psi_{\text{meson}}\rangle$$

Reviews:
[C. W. Bauer et al., PRX Quantum 4, 027001 (2023)]
[Bauer, Davoudi, Klco, Savage, Nature Rev. Phys. 5, 420 (2023)]

[Li, Guo, Lai, Liu, Wang, Xing, Zhang, Zhu (QuNu Collaboration), PRD.105.L111502, PRD.109.036025, Sci.ChinaPhys.Mech.Astron. 66,281011]

thermal properties

$$\langle O \rangle = \text{tr}(\hat{O} e^{-\beta(\hat{H}-\mu\hat{Q})})/Z$$

[Hidaka, Yamamoto, 2409.17349]
[Heyata, Hidaka, JHEP09(2023)126, JHEP07(2024)106]
[Ebner, Muller, Schafer, Seidl, Yao, PRD.109.014504]
[Yao, PRD.108.L031504]
[Czajka, Kang, Ma, Zhao, JHEP08,209]
[Ikeda, Kharzeev, Meyer, SS, PRD.108.L091501]

real-time evolution

$$\partial_t |\Psi(t)\rangle = -i\hat{H}|\Psi(t)\rangle$$

$$\partial_t \hat{\rho}(t) = -i[\hat{H}, \hat{\rho}(t)]$$

$$O(t) = \text{tr}(\hat{O} \hat{\rho}(t))$$

[de Jong, Lee, Mulligan, Plaskon, Ringer, Yao, PRD.106.054508]
[Farrell, Ila, Ciavarella, Savage, PRX Quantum.5.020315; PRD.109.114501]
[Florio, PRD.109.L071501] [Ikeda, Kang, Kharzeev, Qian, Zhao, JHEP10(2024)031]
[Shile Chen, SS, Li Yan, 2412.00662] [Lee, Mulligan, Ringer, Yao, PRD.108.094518]
[Ikeda, Kharzeev, SS, PRD.108.074001] [Wu, Du, Zhao, Vary, PRD.110.056044]
[Ikeda, Kharzeev, Kikuchi, PRD.103.L071502] [Kharzeev, Kikuchi, PRRes.023342]
[Florio, Eosoklakh, Ikeda, Kharzeev, Kozmin, SS, Yu, PRL.131.021902; PRD.110.094029]



Noise in QCs!

Tool(s) to assist Lattice QCD calculation?

Machine Learning!

thermal properties

$$\langle O \rangle = \text{tr}(\hat{O} e^{-\beta(\hat{H}-\mu\hat{Q})})/Z$$

[Hidaka, Yamamoto, 2409.17349]
[Heyata, Hidaka, JHEP09(2023)126, JHEP07(2024)106]
[Ebner, Muller, Schafer, Seidl, Yao, PRD.109.014504]
[Yao, PRD.108.L031504]
[Czajka, Kang, Ma, Zhao, JHEP08,209]
[Ikeda, Kharzeev, Meyer, SS, PRD.108.L091501]

real-time evolution

$$\begin{aligned}\partial_t |\Psi(t)\rangle &= -i\hat{H} |\Psi(t)\rangle \\ \partial_t \hat{\rho}(t) &= -i[\hat{H}, \hat{\rho}(t)] \\ O(t) &= \text{tr}(\hat{O} \hat{\rho}(t))\end{aligned}$$

[de Jong, Lee, Mulligan, Ploskon, Ringer, Yao, PRD.106.054508]
[Farrell, Ila, Ciavarella, Savage, PRX Quantum.5.020315; PRD.109.114501]
[Florio, PRD.109.L071501] [Ikeda, Kang, Kharzeev, Qian, Zhao, JHEP10(2024)031]
[Shile Chen, SS, Li Yan, 2412.00662] [Lee, Mulligan, Ringer, Yao, PRD.108.094518]
[Ikeda, Kharzeev, SS, PRD.108.074001] [Wu, Du, Zhao, Vary, PRD.110.056044]
[Ikeda, Kharzeev, Kikuchi, PRD.103.L071502] [Kharzeev, Kikuchi, PRRes.023342]
[Florio, Eosoklakh, Ikeda, Kharzeev, Kozpin, SS, Yu, PRL.131.021902; PRD.110.094029]

Lattice calculation

$$Z = \text{tr}(e^{-\beta H[\Psi, \Pi]}) = \int \mathcal{D}\Psi e^{-S[\Psi, \dot{\Psi}]}$$

sample $\Psi(\tau) \sim P[\Psi(t)] \propto e^{-\beta L[\Psi, \dot{\Psi}]}$.

expensive to sample uncorrelated configurations $\Psi(\tau)$!

ML: approximate $P[\Psi(t)] \approx P_{\text{ML}}[\Psi(t)]$,

sample $\Psi(\tau) \sim P_{\text{ML}}[\Psi(t)]$

- VAEs and GANs

- D. Giataganas, et al., New J. Phys. 24, 043040 (2022).

- K. Zhou, et al., Phys. Rev. D 100, 011501 (2019).

- J. M. Pawłowski and J. M. Urban, MLST 1, 045011 (2020).

- J. Singh, et al., SciPost Phys. 11, 043 (2021).

- Diffusion Models

- Wang, Aarts, Zhou, JHEP 05 (2024) 060; 2412.13704**

- Autoregressive models

- D. Wu, et al., Phys. Rev. Lett. 122, 080602 (2019).

- L. Wang, et al., CPL 39, 120502 (2022).

- P. Białas, P. Korcyl, and T. Stebel, CPC 281, 108502 (2022).

- Flow-based models

- M. S. Albergo, et al., Phys. Rev. D 100, 034515 (2019).**

- G. Kanwar, et al., Phys. Rev. Lett. 125, 121601 (2020).**

- K. A. Nicoli, et al., Phys. Rev. Lett. 126, 032001 (2021).

- L. Del Debbio, et al., Phys. Rev. D 104, 094507 (2021).

- M. Caselle, et al., JHEP 2022, 15 (2022).

- R. Abbott et al., Phys. Rev. D 106, 074506 (2022).

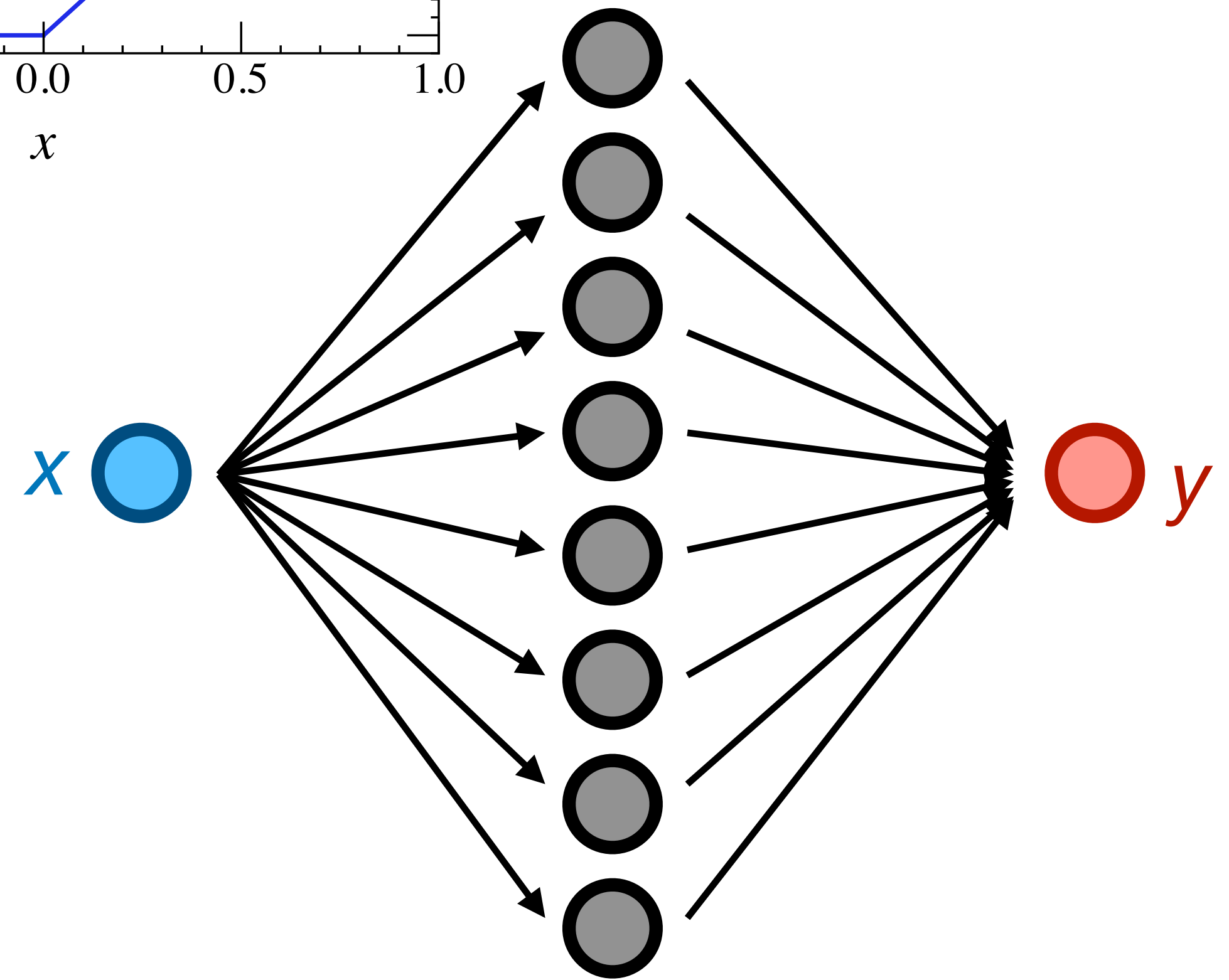
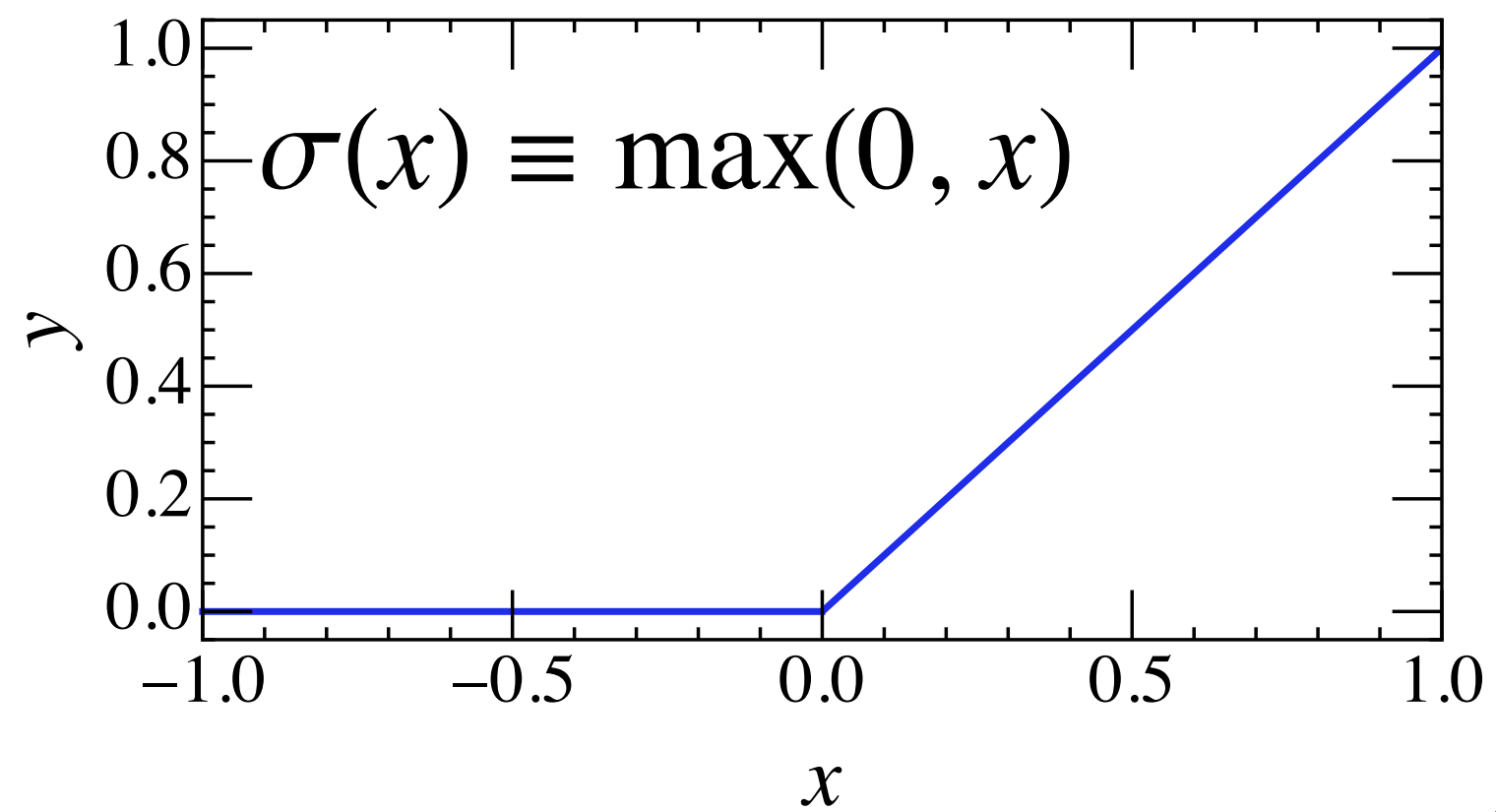
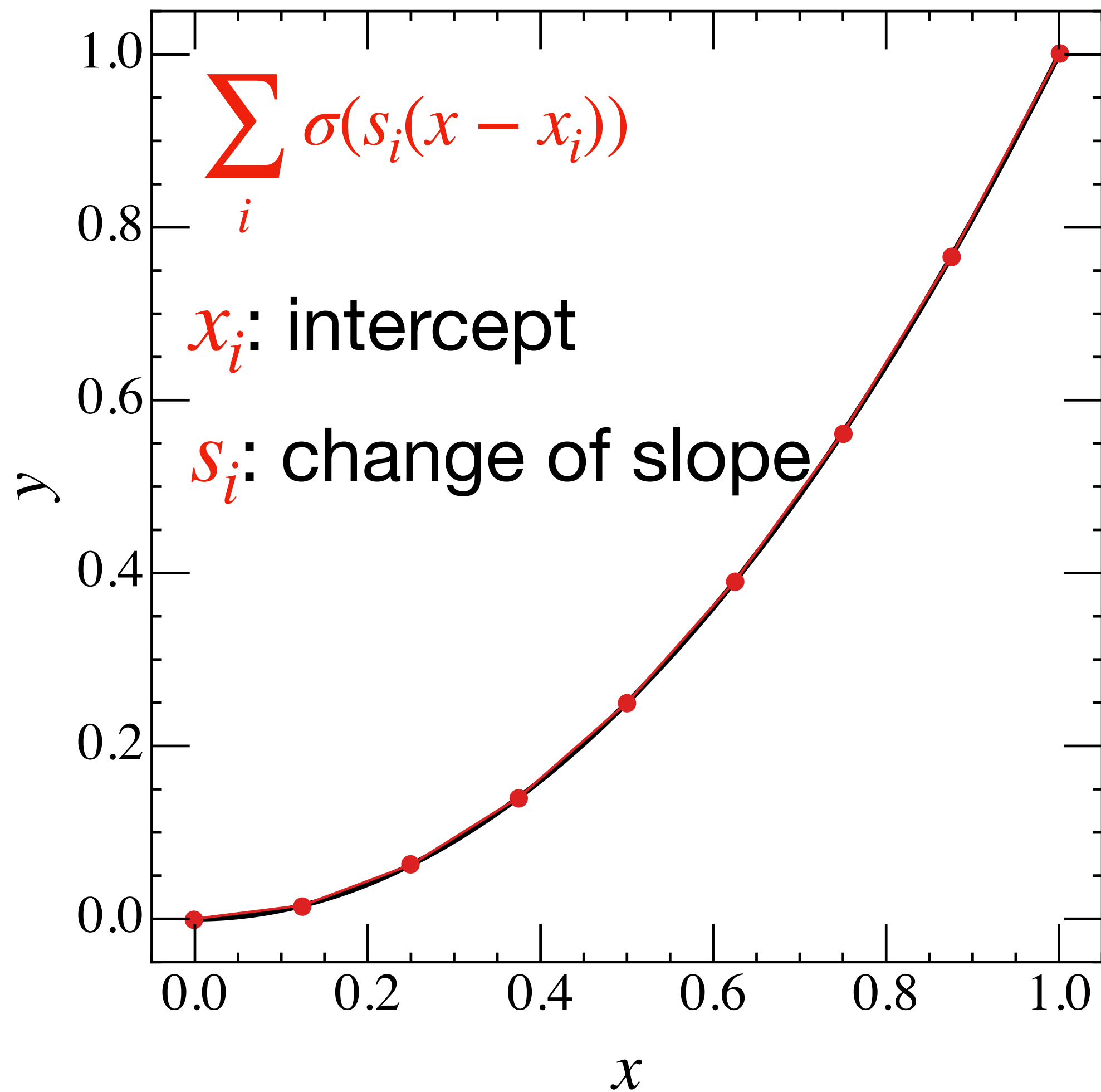
- A. Singha, et al., Phys. Rev. D 107, 014512 (2023).

- S. Chen, et al., Phys. Rev. D 107, 056001(2023).

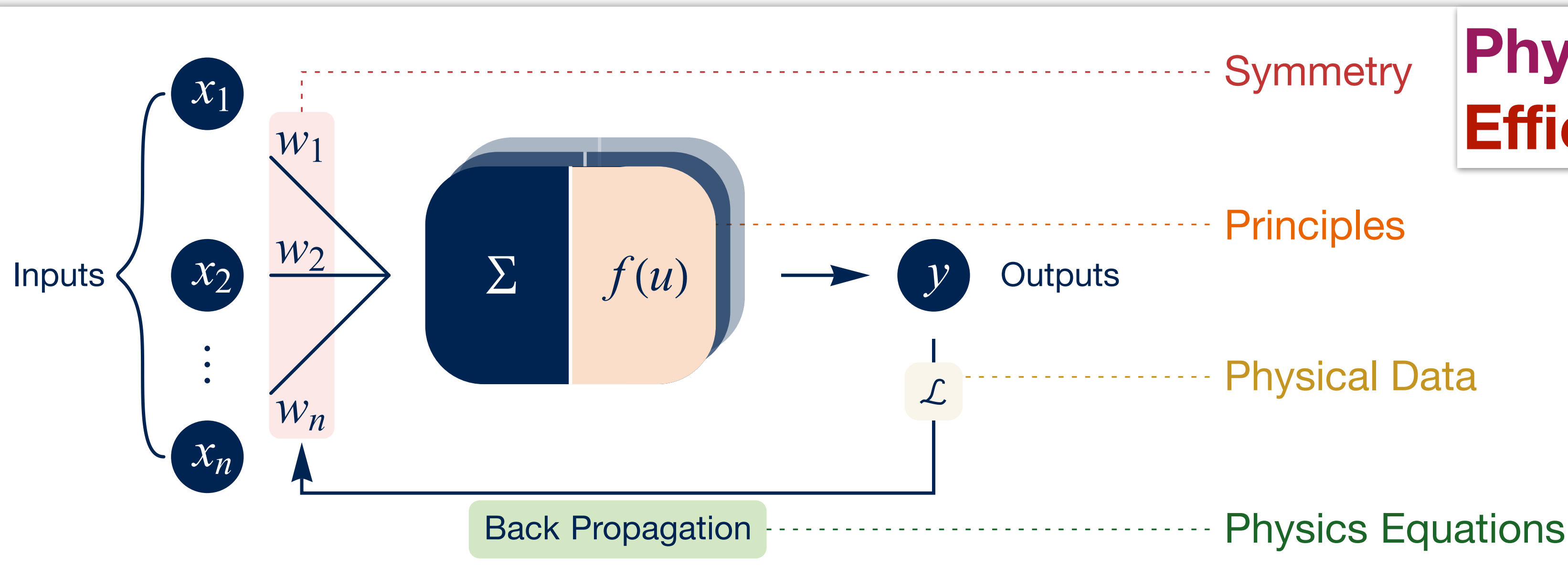
Review

- K. Cranmer, G. Kanwar, S. Racanière, D. J. Rezende, and P. E. Shanahan, Advances in Machine-Learning-Based Sampling Motivated by Lattice Quatum Chromodynamics, Nat. Rev. Phys. 1 (2023).**

--- a general parameterization scheme to approximate continuous functions.



each \bullet represents one of $\sigma(s_i(x - x_i))$



Physics Knowledge in Design Efficiency & Reliability

nature reviews physics <https://doi.org/10.1038/s42254-024-00798-x>

Perspective Check for updates

Physics-driven learning for inverse problems in quantum chromodynamics

Gert Aarts¹, Kenji Fukushima², Tetsuo Hatsuda³, Andreas Ipp⁴, Shuzhe Shi⁵, Lingxiao Wang³ & Kai Zhou^{6,7}

Progress in Particle and Nuclear Physics 135 (2024) 104084

Contents lists available at ScienceDirect

Progress in Particle and Nuclear Physics

journal homepage: www.elsevier.com/locate/ppnp

Review

Exploring QCD matter in extreme conditions with Machine Learning

Kai Zhou^{a,b,*}, Lingxiao Wang^{a,*}, Long-Gang Pang^{c,*}, Shuzhe Shi^{d,e,*}

Check for updates

HIC observed particles → 1st-order phase transition

Pang, Zhou, Su, Petersen, Stocker, Wang, Nat.Comm. 9 (2018)1,210

Neutron Star Mass-Radius → EoS

Fujimoto, Fukushima, Murase, PhysRevD.98,023019

Soma, Wang, **SS**, Stöcker, Zhou, PRD.107.083028; JCAP 98(2020)071

Energy spectrum → potential

SS, Zhou, Zhao, Mukherjee, Zhuang, PhysRevD.105.014017

imaginary time correlation → spectral function

Wang, **SS**, Zhou, PRD.106.L051502; Com.Phys.Comm. (2022) 108547

femtoscopy → hadron interaction

Wang, Zhao, 2411.16343

lattice EoS → quasi particle properties

Li, Lu, Pang, Qin, Phys.Lett.B 844(2023)138088

Physics Knowledge in Design
Efficiency & Reliability

Other Reviews:

Ma, Pang, Wang, Zhou,
Chin.Phys.Lett.40.112101

He, Ma, Pang, Song, Zhou,
Nucl.Sci.Tech.34,6,88

Pang,
Int.J.Mod.Phys.E 33, 06, 2430009

Boehnlein et al,
Rev.Mod.Phys.94.031003

Progress in Particle and Nuclear Physics 135 (2024) 104084

Contents lists available at ScienceDirect

Progress in Particle and Nuclear Physics

journal homepage: www.elsevier.com/locate/ppnp



- ▶ Quantum Computation / Simulation:
 - real-time
 - finite temperature

- ▶ Machine Learning:
 - inverse problems
 - classification