COMPUTATIONAL FRAMEWORKS AND CHALLENGES IN QUANTUM MANY-BODY PHYSICS

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OUTLINE

- Goal: Wild ride (hopefully exciting)
- Computational challenges in quantum many-body systems
- A case study: one-dimensional Heisenberg spin chain
- Density-Matrix-Renormalization-Group (DMRG) versus Monte Carlo

FIRST COMPUTATIONAL CHALLENGE?

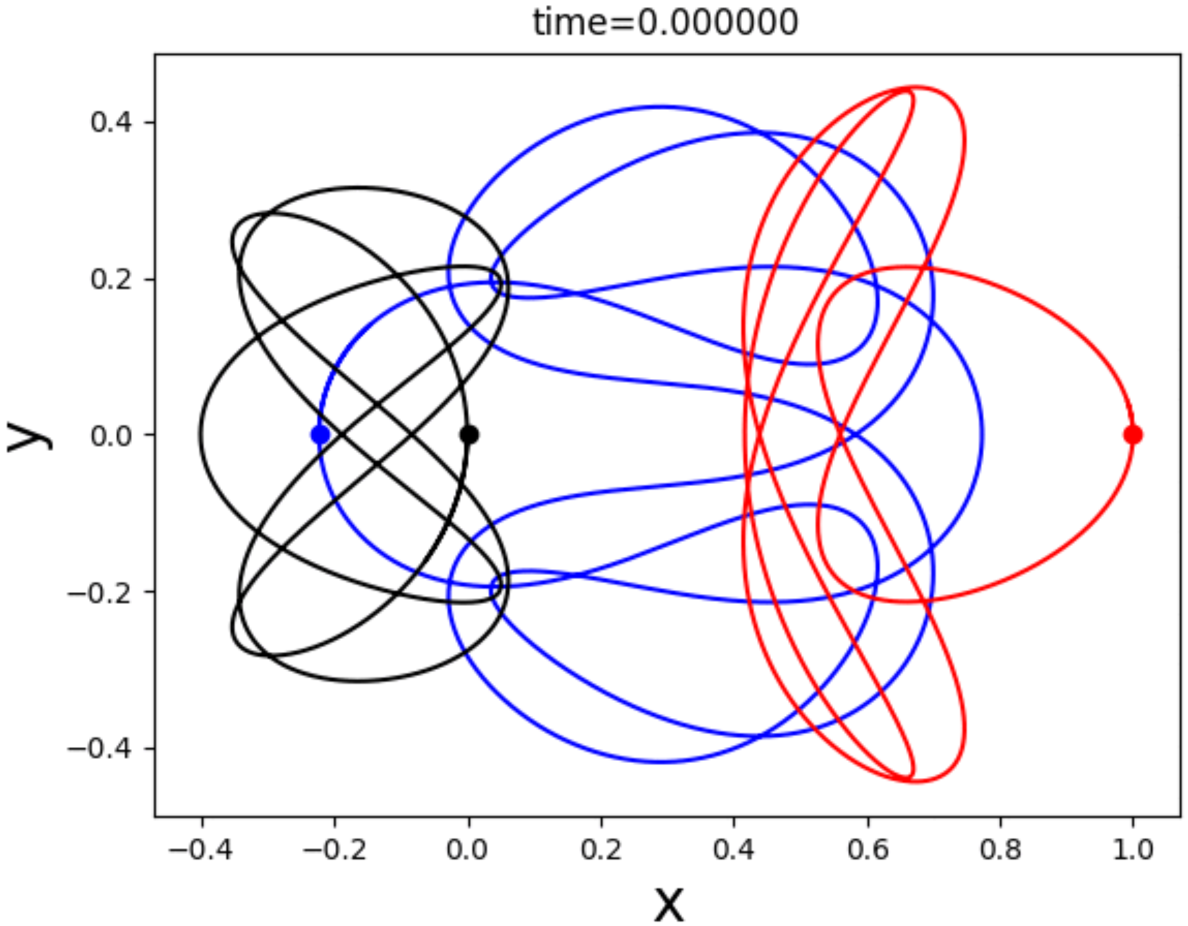
$$\ddot{\mathbf{r}}_1 = Gm_2 \frac{\mathbf{r}_2 - \mathbf{r}_1}{|\mathbf{r}_2 - \mathbf{r}_1|^3} + Gm_3 \frac{\mathbf{r}_3 - \mathbf{r}_1}{|\mathbf{r}_3 - \mathbf{r}_1|^3}$$

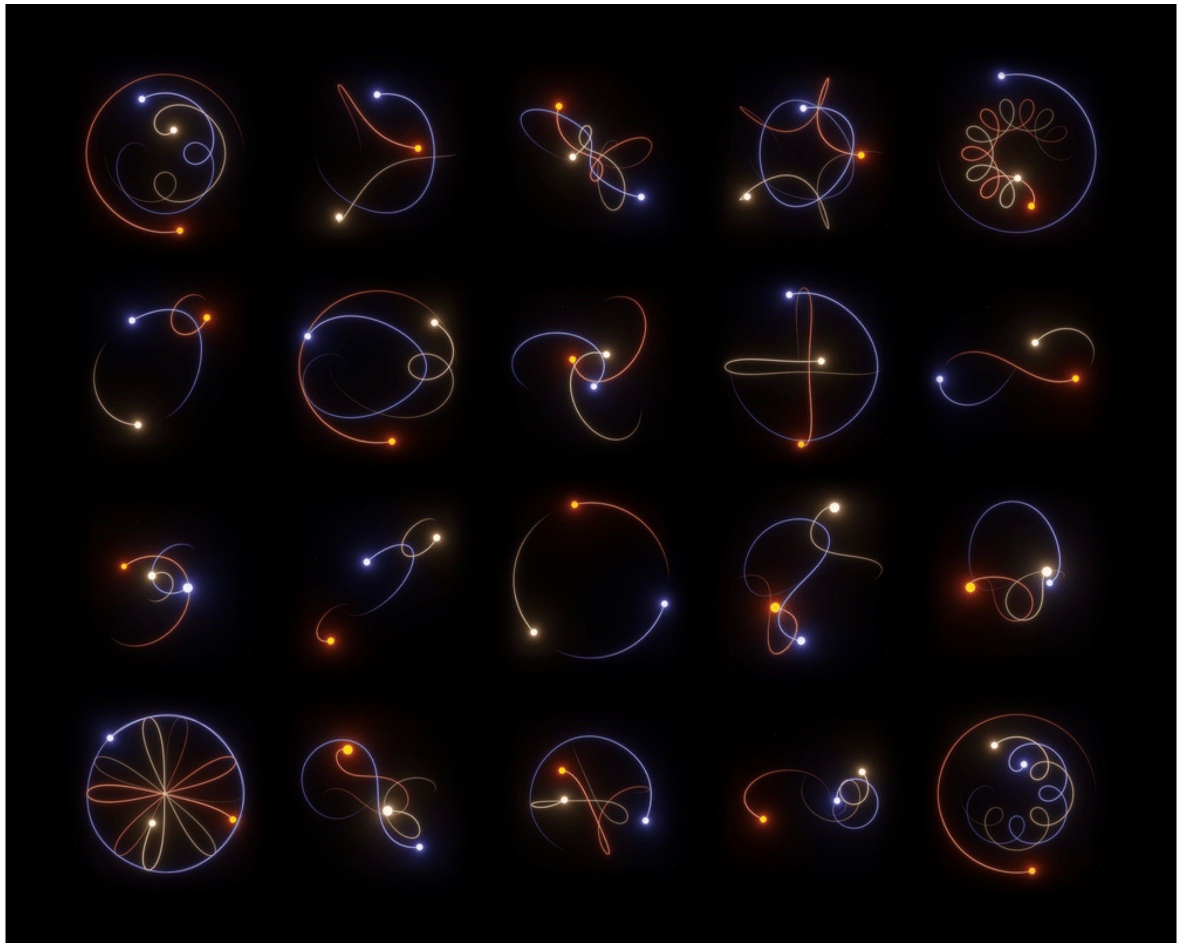
$$\ddot{\mathbf{r}}_2 = Gm_1 \frac{\mathbf{r}_1 - \mathbf{r}_2}{|\mathbf{r}_1 - \mathbf{r}_2|^3} + Gm_3 \frac{\mathbf{r}_3 - \mathbf{r}_2}{|\mathbf{r}_3 - \mathbf{r}_2|^3}$$

$$\ddot{\mathbf{r}}_3 = Gm_1 \frac{\mathbf{r}_1 - \mathbf{r}_3}{|\mathbf{r}_1 - \mathbf{r}_3|^3} + Gm_2 \frac{\mathbf{r}_2 - \mathbf{r}_3}{|\mathbf{r}_2 - \mathbf{r}_3|^3}$$

Generically non integrable problem

Orbits are non periodic, chaotic





https://numericaltank.sjtu.edu.cn/three-body/three-body.htm

ELECTRON'S MAGNETIC MOMENT

$$\alpha^{-1}(Rb) = 137.035998996(85)$$

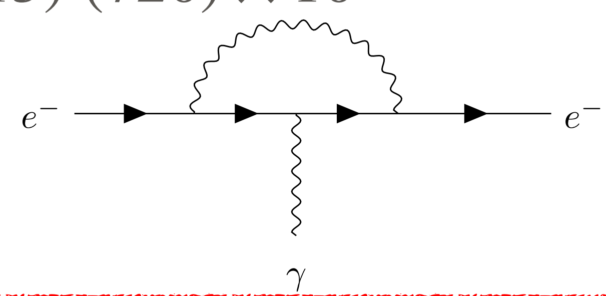
$$\mu = -\frac{g}{2}\mu_B \frac{\mathbf{S}}{\hbar/2}$$

$$a_e^{\text{QED}} = \frac{g-2}{2} = C_1\left(\frac{\alpha}{\pi}\right) + C_2\left(\frac{\alpha}{\pi}\right)^2 + C_3\left(\frac{\alpha}{\pi}\right)^3 + C_4\left(\frac{\alpha}{\pi}\right)^4 + C_5\left(\frac{\alpha}{\pi}\right)^5 + \mathcal{O}\left(\frac{\alpha}{\pi}\right)^6,$$

$$a_e^{\text{SM}}(\alpha) = 1\,159\,652\,182.031\;(15)\;(15)\;(720) \times 10^{-12}$$

$$a_e^{\text{exp}} = 1\,159\,652\,180.73\;(0.28) \times 10^{-12}$$

$$C_1 = \frac{1}{2}$$



5 diagrams

$$C_2 = \frac{197}{144} + \frac{1}{12}\pi^2 - \frac{1}{2}\pi^2 \ln 2 + \frac{3}{4}\zeta(3)$$

7 diagrams

72 diagrams

$$C_3 = \frac{83}{72}\pi^2\zeta(3) - \frac{215}{24}\zeta(5) + \frac{100}{3}\left[\left(a_4 + \frac{1}{24}\ln^4 2\right) - \frac{1}{24}\pi^2\ln^2 2\right] - \frac{239}{2160}\pi^4 + \frac{139}{18}\zeta(3) - \frac{298}{9}\pi^2\ln 2 + \frac{17101}{810}\pi^2 + \frac{28259}{5184}$$

891 diagrams

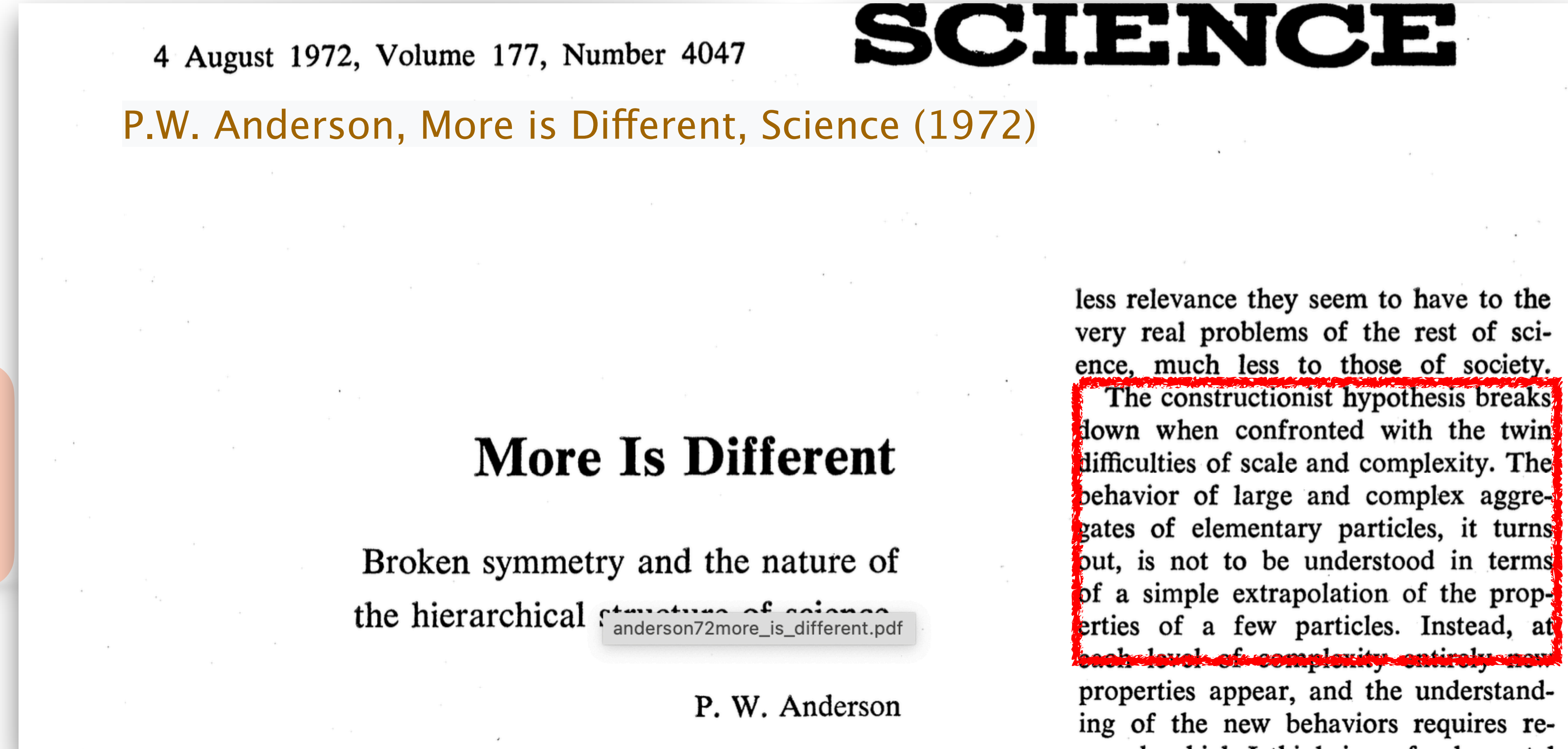
$$C_4 = -\,1.912245764926445574152647167439830054060873390658725345171329$$

$$C_5 = 6.599(223)$$

12672 diagrams

MORE IS DIFFERENT

$$1 + 1 \neq 2$$



4 August 1972, Volume 177, Number 4047
SCIENCE

P.W. Anderson, More is Different, Science (1972)

More Is Different

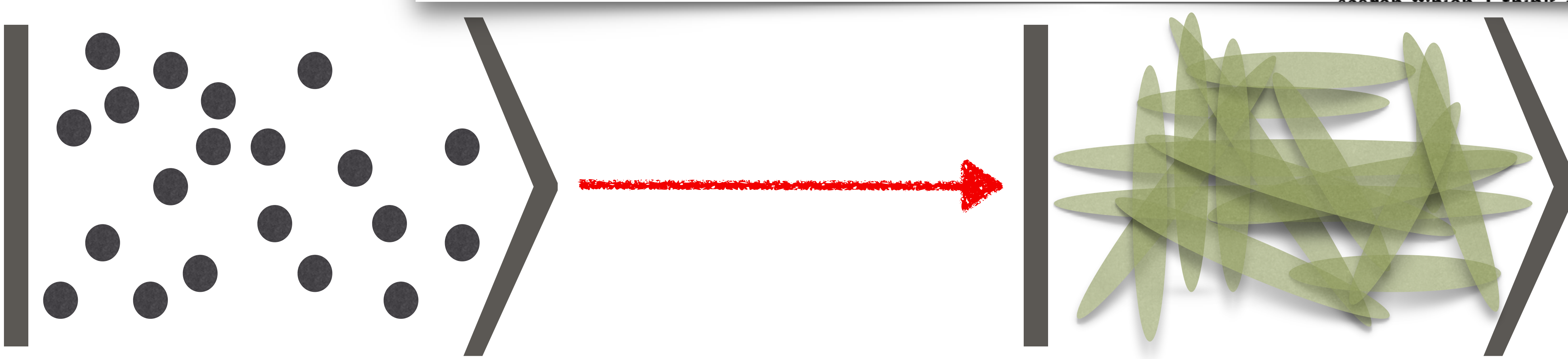
Broken symmetry and the nature of the hierarchical structure of science

anderson72more_is_different.pdf

P. W. Anderson

less relevance they seem to have to the very real problems of the rest of science, much less to those of society.

The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity. The behavior of large and complex aggregates of elementary particles, it turns out, is not to be understood in terms of a simple extrapolation of the properties of a few particles. Instead, at each level of complexity entirely new properties appear, and the understanding of the new behaviors requires re-

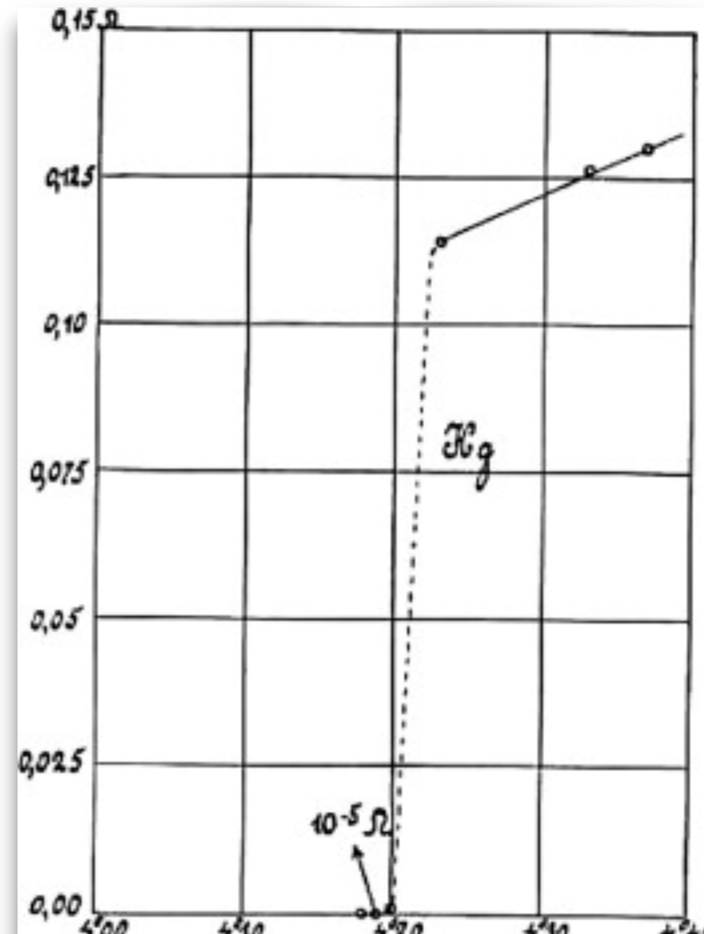


- Quantum many-body systems are more than the "sum" of their constituents

Many-body effects are enhanced in low dimension and "small" local Hilbert space

SUPERCONDUCTIVITY

Heike Kamerlingh Onnes
(1853-1926)



"Mercury practically zero",
Leiden, October 1911

HEISENBERG SPIN-1/2 CHAIN

$$H = J \sum_{j=1}^{L} \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z \right]$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$CuSO_4$

- Exact diagonalization

$$|\, s_1, s_2, s_3, \ldots, s_L \rangle$$

$$s_i = \uparrow, \downarrow$$

$$\langle i \,|\, H \,|\, j \rangle = \Big[\quad \Big]^{2^L}_{2^L}$$

$$|\, \Psi \rangle = \sum_{\{s_j\}} A_{s_1, s_2, \ldots s_L} \,|\, s_1, s_2, \ldots, s_L \rangle$$

SPIN CHAIN HEAVEN

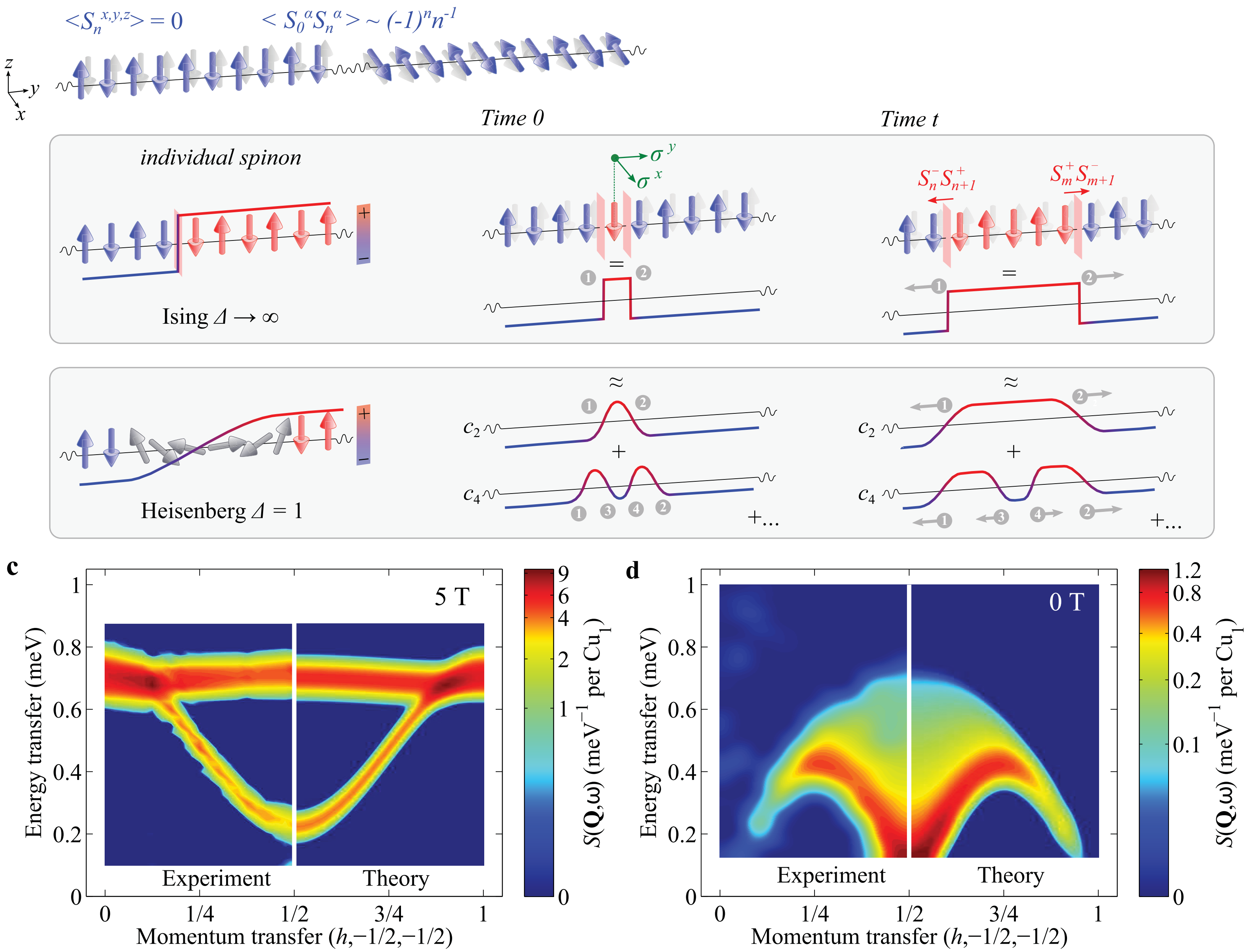
In 2008 Roger Hiorns transformed an empty council flat in Southwark, London into Seizure, a sparkling blue world of copper sulphate crystals. The work was created using 75,000 litres of liquid copper sulphate, which was pumped into the former dwelling to create a strangely beautiful and somewhat menacing crystalline growth on the walls, floor, ceiling and even the bath of the abandoned flat.

GLIMPSE INTO PHYSICS

- Inelastic neutron scattering

Dynamical structure factor

$$\frac{d^2\sigma}{d\Omega d\omega} \propto S^{\alpha\beta}(\mathbf{q},\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt e^{-i\omega t}\sum_l e^{i\mathbf{q}\cdot\mathbf{r}_l}\langle S_0^\alpha(0)S_l^\beta(t)\rangle$$



Ground state is in a "liquid" phase (critical state)

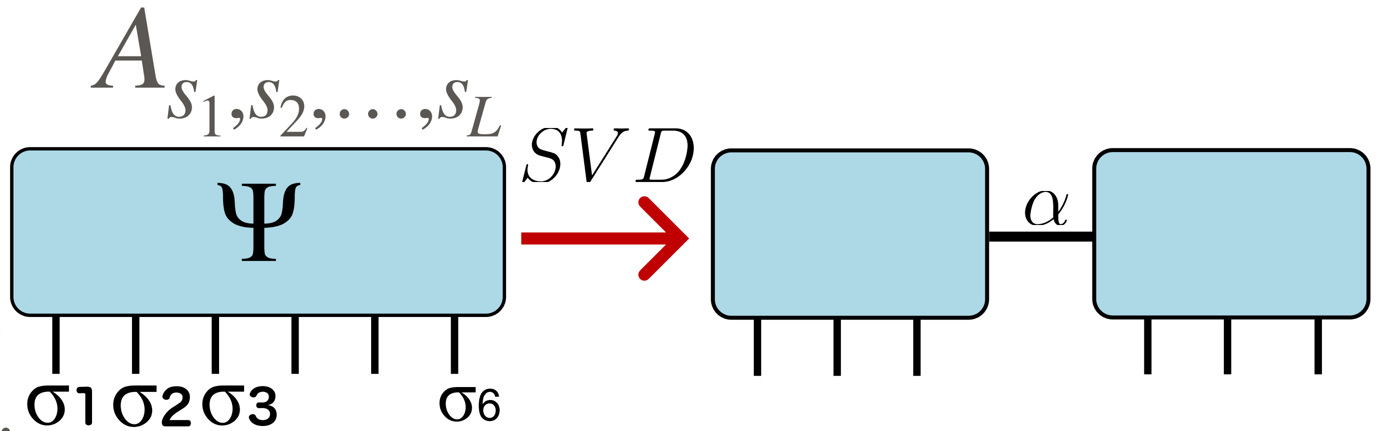
Not just low energy

Two-particle continuum

Deconfined excitations

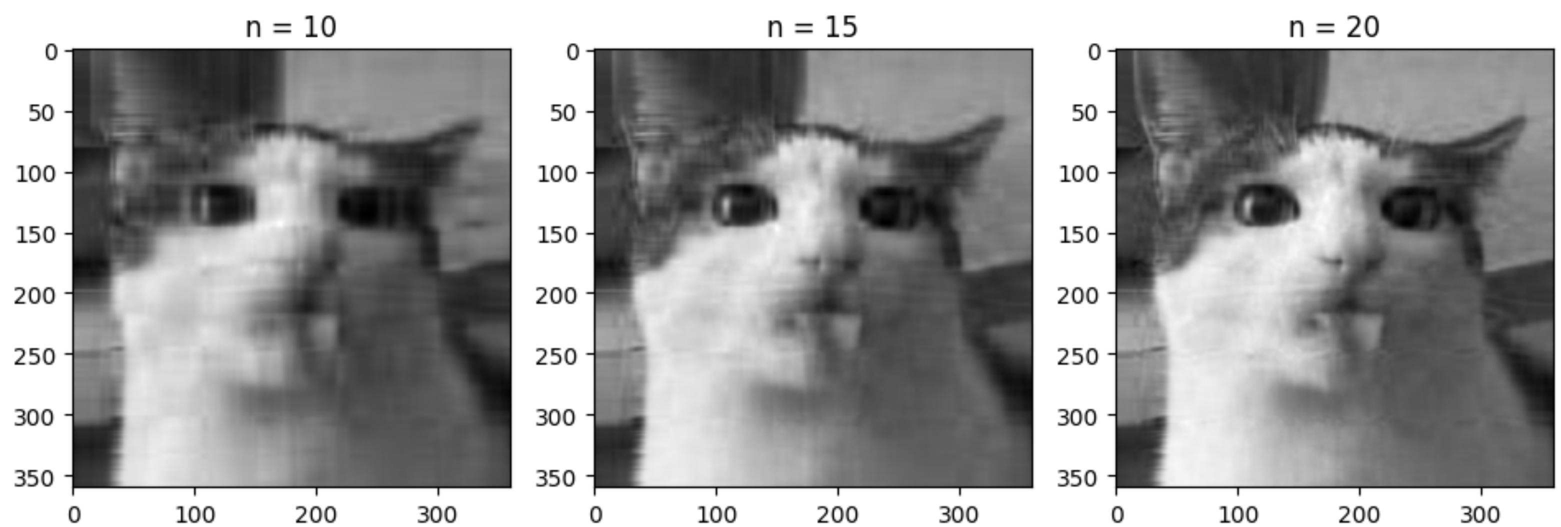
MATRIX PRODUCT STATES

d^L



- Singular Value Decomposition

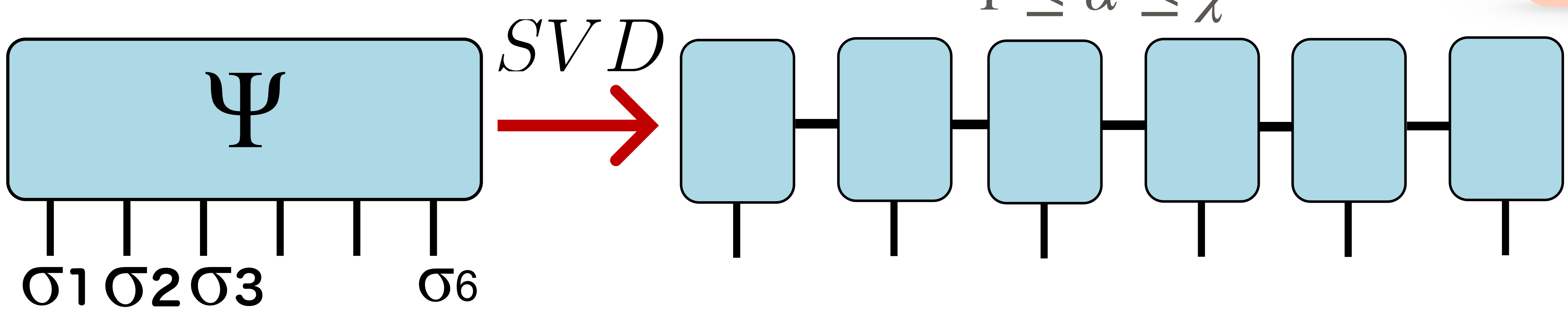
$$M = U\Sigma V^\dagger, \quad \Sigma = \left\{\sqrt{\lambda_1}, \sqrt{\lambda_2}, \ldots, \sqrt{\lambda_n}\right\}$$



- Matrix Product State (MPS) decomposition

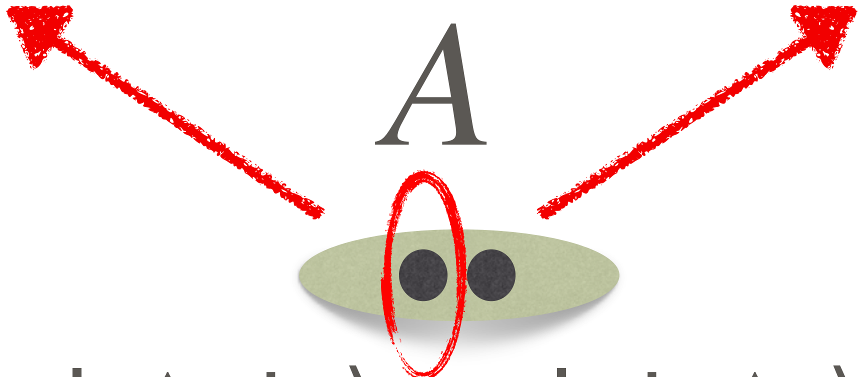
$1 \leq \alpha \leq \chi$

$\chi^2 L d$



WHY IT WORKS

- Entanglement scaling



$$\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

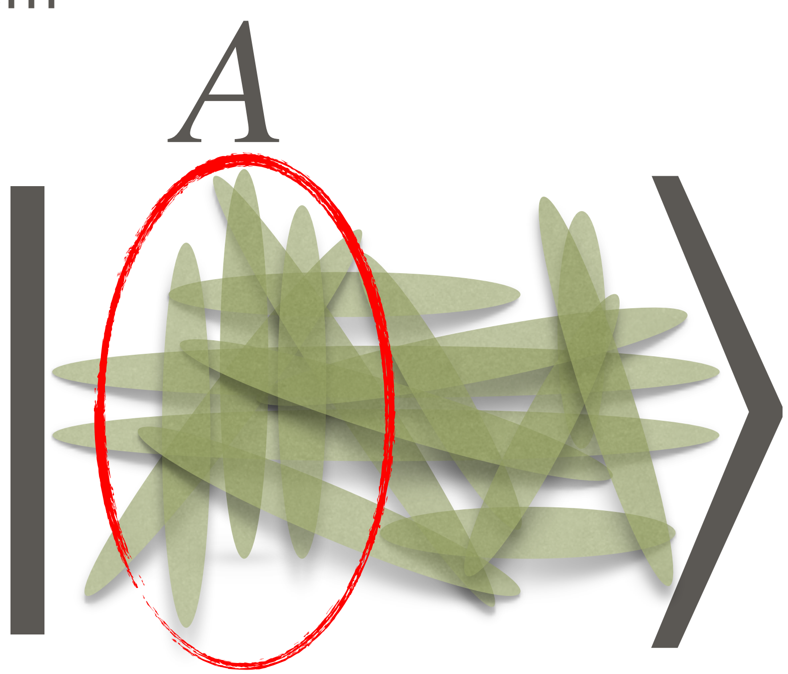
$$\rho_A = \mathrm{Tr}_B |\Psi\rangle\langle\Psi|$$

Von Neuman entropy

$$S_A = -\,\mathrm{Tr}_A \rho_A \ln(\rho_A)$$

$$S_A = \ln(2)$$

- In a many-body system



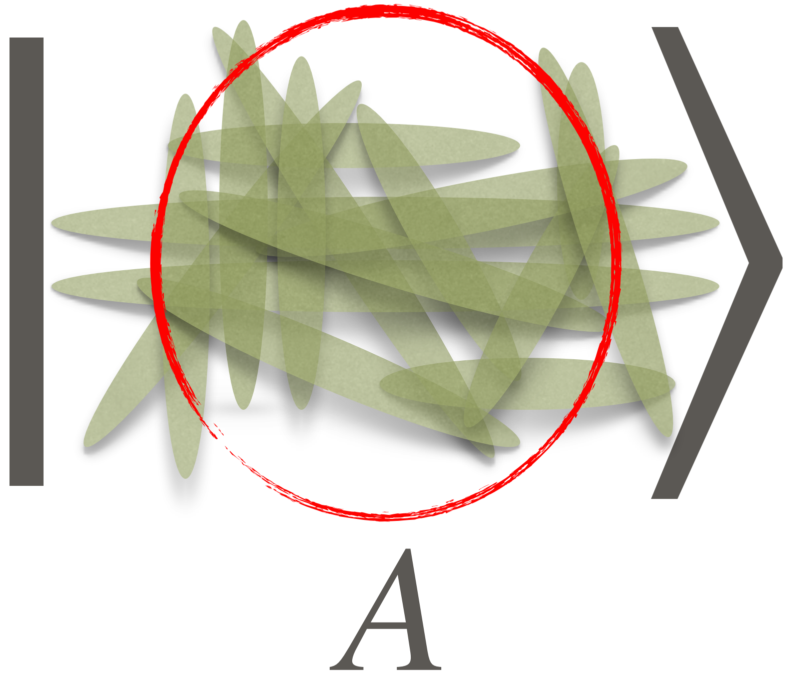
Volume-law scaling

$$S_A^{\max} = |A| \ln(2)$$

ENTANGLEMENT SCALING

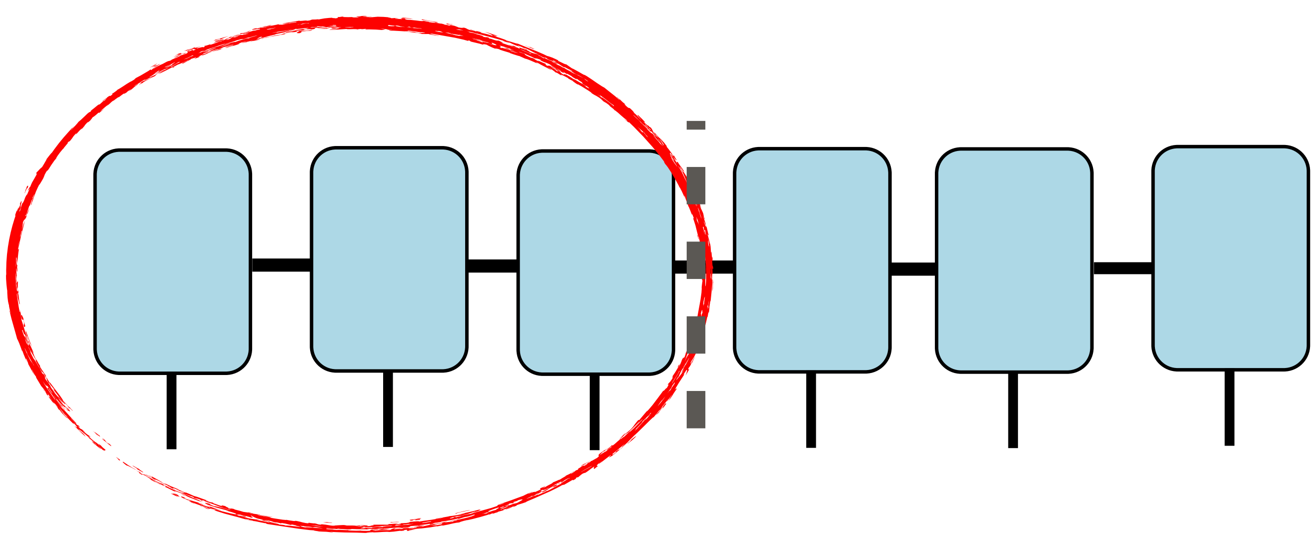
- Area-law scaling in ground-states of local Hamiltonians

M. B. Hastings, JSTAT, P08024 (2007)



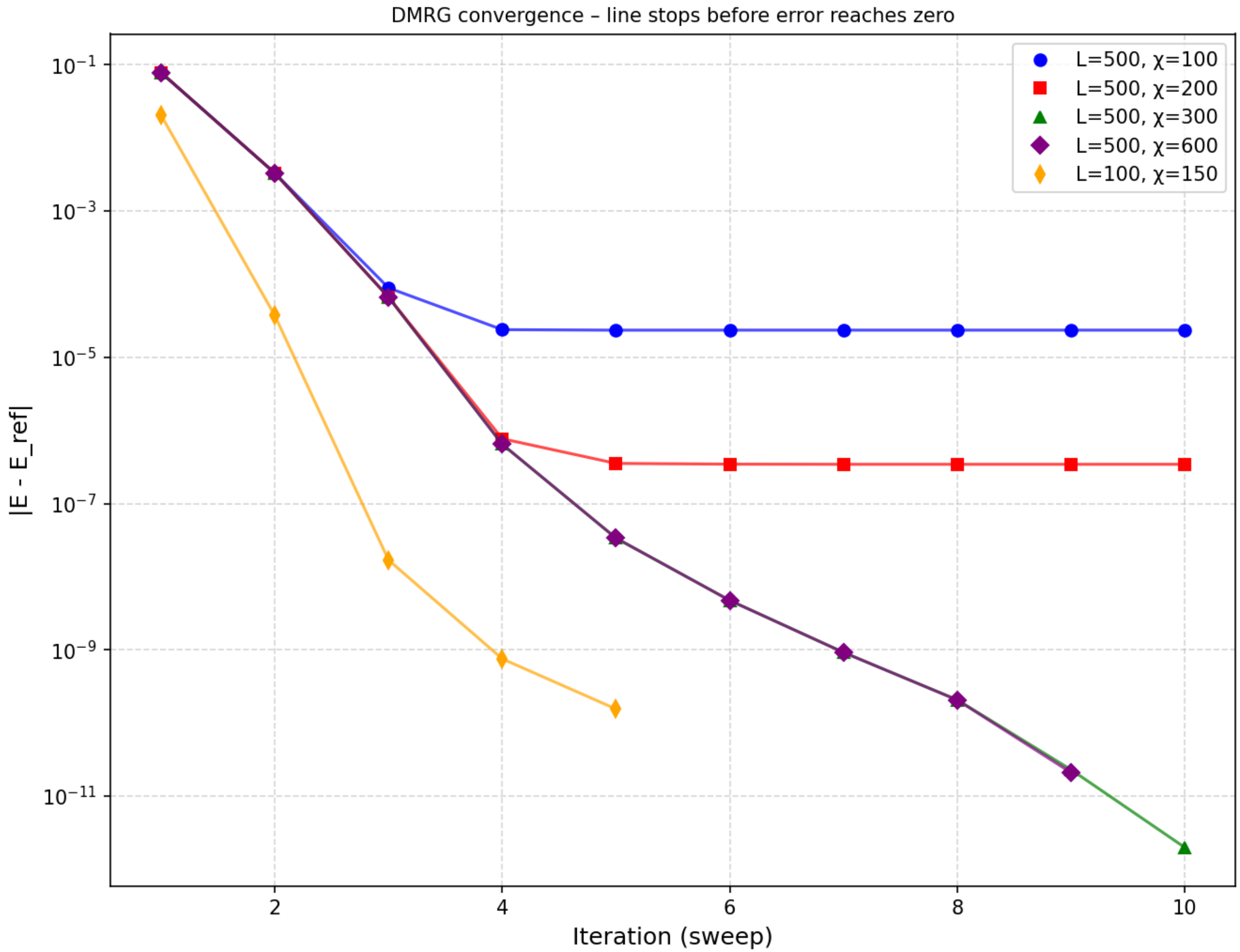
$$S_A \propto |A|^{d-1}$$

- For an MPS we have



$$S_A = -\sum_j \lambda_j \ln(\lambda_j)$$

DENSITY MATRIX RENORMALIZATION GROUP



QUANTUM MONTE CARLO

- Partition function in quantum statistical mechanics

A. Sandvik, Computational Studies of Quantum Spin Systems, AIP Conf.Proc.1297:135,2010

$$Z(T) = \mathrm{Tr}\left(e^{-\beta H}\right)$$

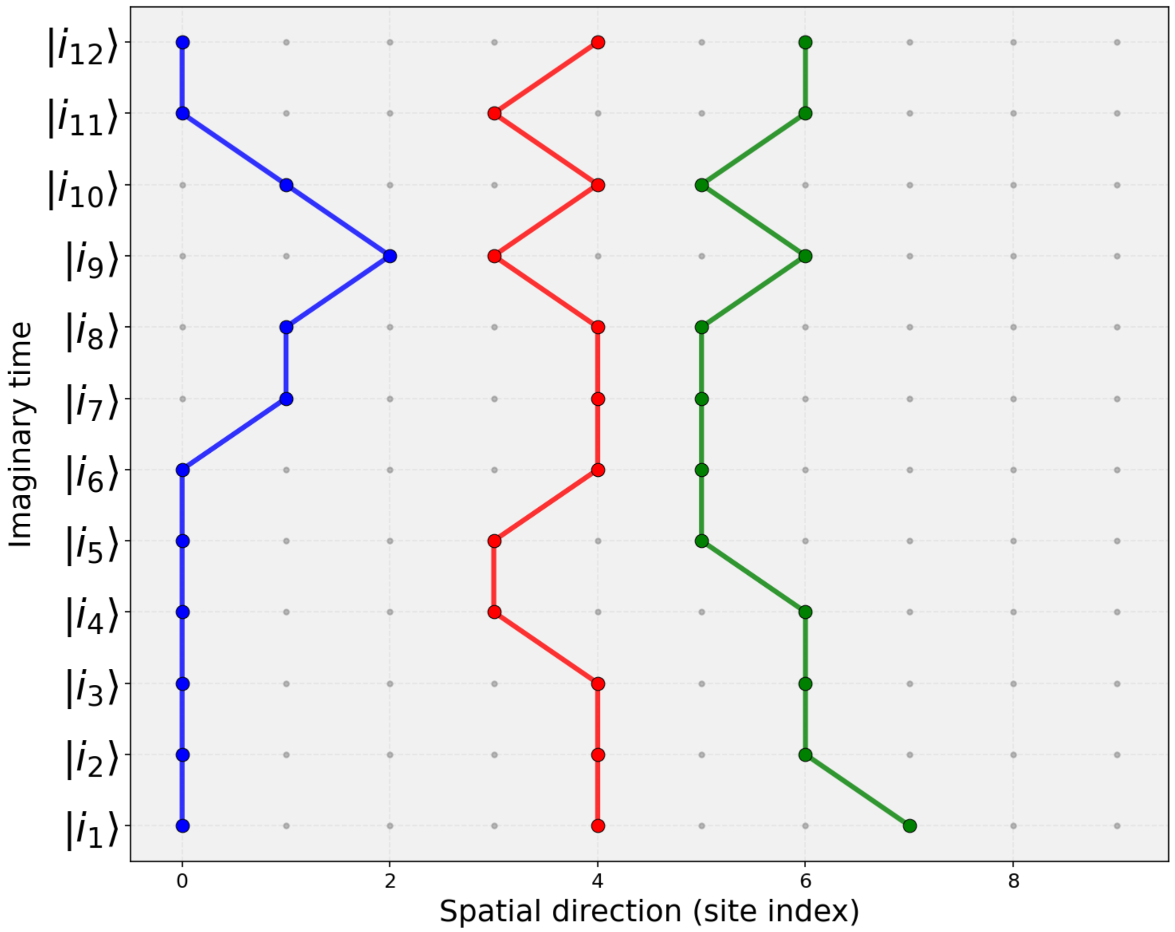
- Expectation values of local observables

$$\langle \mathcal{O} \rangle = \mathrm{Tr}\left(\mathcal{O} e^{-\beta H}\right)$$

- Suzuki-Trotter decomposition

$$Z(T) = \mathrm{Tr}\left(e^{-\Delta\tau H}\right)^M = \sum_{\{(i_1,i_2,\ldots,i_M)\}} \langle i_1 | 1 - \Delta\tau H | i_2 \rangle \langle i_2 | 1 - \Delta\tau H | i_3 \rangle \cdots \langle i_M | 1 - \Delta\tau H | i_1 \rangle$$

QUANTUM MONTE CARLO



Monte Carlo sampling of trajectories

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 21, NUMBER 6 JUNE, 1953

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

Fermions and/or frustration

Configurations can have negative weight (sign problem)

$$\langle \uparrow_i \uparrow_j | e^{-\Delta\tau H_{ij}} | \uparrow_i \uparrow_j \rangle = \langle \downarrow_i \downarrow_j | e^{-\Delta\tau H_{ij}} | \downarrow_i \downarrow_j \rangle = +\, e^{-\Delta\tau/4}$$

$$\langle \uparrow_i \downarrow_j | e^{-\Delta\tau H_{ij}} | \uparrow_i \downarrow_j \rangle = \langle \downarrow_i \uparrow_j | e^{-\Delta\tau H_{ij}} | \downarrow_i \uparrow_j \rangle = +\, e^{\Delta\tau/4} \cosh(\Delta\tau/2)$$

$$\langle \downarrow_i \uparrow_j | e^{-\Delta\tau H_{ij}} | \uparrow_i \downarrow_j \rangle = \langle \uparrow_i \downarrow_j | e^{-\Delta\tau H_{ij}} | \downarrow_i \uparrow_j \rangle = -\, e^{\Delta\tau/4} \sinh(\Delta\tau/2)$$

$$\langle \mathrm{Sgn} \rangle_F = e^{-\beta N_s \Delta f}$$

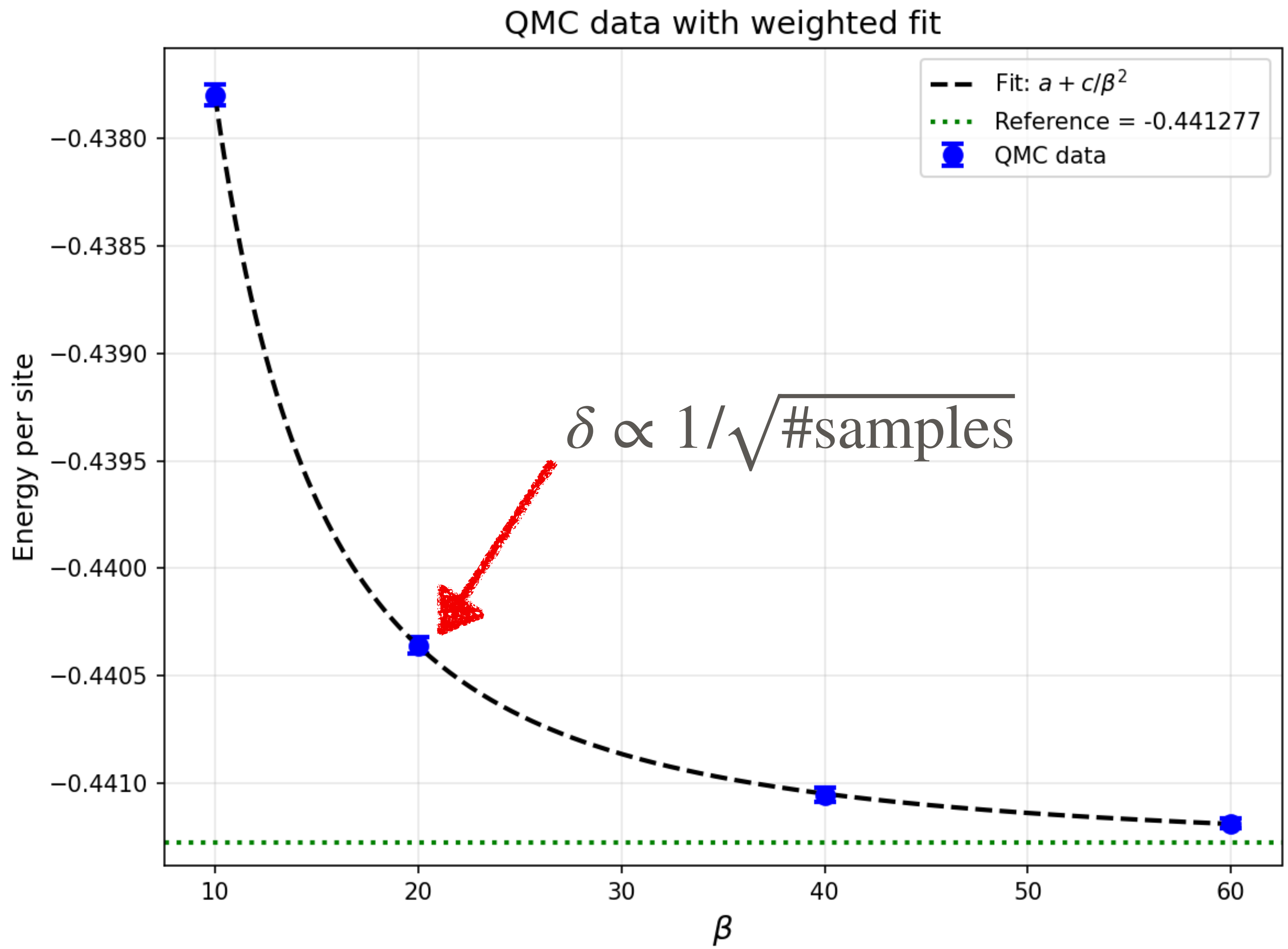
S. Wessel, Monte Carlo simulations of spin models (2013)

Up to date, no general solution of the QMC sign problem is known, although it can be overcome in certain special cases (cf., e.g., [35,51,52]). Moreover, it has been shown that a general solution to the sign problem essentially constitutes an NP-hard challenge [50]. It is however generally suspected, that no polynomial-time solutions to NP-hard problem exist. Hence, we urge the reader to contact us immediately in case she or he finds a serious path to a generic solution of the QMC sign problem! In the mean time, we hope to have stimulated your interest in

CONVERGENCE OF QMC

Finite-temperature corrections

$$\delta \propto 1/\beta^2$$



FIELD THEORY CONTENT

$$H = J \sum_{j=1}^{L} \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y \right]$$

"vacuum state"

"Tower of excitations"

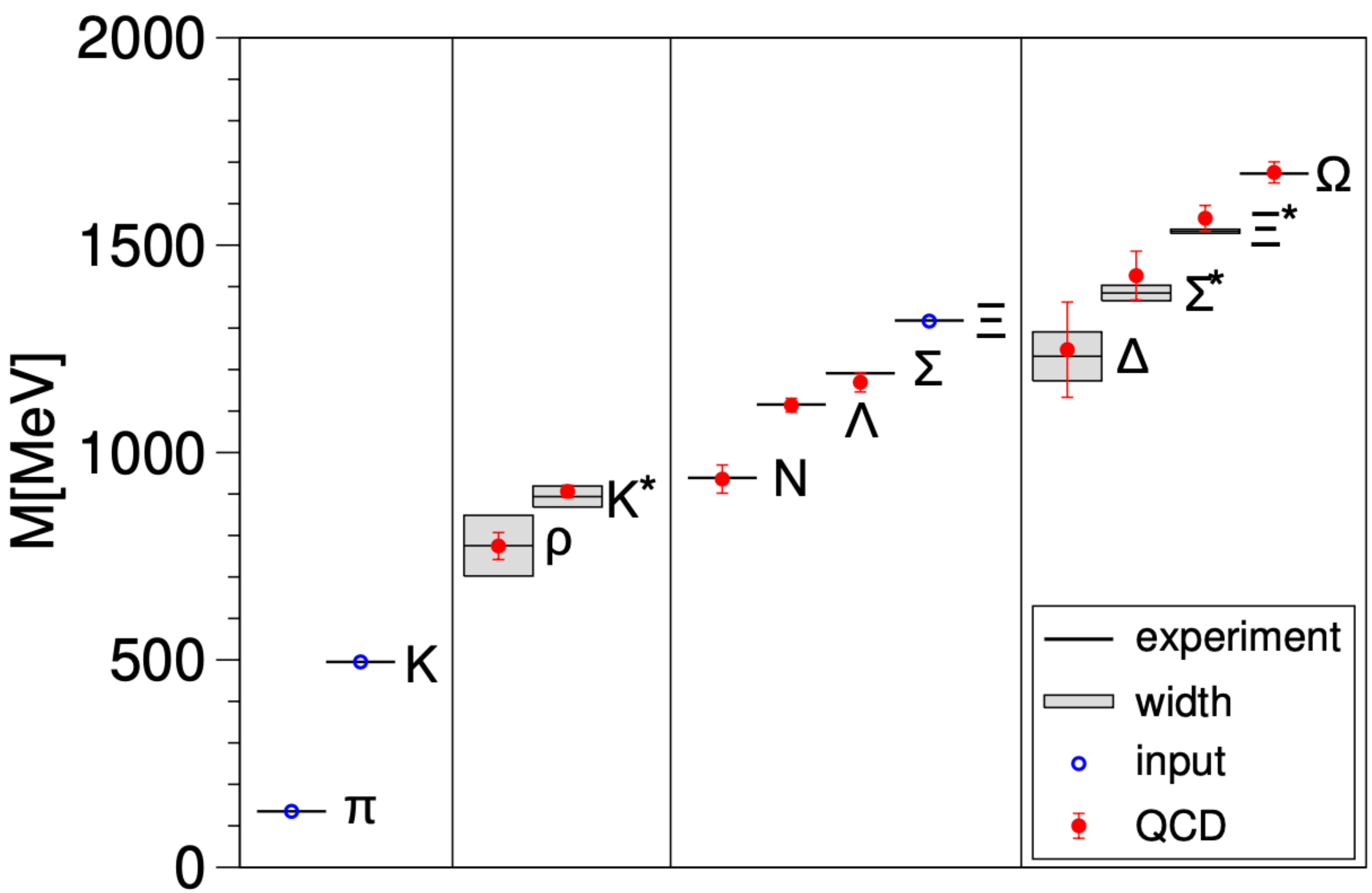
Name of excitation	Field	$(h, \bar{h})$	State $(n_F = N/2)$	$(h{:}p)$	$N = 8$ example
Ground state	$\mathbf{1}$	$(0, 0)$	$\lvert n_F\rangle$	$(:)$	○○●●●●○○
(a)	$e^{-i\phi}$	$(1/2, 0)$	$d_{(n_F-1)/2}\lvert n_F\rangle$	$(1:)$	○○●●●○○○
(b)	$e^{i\phi+i\bar{\phi}}$	$(1/2, 1/2)$	$d^\dagger_{n_F/2+1/2}\, d^\dagger_{-n_F/2-1/2}\lvert n_F\rangle$		○●●●●●●○
Umklapp	$e^{i\phi-i\bar{\phi}}$	$(1/2, 1/2)$	$d_{-(n_F-1)/2}\, d^\dagger_{(n_F+1)/2}\lvert n_F\rangle$		○○○●●●●○
Particle–hole	$i\partial\phi$	$(1, 0)$	$d_{(n_F-1)/2}\, d^\dagger_{(n_F+1)/2}\lvert n_F\rangle$	$(1:1)$	○○●●●○●○
R–L particle–hole	$\bar{\partial}\bar{\phi}\partial\phi$	$(1, 1)$	$d_{(n_F-1)/2}\, d^\dagger_{(n_F+1)/2}\, d_{-(n_F-1)/2}\, d^\dagger_{-(n_F+1)/2}\lvert n_F\rangle$		○●○●●○●○
	—	—	$d_{(n_F-1)/2}\, d^\dagger_{(n_F+3)/2}\lvert n_F\rangle$	$(1:2)$	○○●●●○○●

CONFORMAL FIELD THEORY

LATTICE RESULT

LATTICE QCD DETERMINATION OF HADRON MASSES

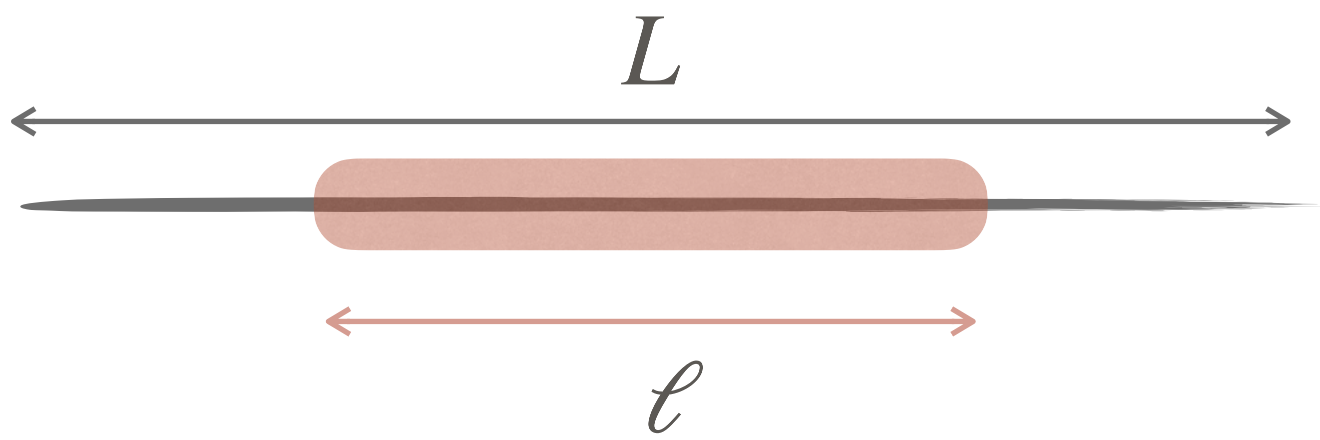
Budapest-Marseille-Wuppertal Collaboration, Science 322, 1224 (2008)



CHECK OF UNIVERSALITY

- Renyi entanglement entropies

$$S_A^{(n)} = \frac{1}{1-n} \ln \mathrm{Tr}_A \rho_A^n$$



- Renyi excess entropy function

Excess entropy

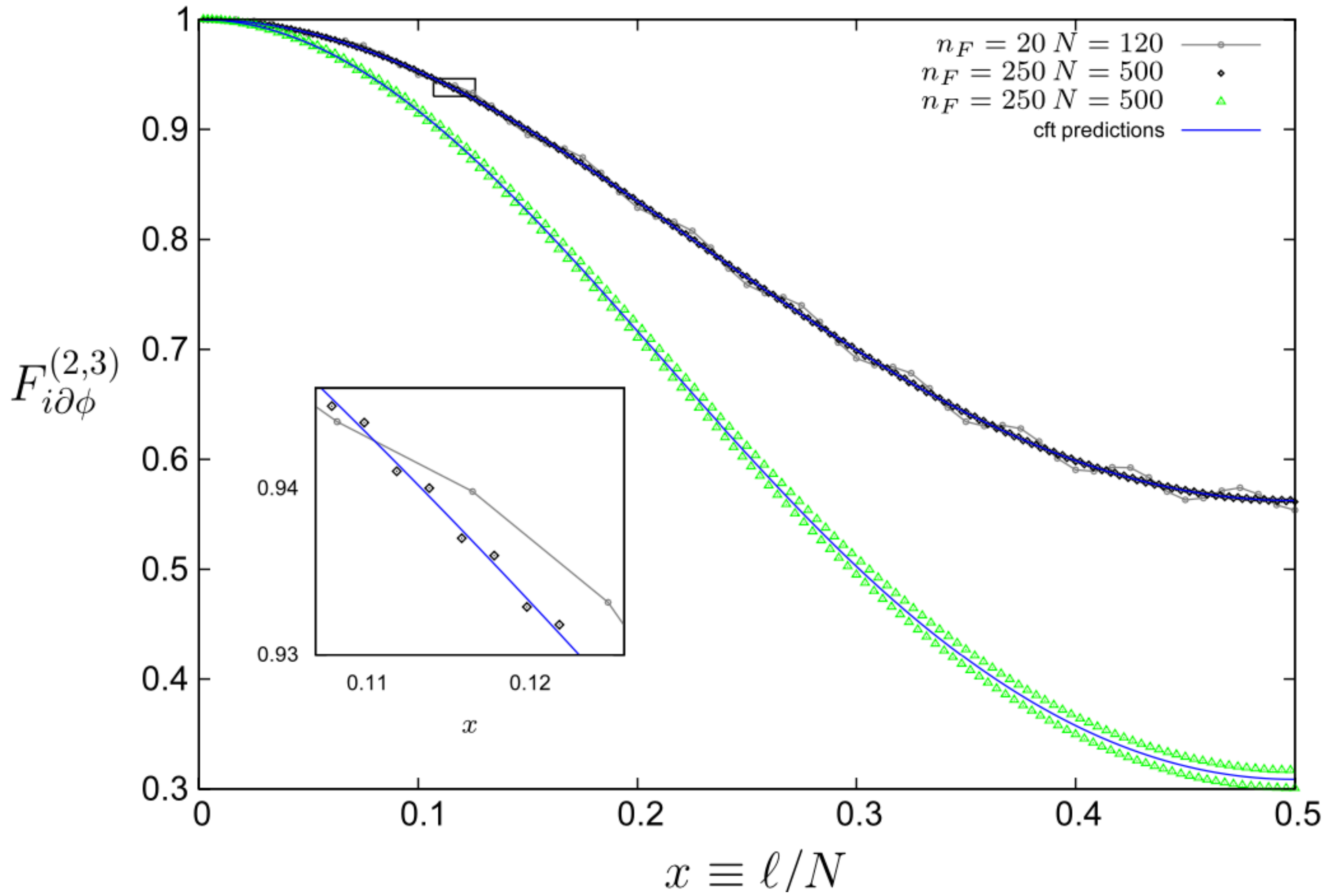
$$F_\Upsilon^{(n)} = \exp[(n-1)(S_\Upsilon^{(n)}(x) - S_{\mathrm{GS}}^{(n)}(x))]$$

$$x = \ell / L$$

- Conformal Field Theory vacuum correlator

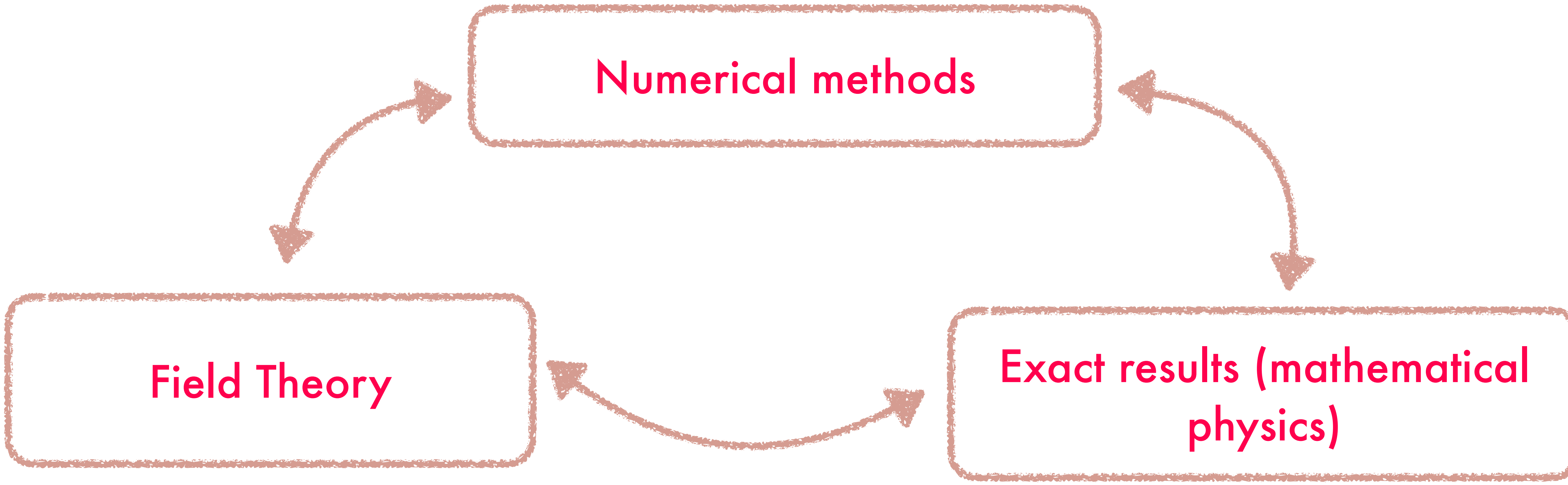
$$F_\Upsilon^{(n)}(A) \equiv F_\Upsilon^{(n)}(x) = \lim_{w \to -i\infty} \frac{\langle \prod_{k=0}^{n-1} \Upsilon_k(w,\bar{w}) \Upsilon_k^\dagger(-w,-\bar{w}) \rangle_{\mathcal{R}_n}}{\langle \Upsilon_0(w,\bar{w}) \Upsilon_0^\dagger(-w,-\bar{w}) \rangle_{\mathcal{R}_1}^n}.$$

Berganza, Alcaraz, Sierra, JSTAT, (2012) P01016



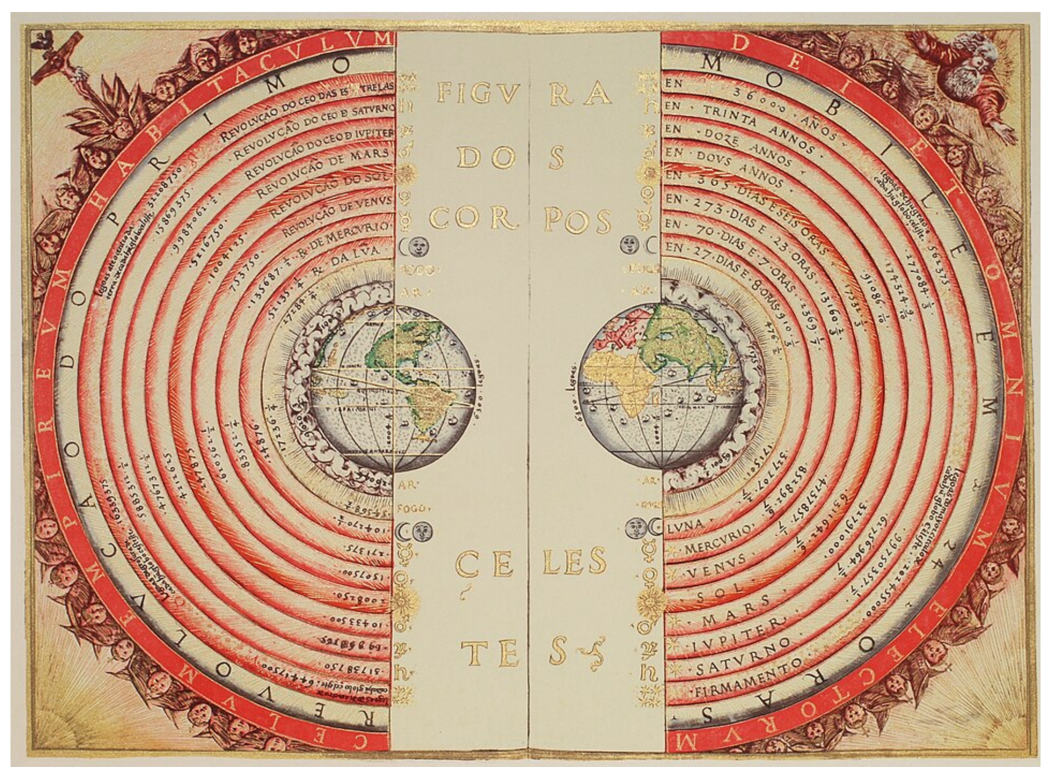
CONCLUSIONS

- Synergistic view



- Ready for paradigm change

"Ptolemy curse"



THANK YOU