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Approximate optimization with tensor networks

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Tensors from the physics viewpoint

Fundusze Europejskie
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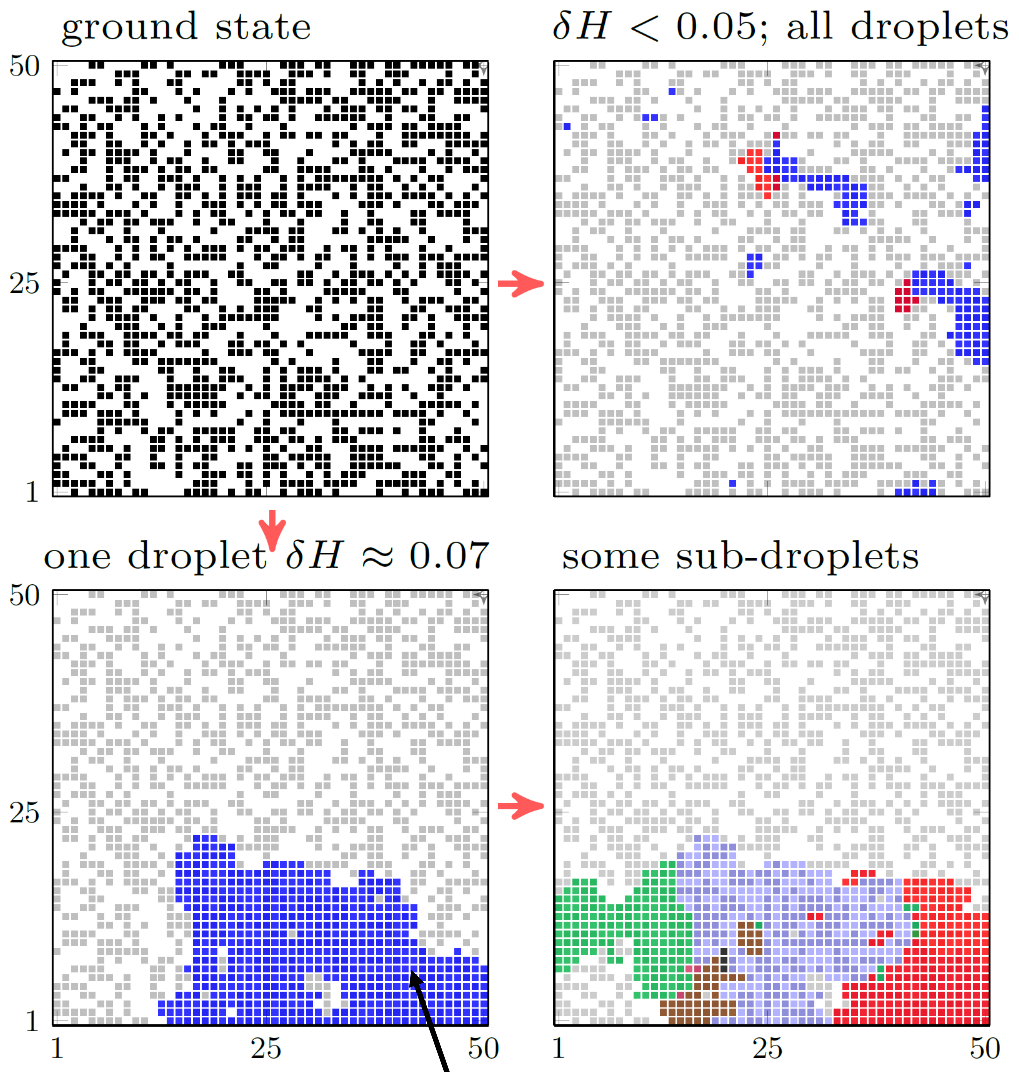
Tensor networks for 2D spin-glass systems:

$$H(\mathbf{s}) = \sum_{\langle i,j\rangle \in \mathcal{E}} J_{ij} s_i s_j + \sum_{i=1}^{N} J_{ii} s_i$$

Edwards-Anderson model

single instance of disorder



Low-energy droplet (Fisher& Huse `86)

PHYSICAL REVIEW E **104**, 025308 (2021)

Approximate optimization, sampling, and spin-glass droplet discovery with tensor networks

Marek M. Rams[1,*] Masoud Mohseni,[2,†] Daniel Eppens,[2] Konrad Jałowiecki,[3] and Bartłomiej Gardas[4,5,‡]
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[2]*Google Quantum Artificial Intelligence Lab, Venice, California 90291, USA*
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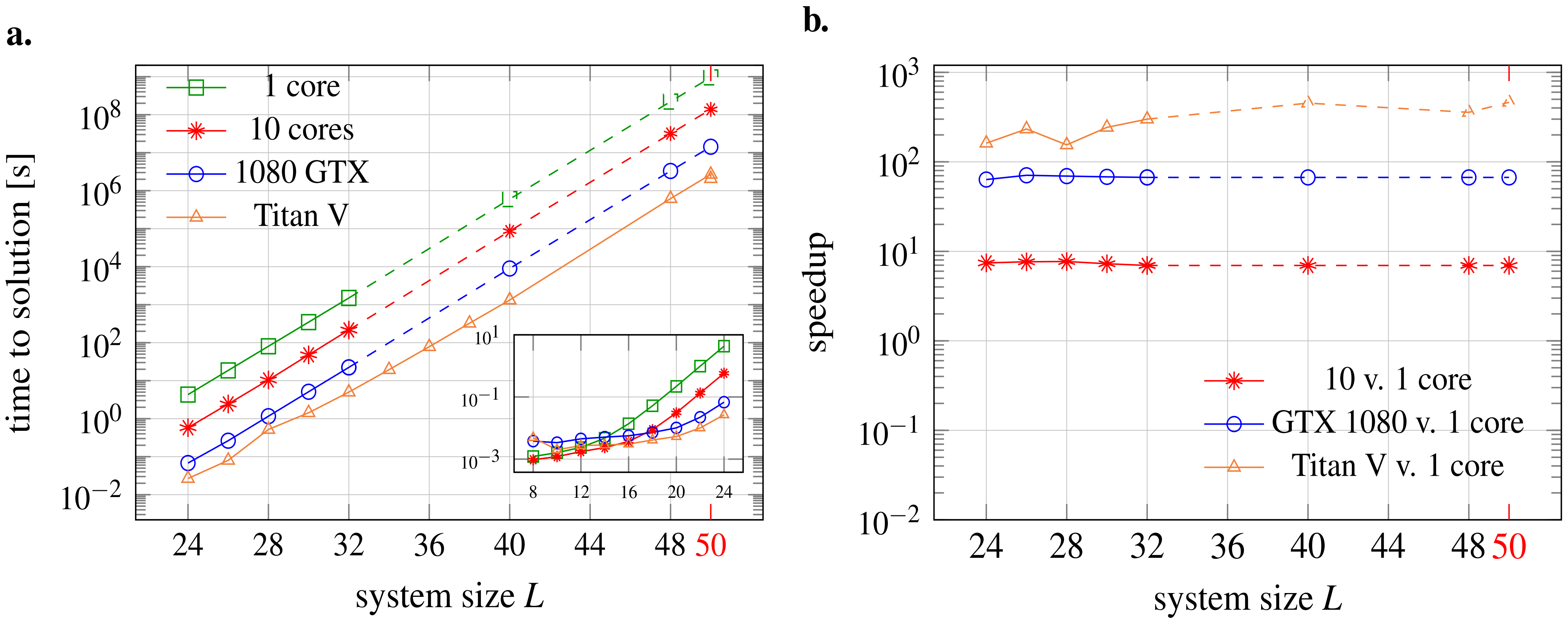
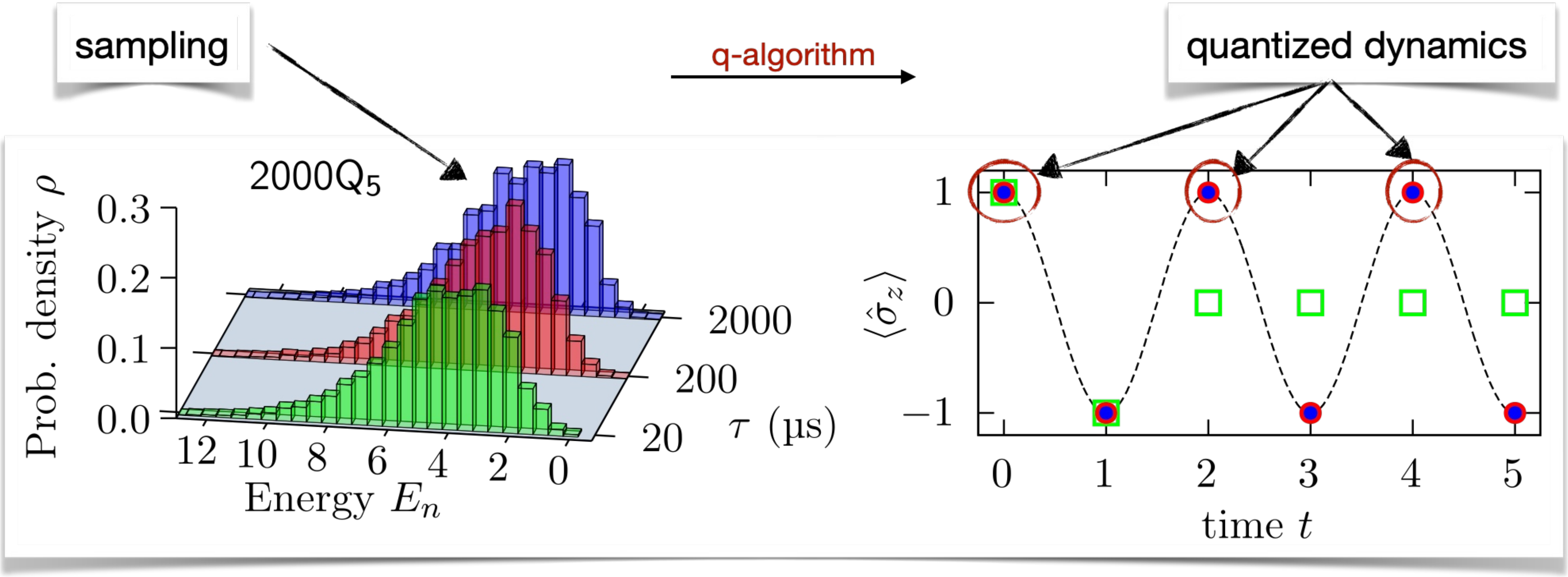
[5]*Jagiellonian University, Marian Smoluchowski Institute of Physics, Łojasiewicza 11, 30-348 Kraków, Poland*

Why not to Brute-Force?



K. Jałowiecki, M. M. Rams, B. Gardas, *"Brute-forcing spin-glass problems with CUDA"*, [Comput. Phys. Commun. **260,** 107728 (2021)].

Quantum annealer simulating Rabi oscillations **(parallel in time)**



$$i\frac{\partial|\psi\rangle}{\partial t} = \hat{\sigma}_x|\psi\rangle \quad \xrightarrow{\text{c-algorithm}} \quad \langle\psi|\hat{\sigma}_z|\psi\rangle \sim \cos(\omega t)$$

(Schrodinger equation) (continuous dynamics)

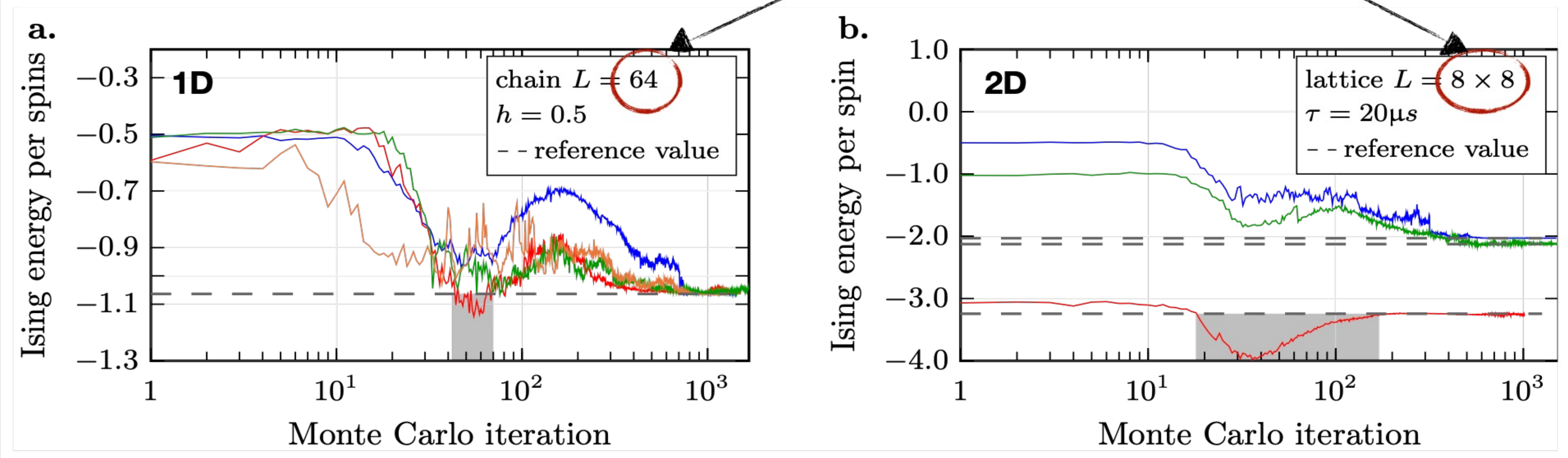
K. Jałowiecki, A. Więckowski, P. Gawron, B. Gardas, "*Parallel in time dynamics with quantum annealers*", Sci. Rep. **10**, 13534 (2020).

Quantum annealer as a **artificial neural network**

- The transverse field Ising model.

- The paradigmatic spin system.

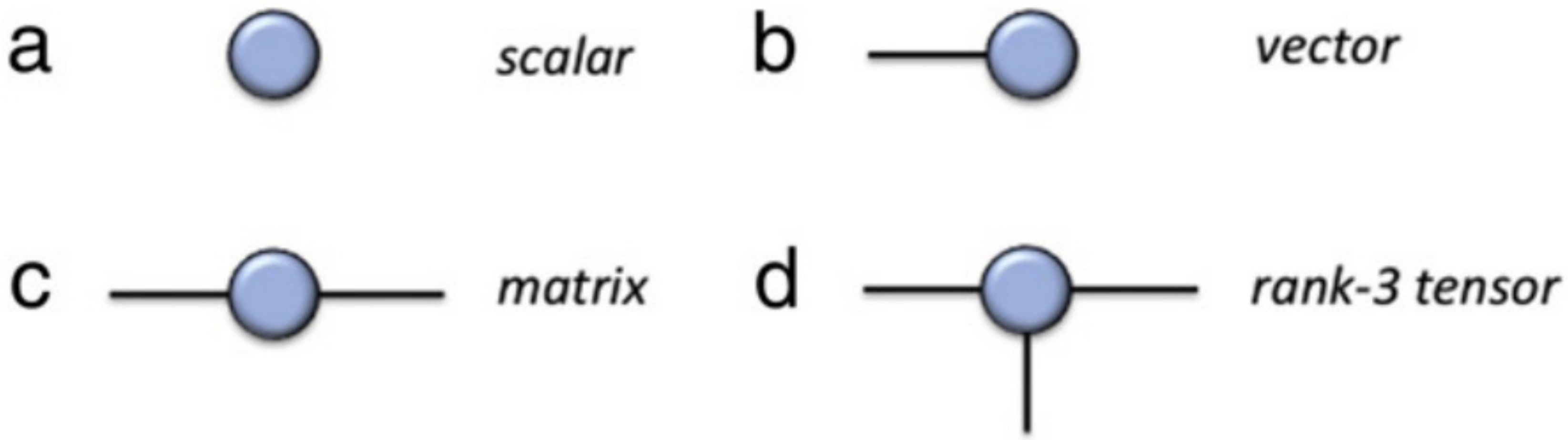
$$H = -h \sum_{i \leq L} \hat{\sigma}_i^x - \sum_{\langle i, j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z$$



BG, et al., "*Quantum neural networks to simulate many-body quantum systems*", Phys. Rev. B **98**, 184304 (2018).

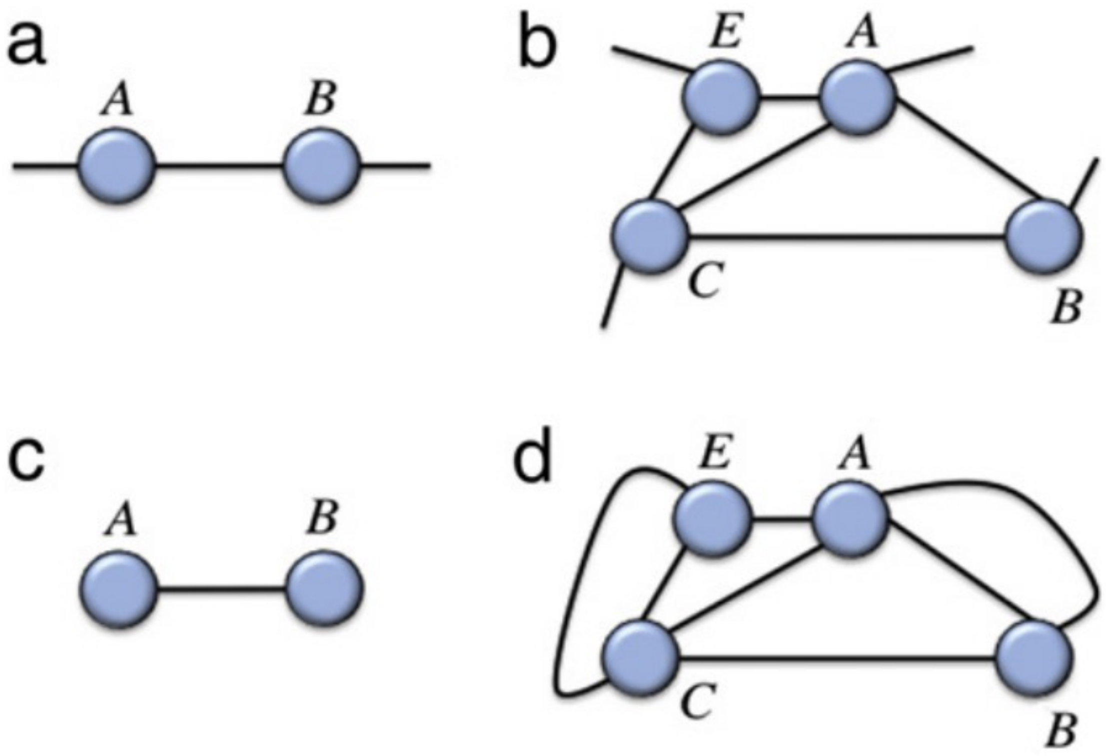
Back to tensors

Oversimplified take on tensors …



R. Orús, “*A practical introduction to tensor networks*: … ” Annals of Physics **349**, 117-158 (2014).

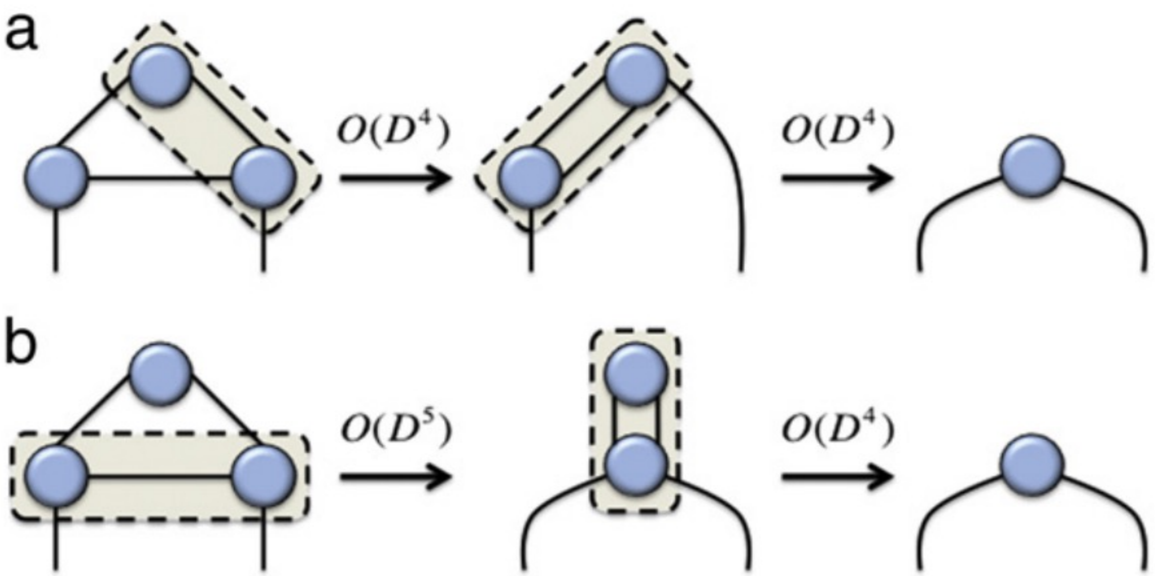
… and tensor networks …



$$F_{\gamma\omega\rho\sigma} = \sum_{\alpha,\beta,\delta,\nu,\mu=1}^{D} A_{\alpha\beta\delta\sigma} B_{\beta\gamma\mu} C_{\delta\nu\mu\omega} E_{\nu\rho\alpha}$$

R. Orús, “*A practical introduction to tensor networks*: … ” Annals of Physics **349**, 117-158 (2014).

… and their contraction:

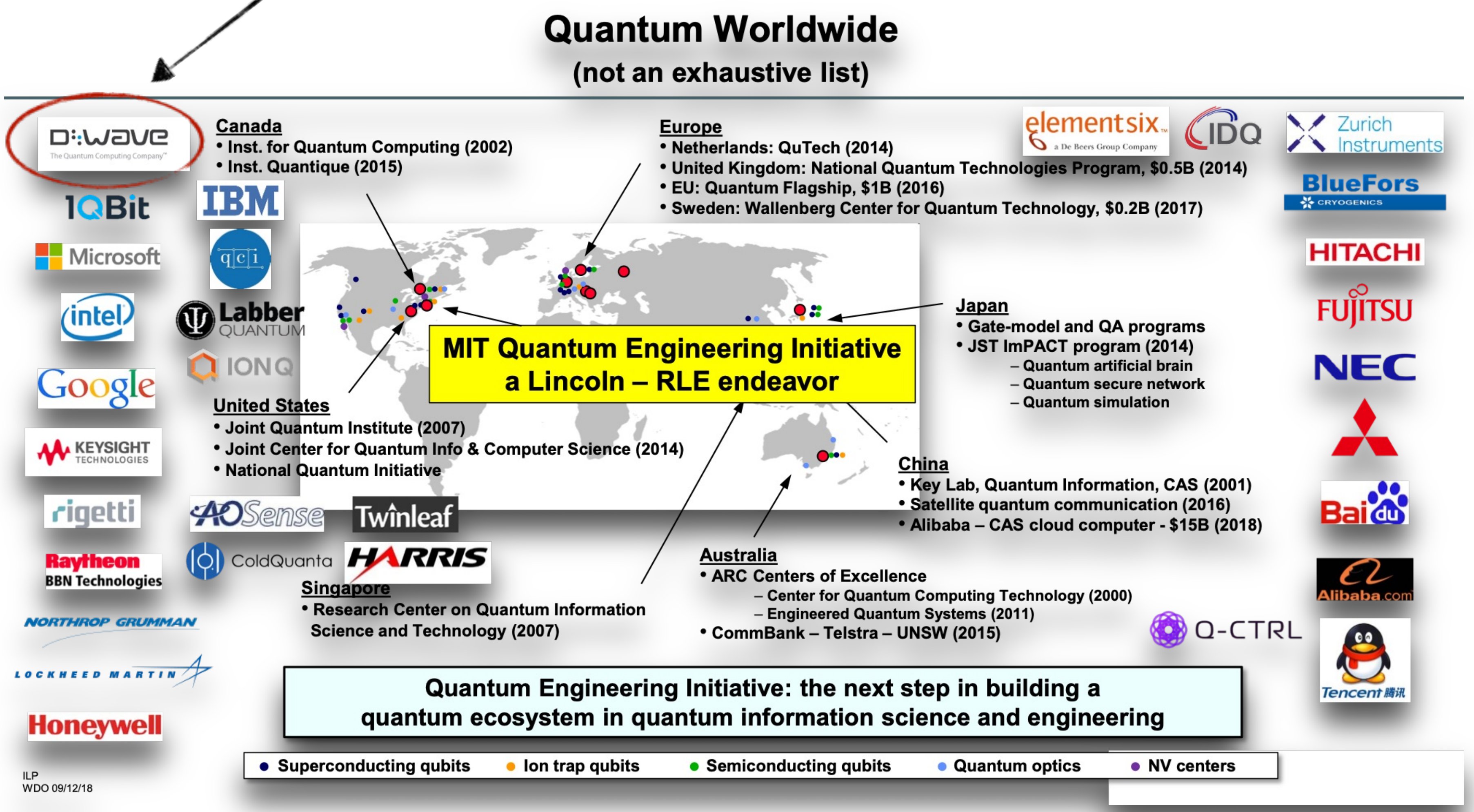


R. Orús, "*A practical introduction to tensor networks*: … " Annals of Physics **349**, 117-158 (2014).

Oversimplified take on quantum computation…

- “the tip of the iceberg”

annealing ⟷ gate model

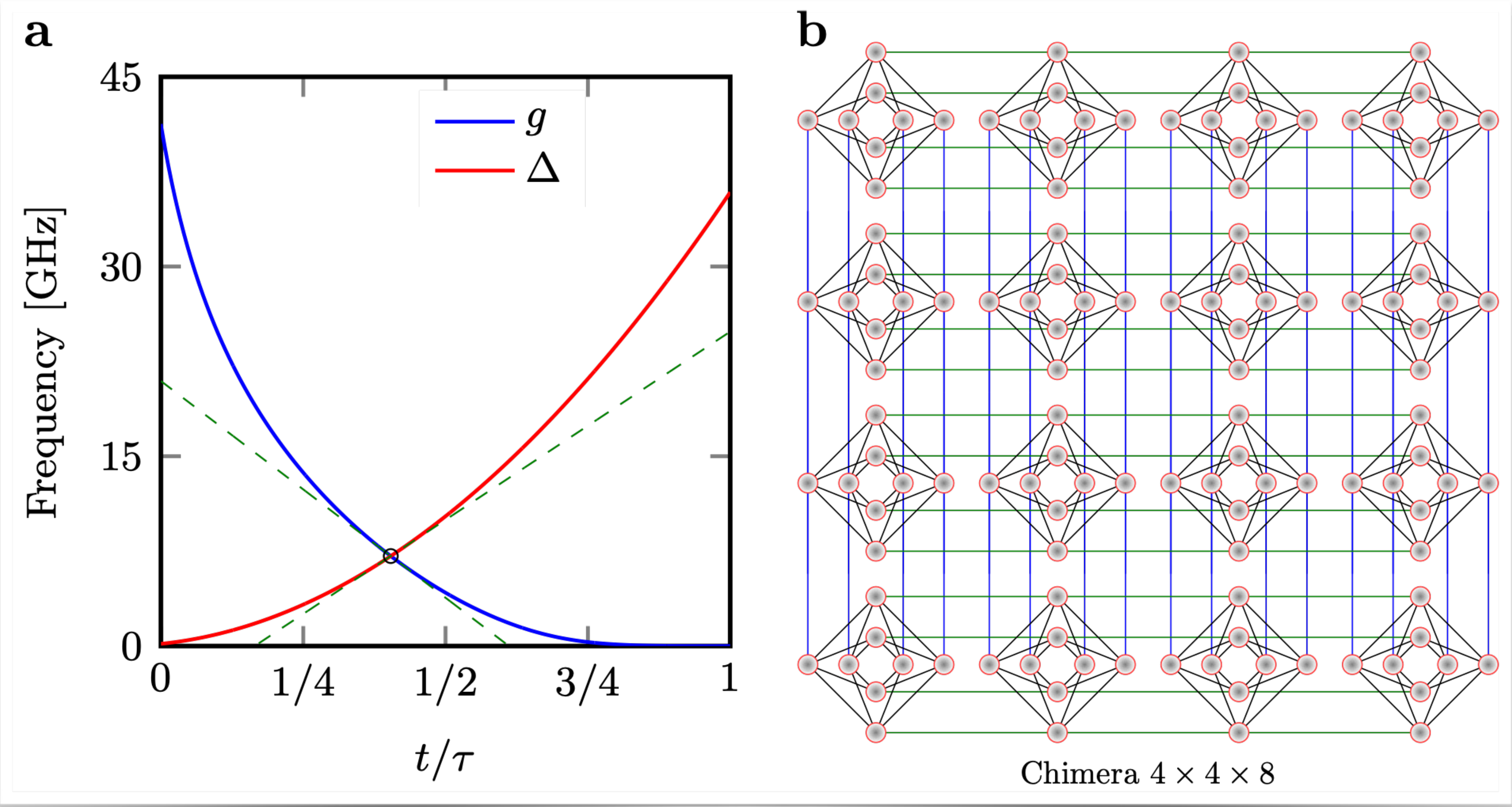


Source: William D. Oliver (MIT)

Quantum correspondence

D-Wave quantum annealer(s)

$$H(t)/(2\pi\hbar) = -g(t)\sum_{i=1}^{L}\sigma_i^x - \Delta(t)\left(\sum_{\langle i,j\rangle\in\mathcal{E}} J_{ij}\sigma_i^z\sigma_j^z + \sum_{i\in\mathcal{V}} h_i\sigma_i^z\right)$$



Transfer matrix

$$H(\mathbf{s}) = \sum_{\langle i,j\rangle \in \mathcal{E}} J_{ij} s_i s_j + \sum_{i=1}^{N} J_{ii} s_i$$

Boltzmann distribution

$$p(\boldsymbol{s}) \sim \exp[-\beta H(\boldsymbol{s})]$$

Partition function

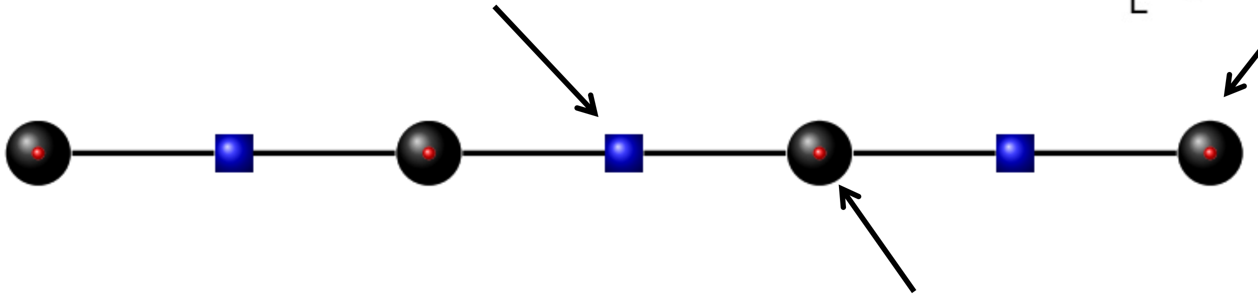
$$Z = \sum_{\mathbf{s}} e^{-\beta H(\mathbf{s})}$$

$$H(\mathbf{s}) = \sum_{\langle i,j\rangle \in \mathcal{E}} E_{i,j}(s_i, s_j) + \sum_{i=1}^{N} E_i(s_i)$$

For 1D chain:

$$\begin{bmatrix} e^{-\beta E_{i-1,i}(\uparrow,\uparrow)} & e^{-\beta E_{i-1,i}(\uparrow,\downarrow)} \\ e^{-\beta E_{i-1,i}(\downarrow,\uparrow)} & e^{-\beta E_{i-1,i}(\downarrow,\downarrow)} \end{bmatrix} \qquad \begin{bmatrix} e^{-\beta E_N(\uparrow)} \\ e^{-\beta E_N(\downarrow)} \end{bmatrix}$$

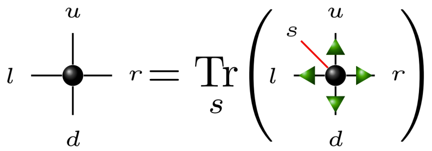
$$Z =$$



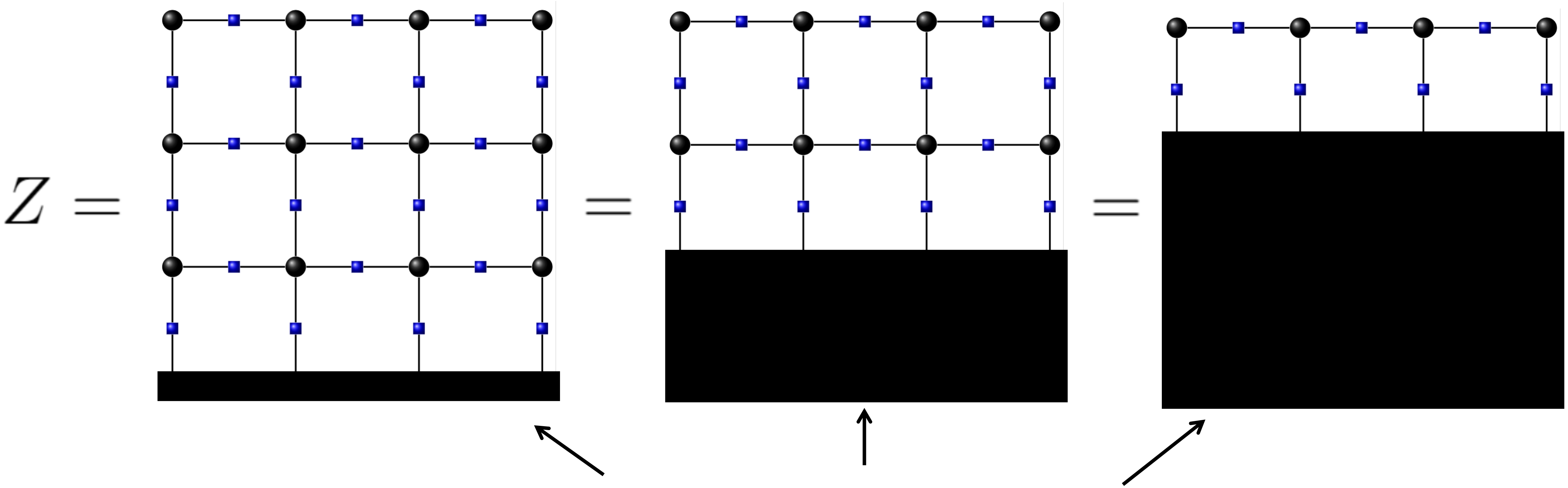
$$\begin{bmatrix} e^{-\beta E_i(\uparrow)} & 0 \\ 0 & e^{-\beta E_i(\downarrow)} \end{bmatrix}$$

Tensor network

For 2D square lattice: $N = L \times L$

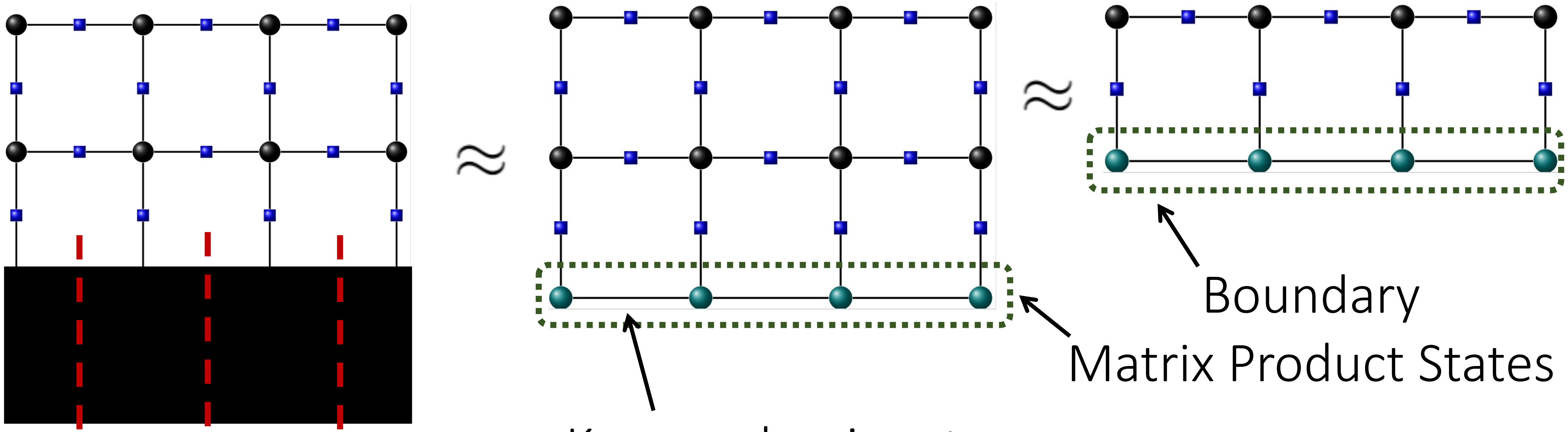


$$= \mathrm{Tr}_s\left(e^{-\beta H(s)}\tilde{\delta}_{sl}\tilde{\delta}_{sr}\tilde{\delta}_{su}\tilde{\delta}_{sd}\right)$$



Boundary MPS; 2^L elements

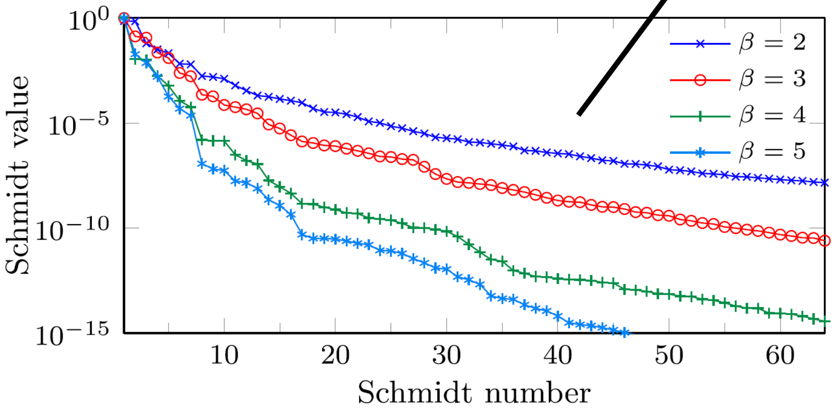
Low-rank approximation



SVD

Keep χ dominant singular values

Boundary
Matrix Product States

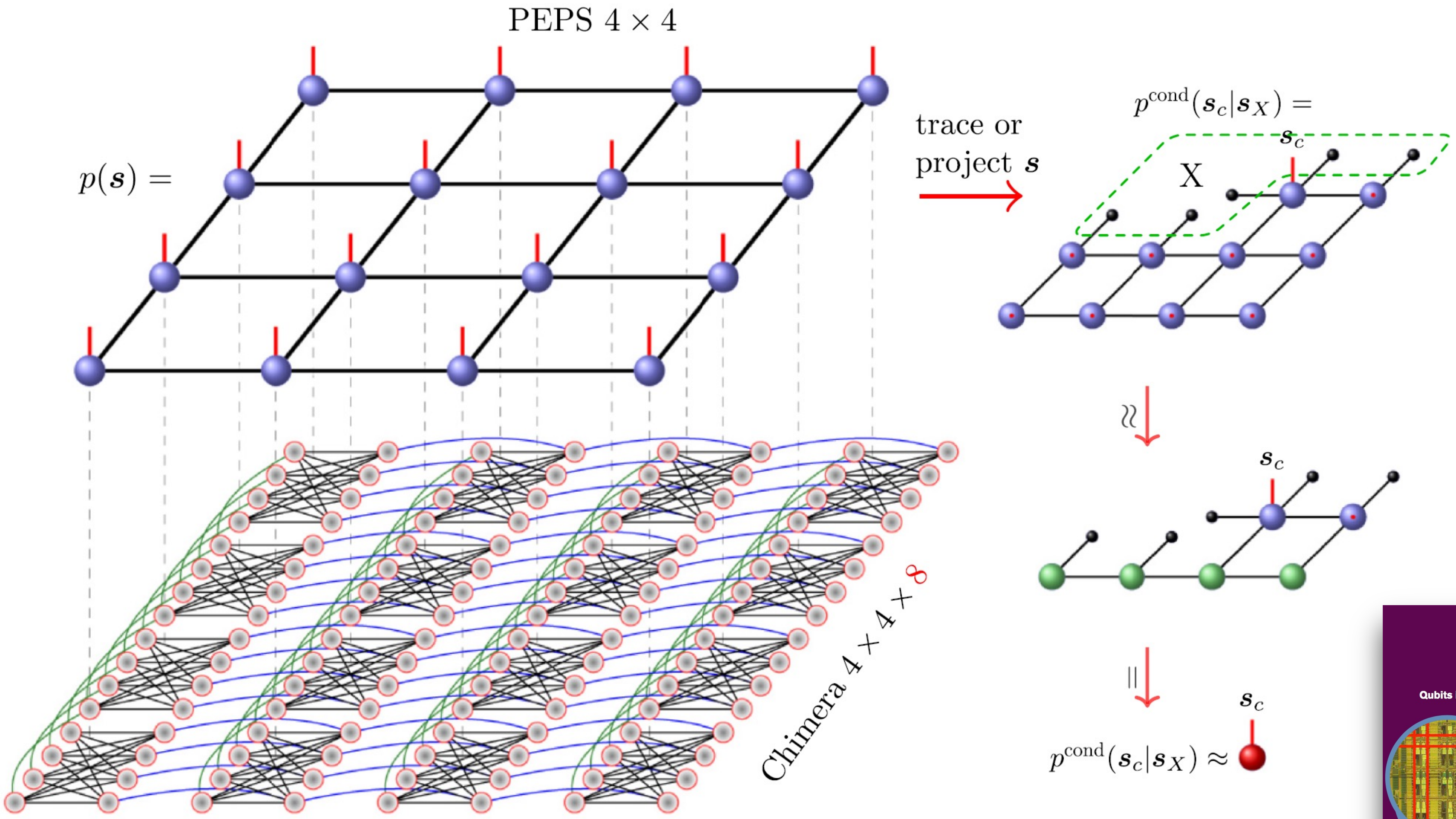


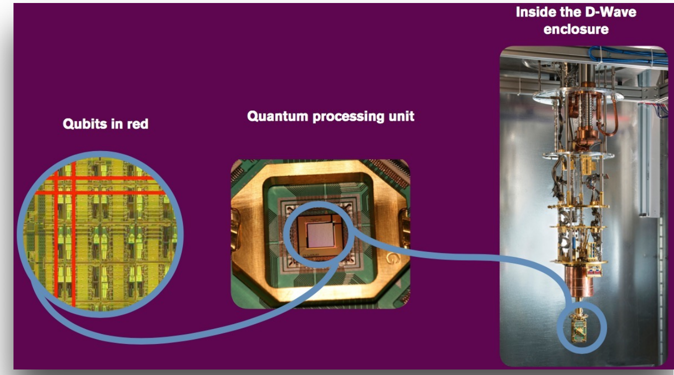
Advances in Physics
Vol. 57, No. 2, March–April 2008, 143–224
Taylor & Francis
Taylor & Francis Group

Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems

F. Verstraete[a*], V. Murg[b] and J.I. Cirac[b]

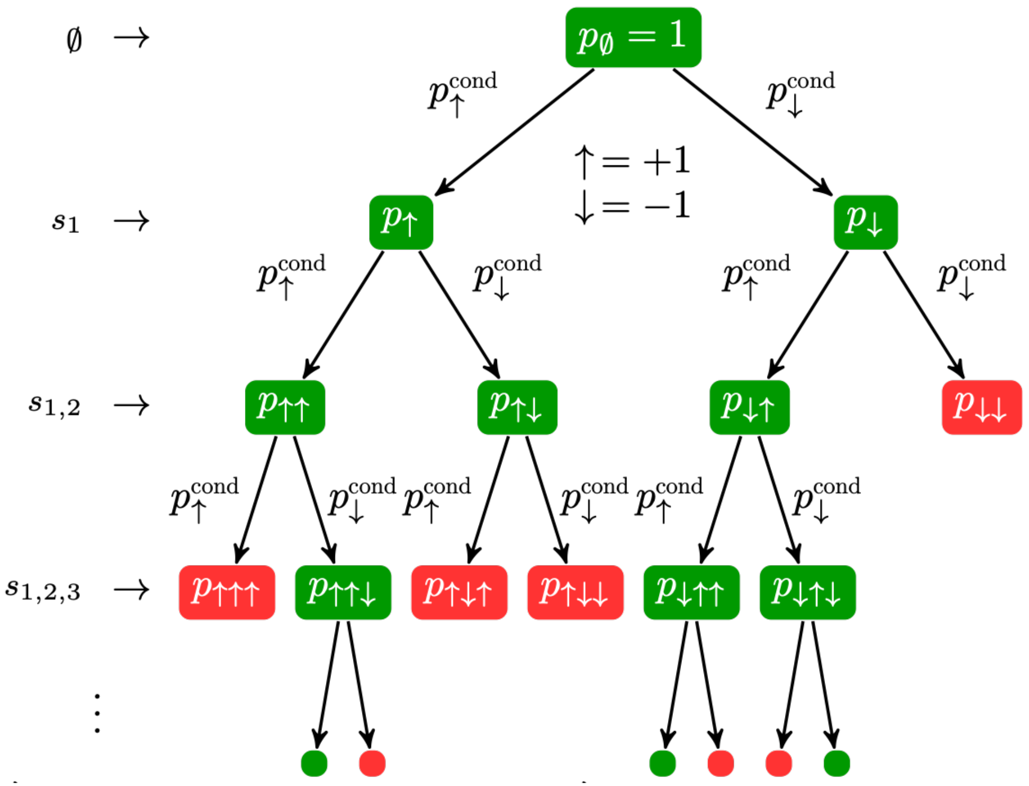
Approximate Oracle to calculate marginal and conditional probabilites



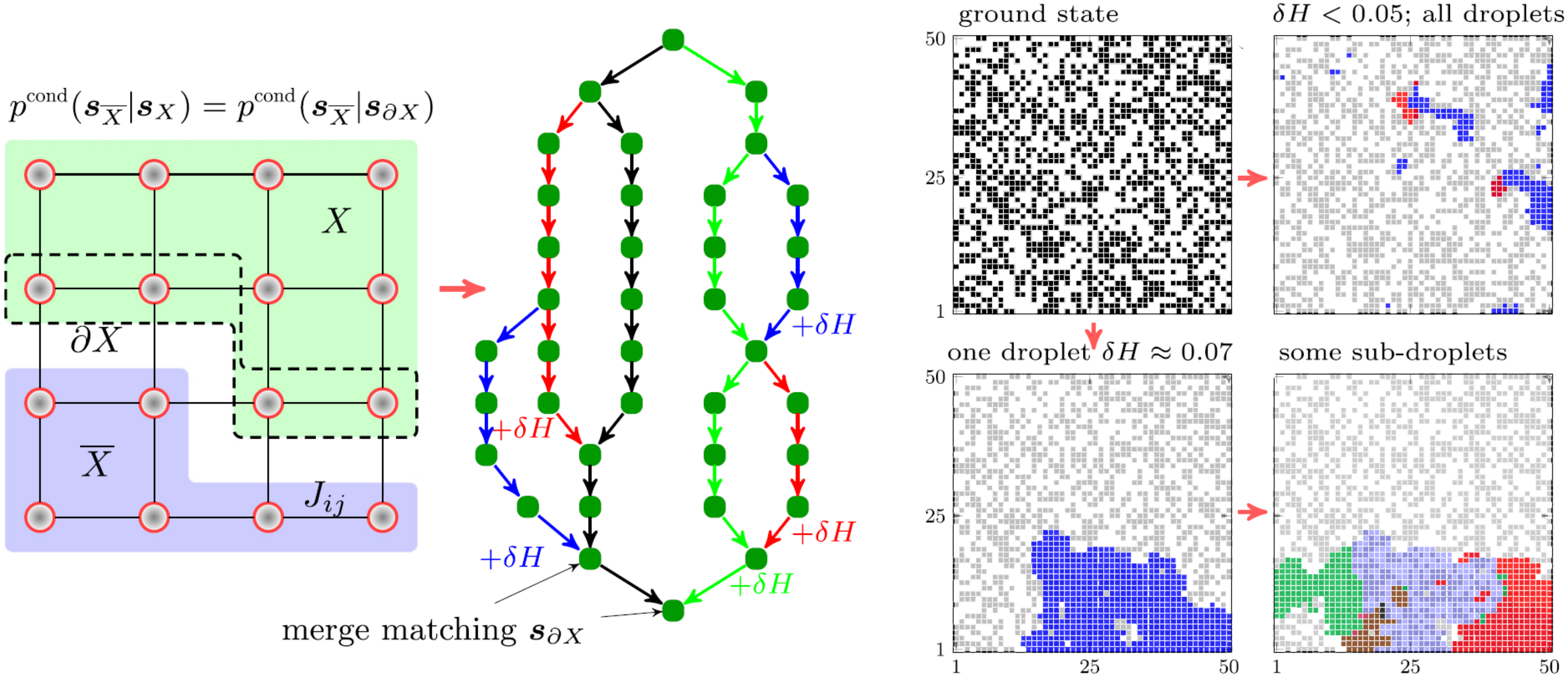


Branch and bound search strategy

Marginal probabilities: $p(s_1, s_2, \ldots, s_k) \sim \mathrm{Tr}\left[\mathcal{P}_{(s_1,s_2,\ldots,s_k)} e^{-\beta H(\boldsymbol{s})}\right]$



Droplet revealing branch and bound



Why it breaks …

PRL 98, 140506 (2007) PHYSICAL REVIEW LETTERS week ending 6 APRIL 2007

Computational Complexity of Projected Entangled Pair States

Norbert Schuch,[1] Michael M. Wolf,[1] Frank Verstraete,[2] and J. Ignacio Cirac[1]

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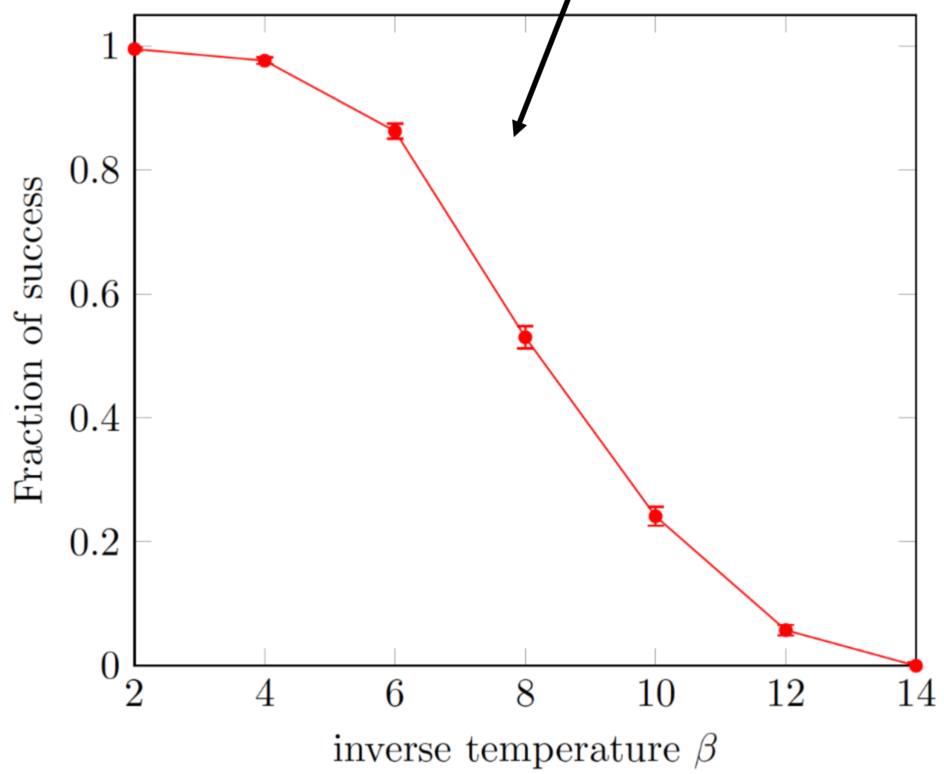
[2]*Fakultät für Physik, Universität Wien, Boltzmanngasse 5, A-1090 Wien, Austria*

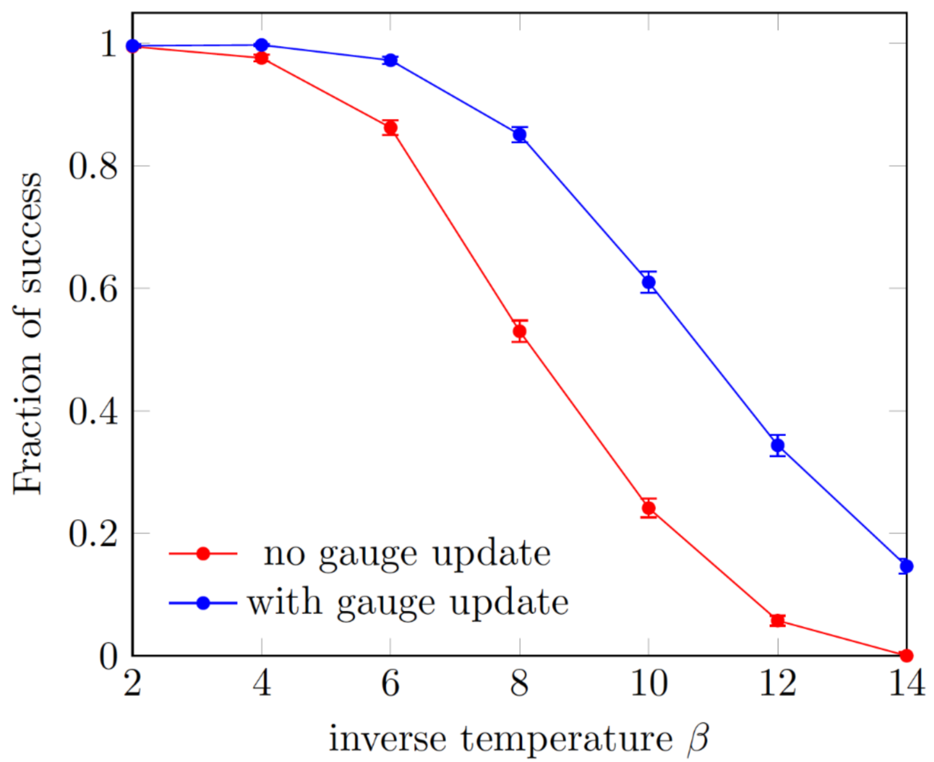
(Received 7 November 2006; published 4 April 2007)

We determine the computational power of preparing projected entangled pair states (PEPS), as well as the complexity of classically simulating them, and generally the complexity of contracting tensor networks. While creating PEPS allows us to solve *PP* problems, the latter two tasks are both proven to be *#P*-complete. We further show how PEPS can be used to approximate ground states of gapped Hamiltonians and that creating them is easier than creating arbitrary PEPS. The main tool for our proofs is a duality between PEPS and postselection which allows us to use existing results from quantum complexity.

Stability

Inaccurate contraction





stability (small β) resolution (large β)

Heuristic gauge fixing

A. Dziubyna, T. Śmierzchalski, B. Gardas, M.R., in prep.

Some benchmarks: time to solution

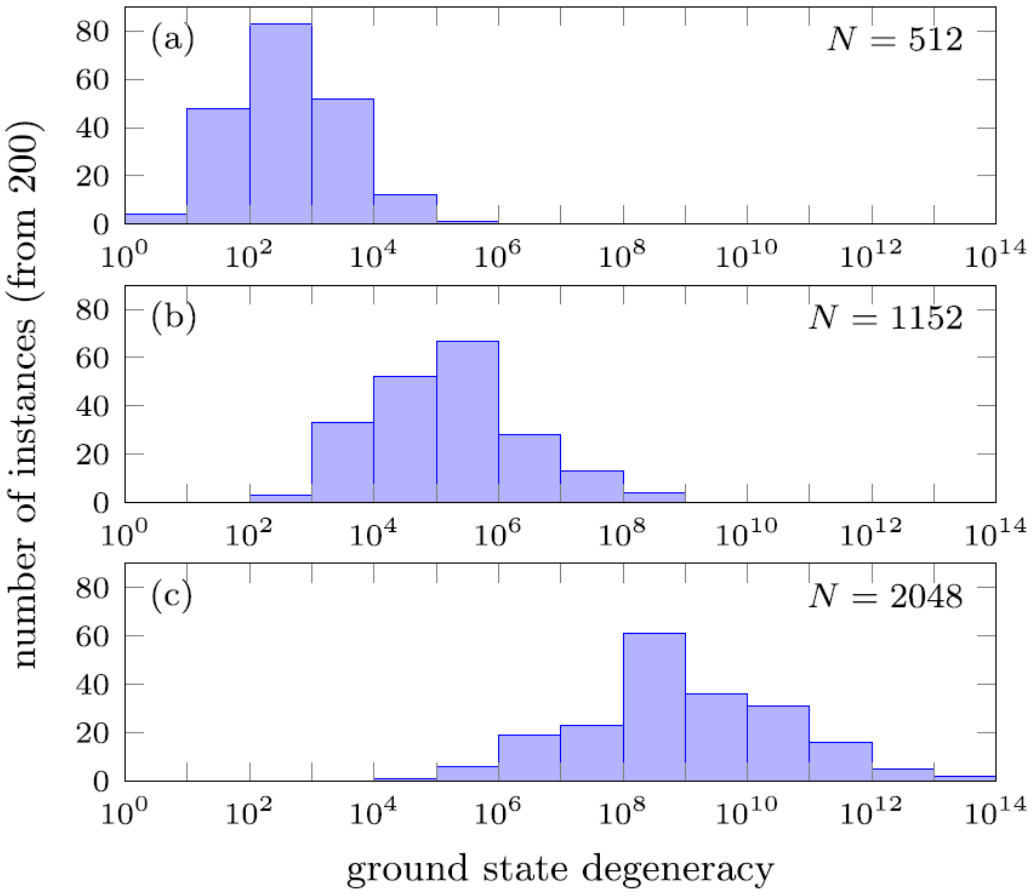
Old library -> tnac4o

Method	Approx. ratio	$N = 512$	$N = 1152$	$N = 2048$
This article	g.s.	30s	150s	450s
PT (adaptive)	g.s.	800s	—	—
PT (geometric)	0.01	0.53s	4.16s	—
PT (geometric)	0.005	2.51s	56.4s	—
PT (geometric)	0.001	158.4s	Timed-out	—
PT (geometric)	0.0001	897.6s	Timed-out	—
DWave $2000Q_6$	0.01	0.003s	0.006s	0.02s
DWave $2000Q_6$	0.005	0.2s	Timed-out	Timed-out
DWave $2000Q_6$	0.001	Timed-out	Timed-out	Timed-out

DWave „chimera” graph

Benchmarks: counting

DWave „chimera” graph $J_{ij} \in \{\pm 1, \pm 2, \pm 4\}$



vs

PHYSICAL REVIEW E **99**, 063314 (2019)

Fair sampling of ground-state configurations of binary optimization problems

Zheng Zhu,[1] Andrew J. Ochoa,[1] and Helmut G. Katzgraber[2,1,3]

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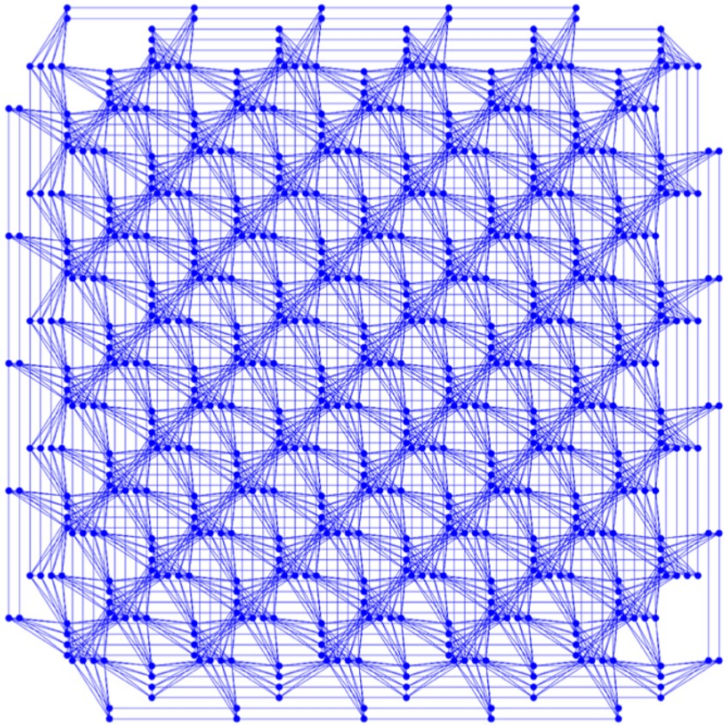
[2]*Microsoft Quantum, Microsoft, Redmond, Washington 98052, USA*
[3]*Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, New Mexico 87501, USA*

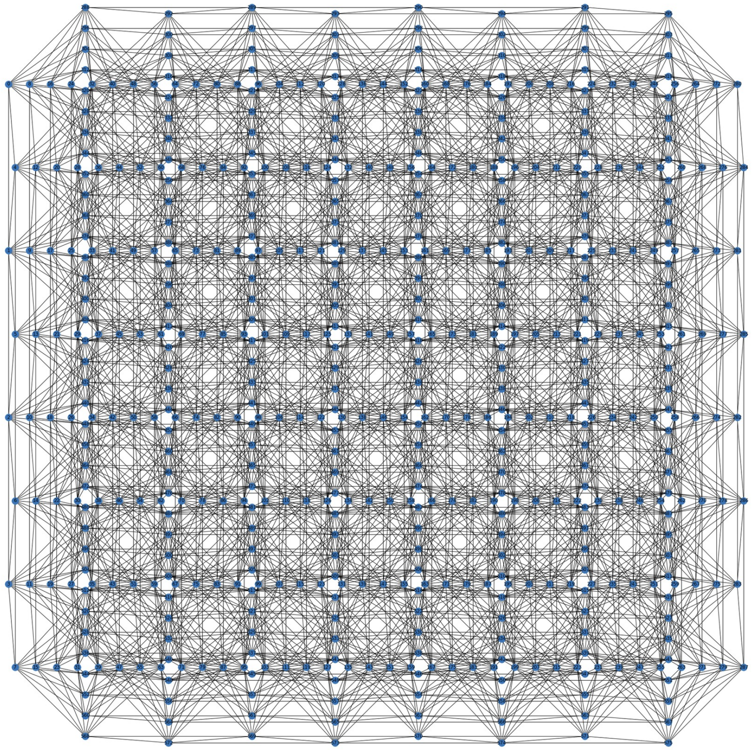
PT and PT + ICM
maximal degeneracy
reported for N=1152
is 10^6

Limitations (large unit cells)

DWave „pegasus” graph



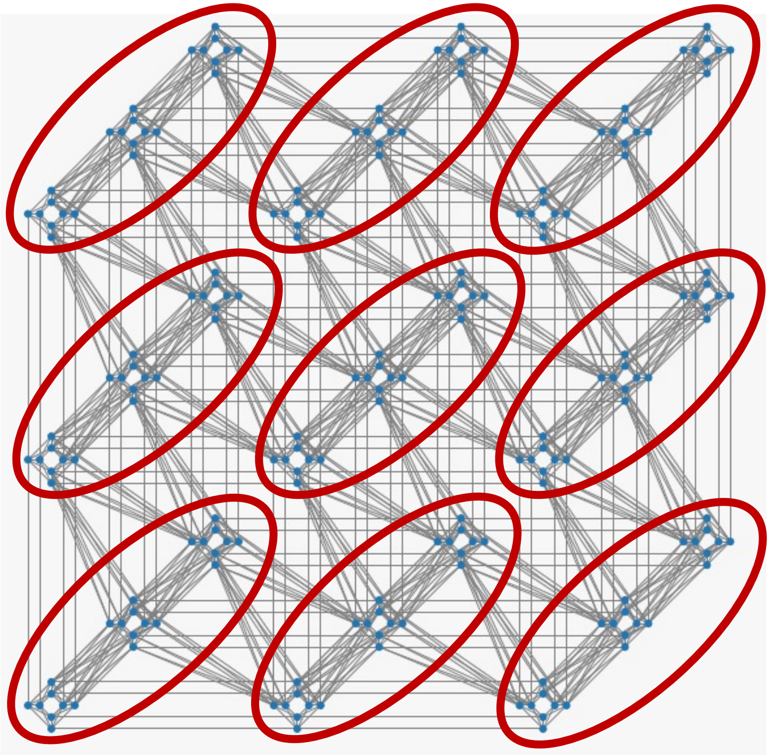
DWave „zephyr” graph

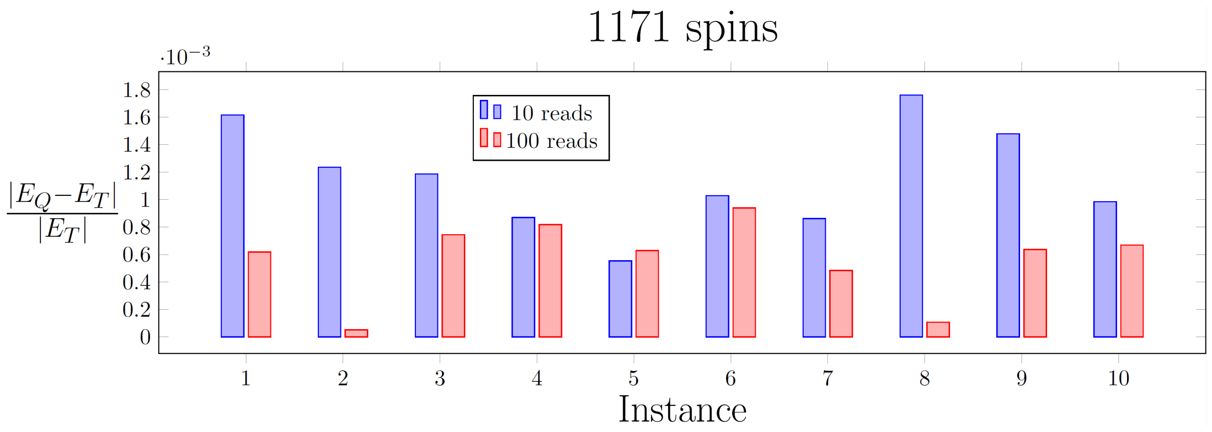


Limitations (large unit cells)

github.com/euro-hpc-pl/SpinGlassPEPS.jl

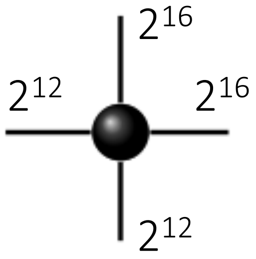
(almost) „pegasus” graph





TN approach still can be executed.

Huge tensors



24 spins in a unit cell

Sparseness + GPU

T. Śmierzchalski, A. Dziubyna, M.R., B. Gardas, in prep.

Thank you!