Quantum AI to simulate many body quantum systems

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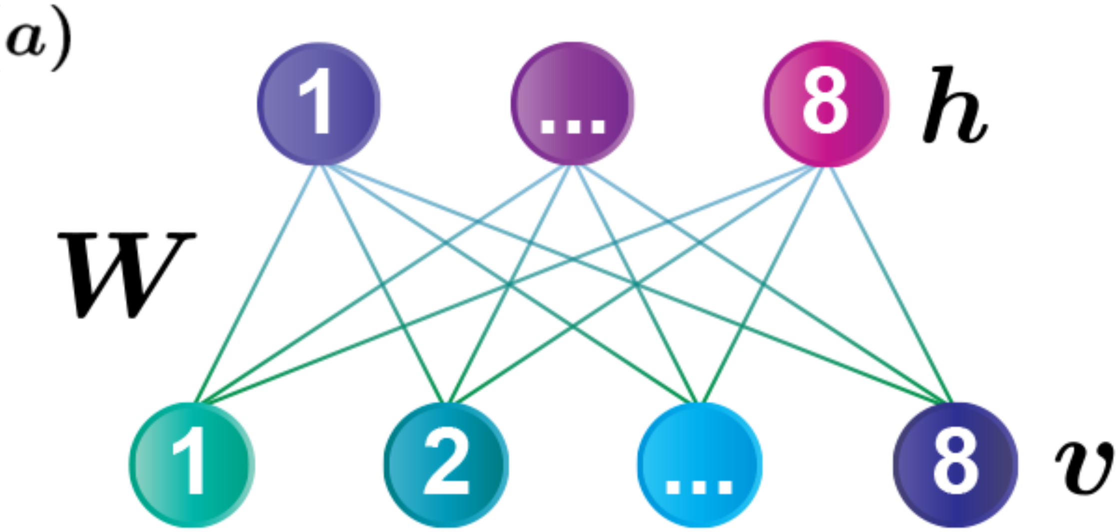
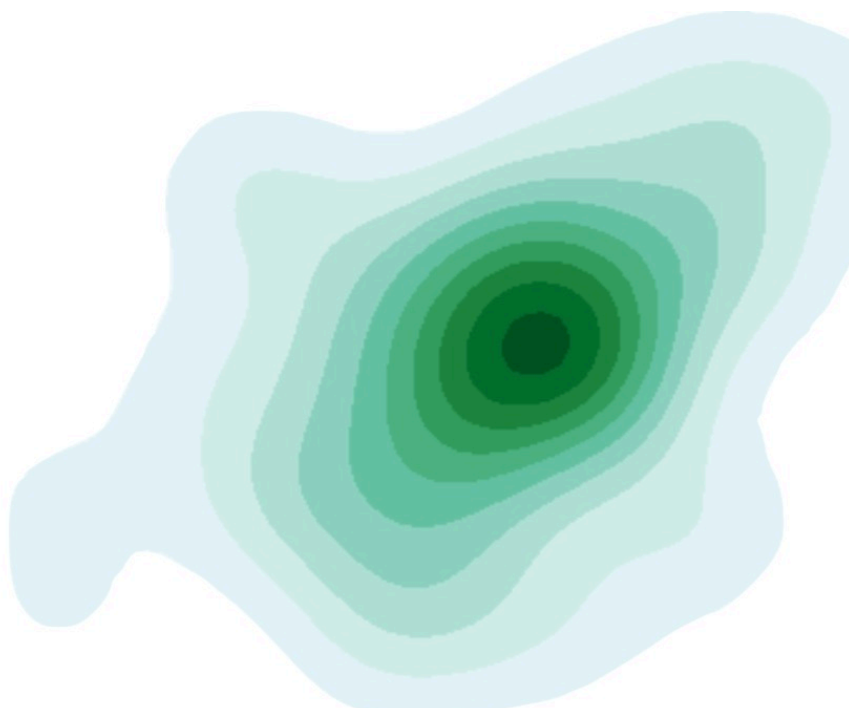
Physicists	Computer scientists
Degrees of freedom (physical or virtual)	Neurons (visible or hidden)
Variational Monte Carlo	Unsupervised learning
A clever ansatz	Neural network (e.g. RBM)
Stochastic Reconfiguration	Learning stage
$\vdots$	$\vdots$

$$\phi(\boldsymbol{v}, \boldsymbol{h})$$

(a)



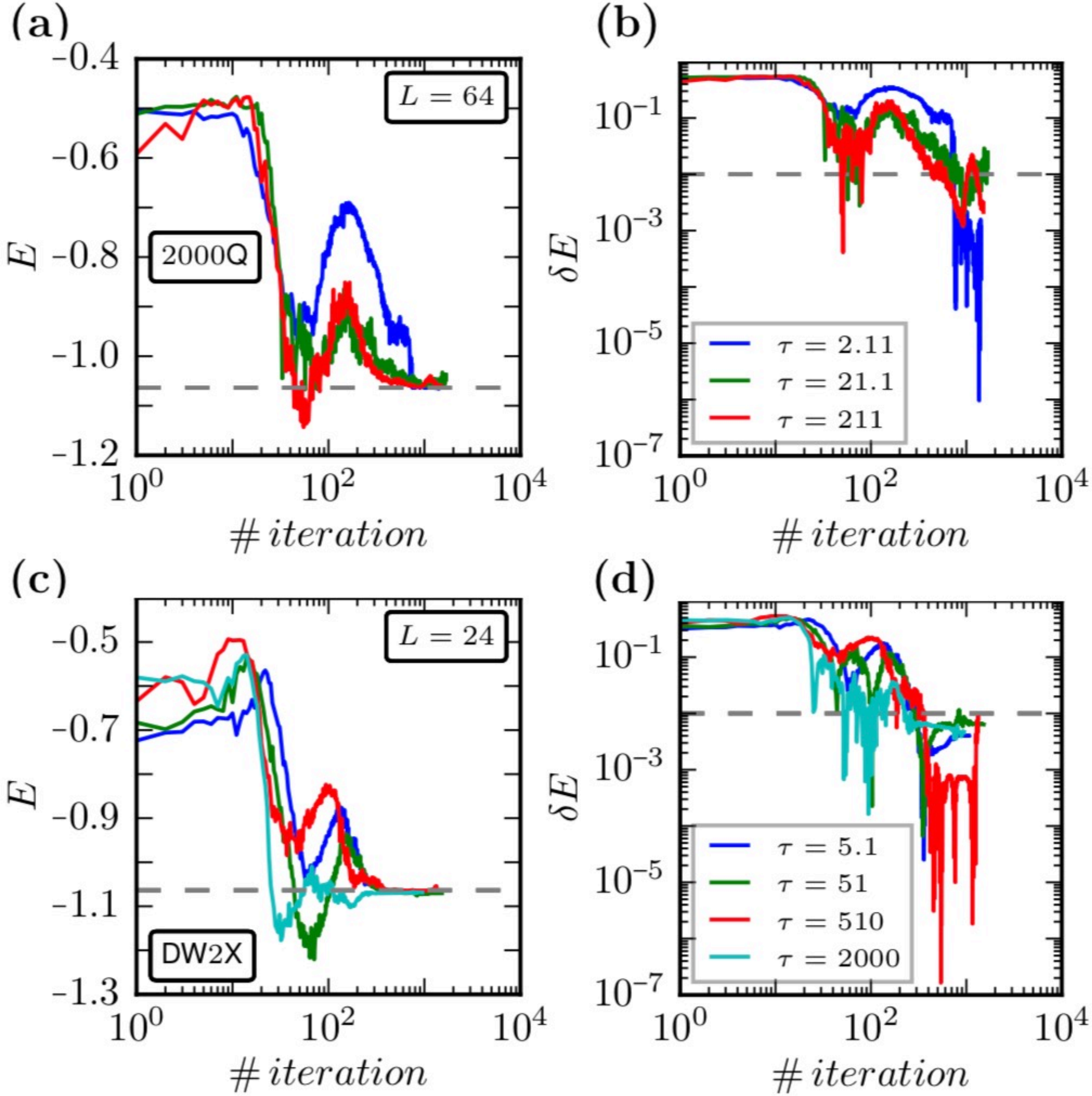
- Why do we want to build a quantum computer?



$$H\left|\Psi\right\rangle = E_0\left|\Psi\right\rangle$$

Stuff we use:

- Exact Diagonalization $L \sim \mathcal{O}(10^2)$
- Tensor Networks $L \sim \mathcal{O}(10^4)$
- Monte Carlo $L \sim \mathcal{O}(10^3)$



Main Result

DW2X - Los Alamos

2000Q - Burnaby

$$\delta E = \left| \frac{E - E_{\text{exact}}}{E_{\text{exact}}} \right|$$

$$E_{\text{exact}} = -1.0635$$

$$\delta E = \mathcal{O}(10^{-2})$$

BG, Marek M. Rams and J. Dziarmaga, *in preparation.*

- How did we get here?

$$|\Psi\rangle = \sum_{\boldsymbol{v}} \Psi(\boldsymbol{v}) \, |\boldsymbol{v}\rangle$$

- The idea is to take Restricted Boltzmann Machine,

$$\Psi(\boldsymbol{v}) = \sqrt{\sum_{\boldsymbol{h}} e^{-\phi(\boldsymbol{v},\boldsymbol{h})}}$$

$$\phi(\boldsymbol{v},\boldsymbol{h}) = \boldsymbol{a}\cdot\boldsymbol{v} + \boldsymbol{b}\cdot\boldsymbol{h} + \boldsymbol{h}\cdot\boldsymbol{W}\cdot\boldsymbol{v}$$

to find the ground state energy of the Ising model (both 1D and 2D)

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

- How do we go about doing this?

$$E_0 \leq \langle\phi| H |\phi\rangle$$

- Now everything seems easy …

$$\boldsymbol{p} = [\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{W}]$$

$$\boldsymbol{p}^{(k+1)} = \boldsymbol{p}^{(k)} - \gamma_k F(\langle\langle f \rangle\rangle_\rho, \boldsymbol{p}^{(k)})$$

… except it is not

Monte Carlo averages

- How to take advantage of a D-Wave annealer?

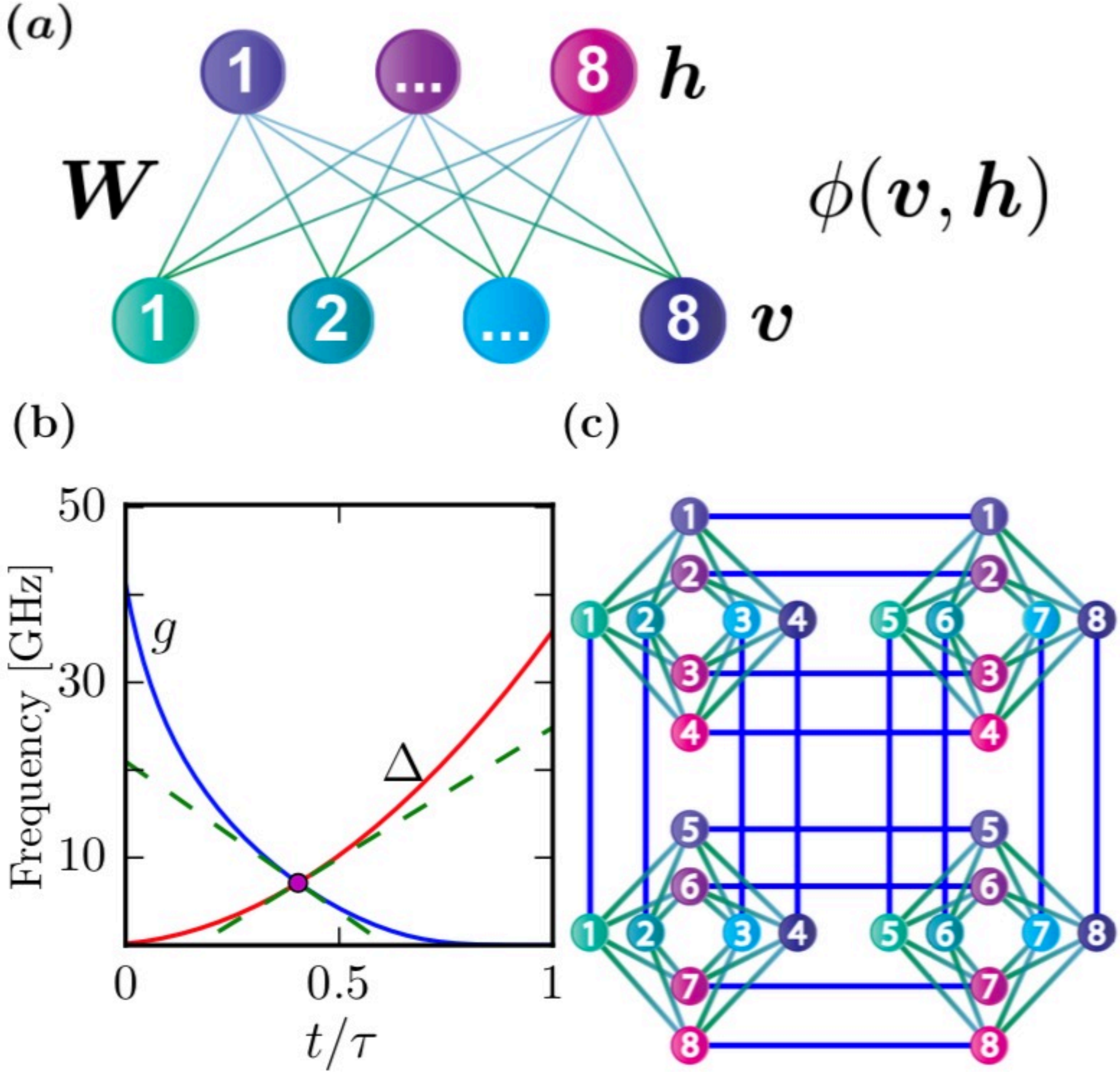
$$\langle\langle f \rangle\rangle_\rho = \sum_{\boldsymbol{v}} \rho(\boldsymbol{v}) f(\boldsymbol{v}) \approx \sum_{\boldsymbol{v},\boldsymbol{h}} p(\boldsymbol{v},\boldsymbol{h}) f(\boldsymbol{v})$$

$$= \sum_{\boldsymbol{\sigma}} p(\boldsymbol{\sigma}) f(\boldsymbol{\sigma}) \approx \frac{1}{N} \sum_{i=1}^{N} f(\boldsymbol{\sigma}_i)$$

- This is fast, *incredibly* fast …

$\mathcal{O}(\mu s) - \mathcal{O}(ms)$ to search 2^{2048} configurations

… depending on the annealing time and the number of samples requested.



(a)
1
...
8
h
W
φ(v, h)
1
2
...
8
v
(b)
(c)
50
30
10
Frequency [GHz]
g
Δ
0
0.5
1
t/τ
1
2
3
4
5
6
7
8

Summary

Simple, yet non-trivial systems can be simulated using quantum computers

- **Dynamics is also possible** … *although not discussed here*
- ***1D* and *2D* systems are not conceptually different** … *this is great*
- **Thermal states may be addressed as well** … *it is worth checking*
- **Much simpler than Tensor Networks** … *students may play with it*
- **New possibilities that we even don't know about** … *fresh take on QM*

Thank you!