Parallel in time dynamics with quantum annealers

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Motivation (why now?)

- **(Adiabatic) quantum computing**
  - growing hardware support (D-Wave, Rigetti, IBM)
  - Big players (IBM, Microsoft, Google) are involved
  - It is *fairly* easy to get access

- **Real life problems …**
  - Indispensable for solving optimization problems (here on Earth)
  - New materials design and space exploration
  - Computationally as complicated as it gets (although not entirely hopeless)

The idea

- Feynman’s dream of quantum computation (1960)
- We are slowly entering an era were quantum ``computers” (annealers) perform (assist) simulations of physical (quantum) systems.
- However, due to various limitations, only static simulations (e.g. ground state serach) have been tried thus far.
- At this point some neural networks are involved.
- What about dynamics (e.g. time dependent phenomenon)?
- Turns out that static and dynamics are not that different after all… ⟵ key concept !

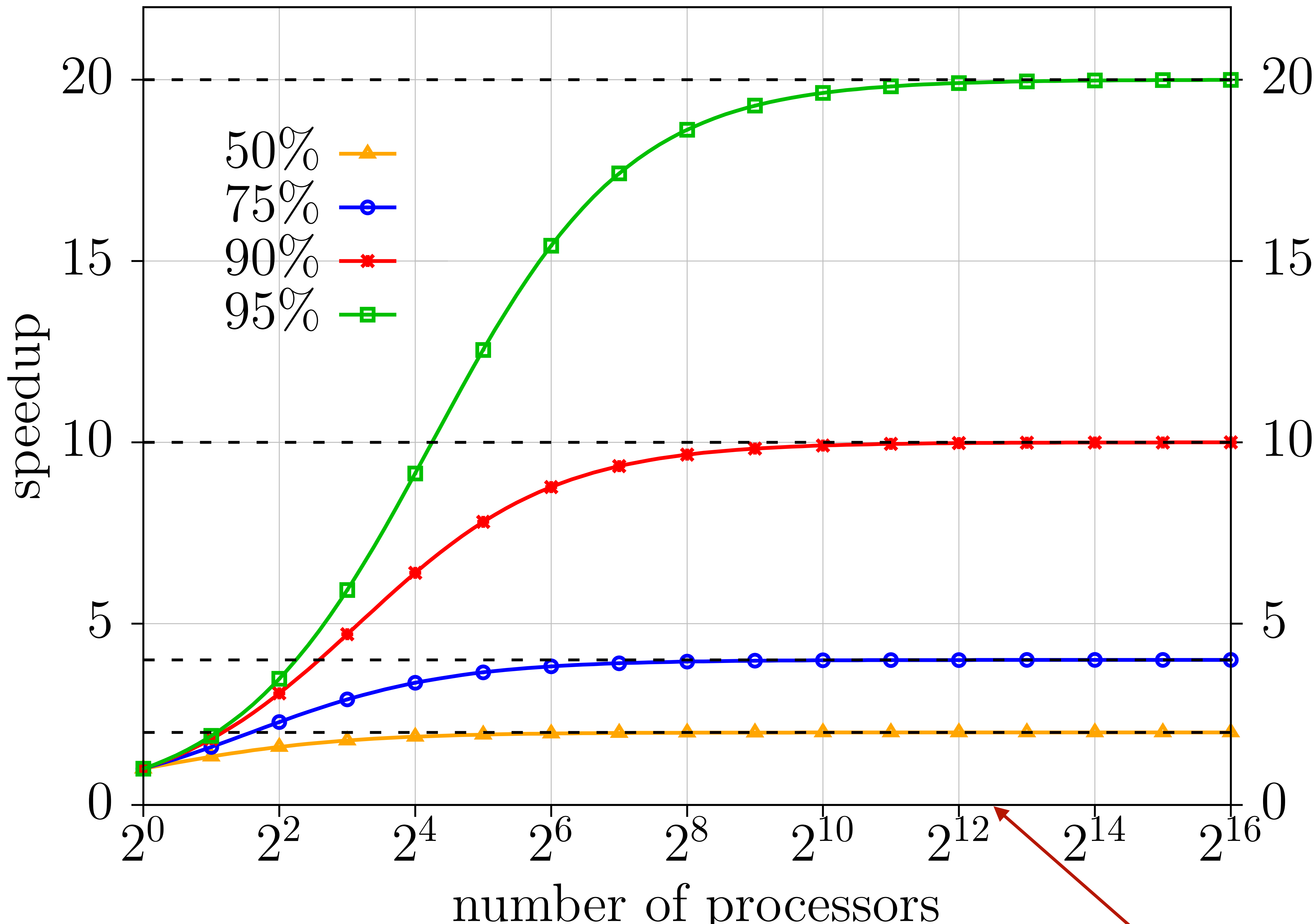
- Two-fold motivation:

  — Investigate how well quantum annealers are suited for dynamical simulations

  — Provide possibly hard instances to benchmark quantum computers

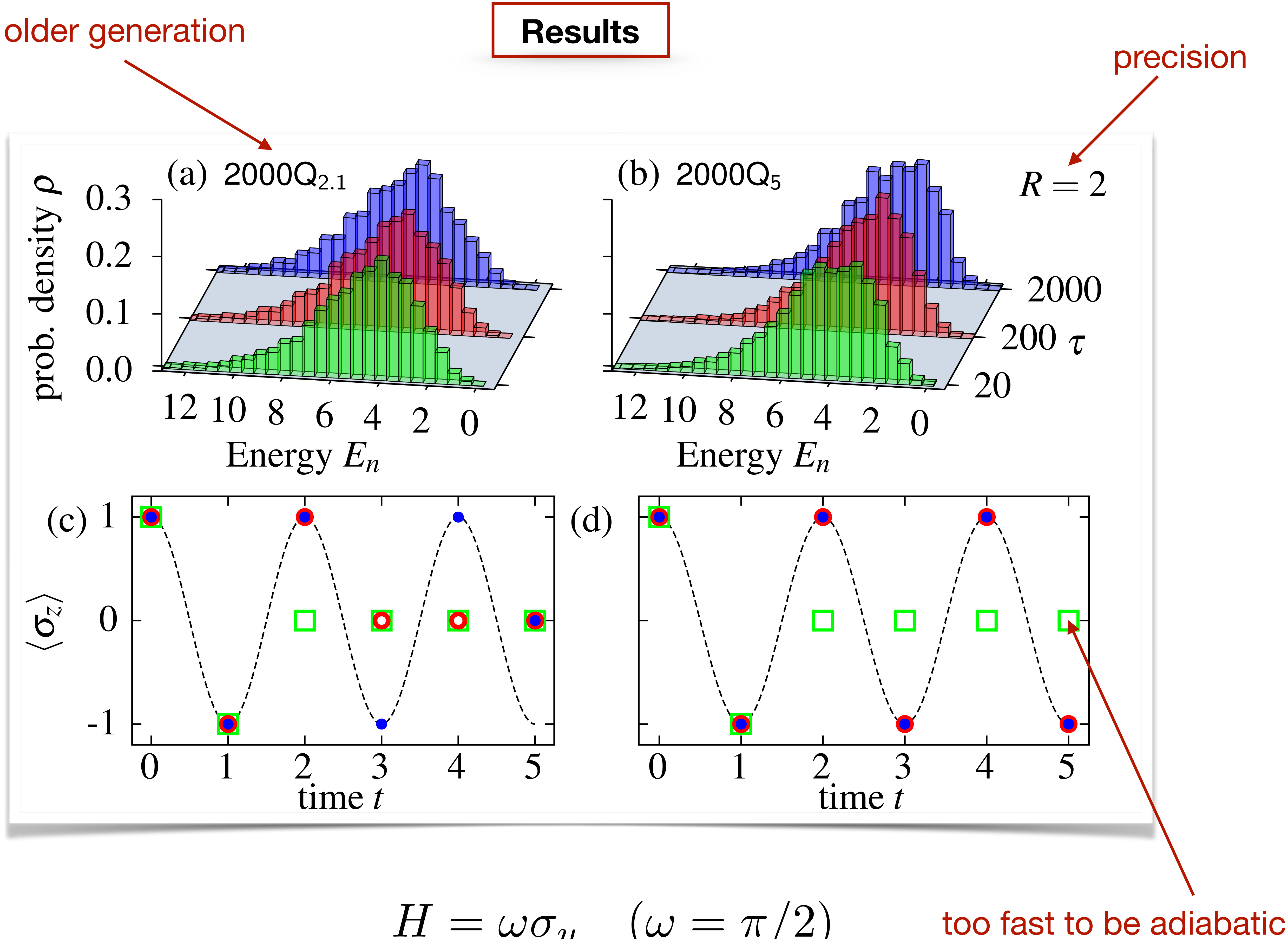
win-win scenario

A technical note #1 …



GPUs have 5000+ CUDA cores

Results

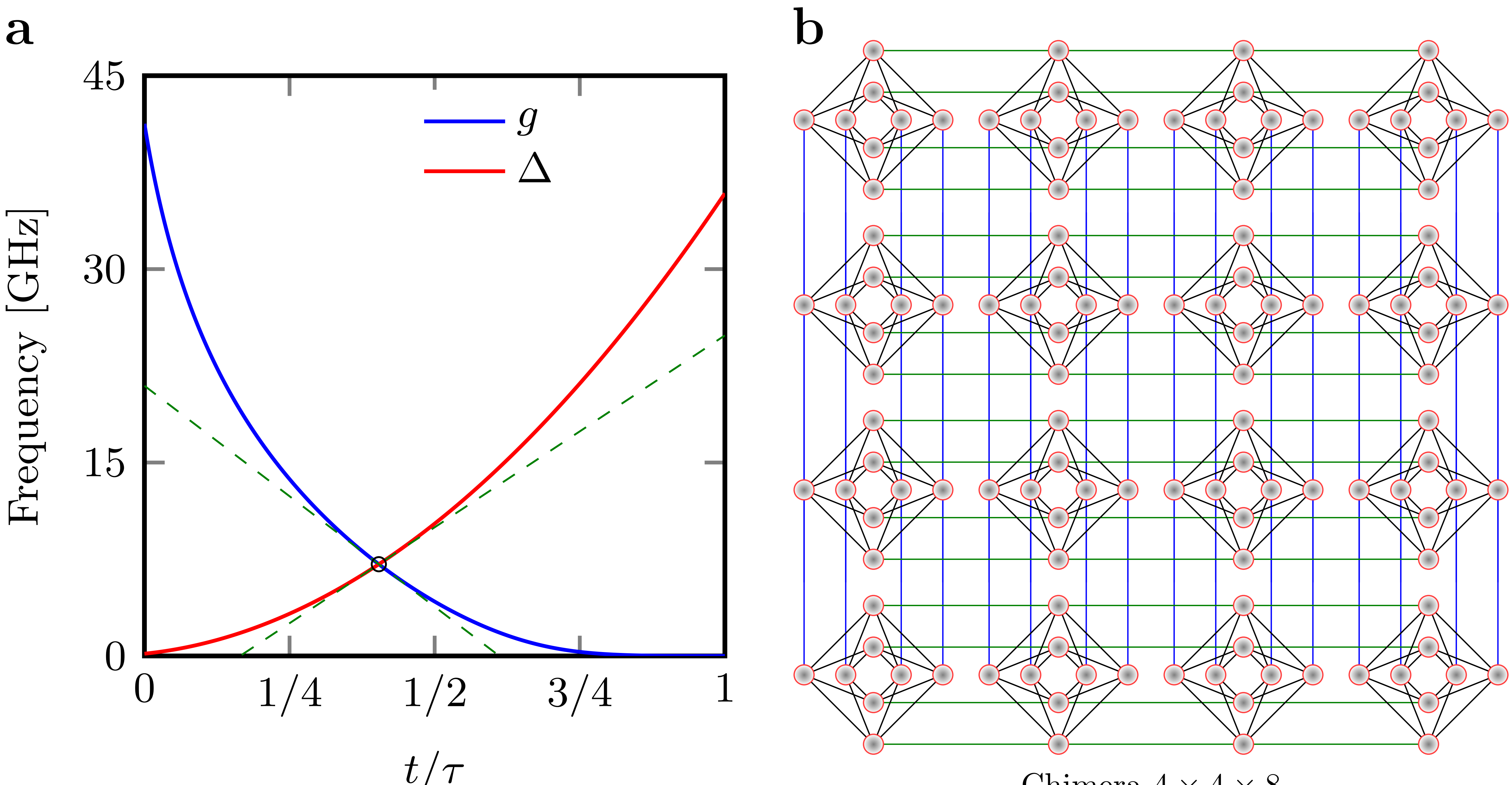


$$H = \omega\sigma_y \quad (\omega = \pi/2)$$

quick reminder:

D-Wave quantum annealer(s)

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



Chimera $4 \times 4 \times 8$

- To begin with, consider a Schrödinger like equation:

not necessary hermitian!

$$\frac{\partial |\psi(t)\rangle}{\partial t} = K(t)\,|\psi(t)\rangle,$$

with known (unique!) solution generated by

$$U(t,t_0) = \mathcal{T}\exp\left(\int_{t_0}^{t} K(\tau)d\tau\right),$$

and a particularly useful property:

“gate” decomposition

$$U(t,t_0) = U_{N-1}\cdots U_{n+1}U_n\cdots U_0;$$

- Now, one may consider the following state

clock states (measure time)

$$|\Psi\rangle = \sum_{n=0}^{N-1} |t_n\rangle \otimes |\psi(t_n)\rangle \, ,$$

being a superposition of the solution states at different moments of time.

- Additionally, let define the **clock operator**:

$$\mathcal{C} = \sum_{n=0}^{N-2} \left(|t_{n+1}\rangle\langle t_{n+1}| \otimes I - |t_{n+1}\rangle\langle t_n| \otimes U_n + \text{h.c.}\right)$$

- Then, clearly

zero energy ground state!

$$\mathcal{C}|\Psi\rangle = 0|\Psi\rangle$$

A technical note #2 …

- An *initial* or a *boundary* condition can be imposed via an additional penalty:

$$(\mathcal{C} + \mathcal{C}_0)|\Psi\rangle = 0,$$

- For instance,

$$\mathcal{C}_0 = |t_0\rangle \langle t_0| \otimes (I - |\psi_0\rangle \langle \psi_0|),$$

results in

$$|\psi(t_0)\rangle = |\psi_0\rangle.$$

- Lets look at this problem differently, namely

$$\mathcal{A}|\Psi\rangle \equiv \mathcal{A}\begin{pmatrix} |\psi(t_0)\rangle \\ |\psi(t_1)\rangle \\ \vdots \\ |\psi(t_N)\rangle \end{pmatrix} = \begin{pmatrix} |\psi_0\rangle \\ 0 \\ \vdots \\ 0 \end{pmatrix} \equiv |\Phi\rangle,$$

where

highly sparse

$$\mathcal{A} = \begin{pmatrix} 2I & -U_0^\dagger & 0 & \cdots & \\ -U_0 & 2I & -U_1^\dagger & & \\ 0 & -U_1 & 2I & & \\ & \vdots & \ddots & \ddots & \\ & & -U_{N-2} & 2I & -U_{N-1}^\dagger \\ & & 0 & -U_{N-1} & I \end{pmatrix}.$$

- Thus, now one “only” needs to solver a linear system:

$$f(\mathbf{x}) = \|\mathcal{A}\,|\mathbf{x}\rangle - |\Phi\rangle\,\|^2$$

optimization problem

- In special cases (hermitian systems) one can simplify to

$$f(\mathbf{x}) = \frac{1}{2}\langle\mathbf{x}|\,\mathcal{A}\,|\mathbf{x}\rangle - \langle\mathbf{x}|\Phi\rangle$$

since

$$\nabla f(\mathbf{x}) = \mathcal{A}\,|\mathbf{x}\rangle - |\Phi\rangle \qquad \nabla^2 f(\mathbf{x}) = \mathcal{A} > 0.$$

This is *almost* what current quantum annealers can do for us

A technical note #3 …

- Fix-point arithmetic on quantum annealers:

$$x_i = 2^D \left(2 \sum_{\alpha=0}^{R-1} q_i^\alpha 2^{-\alpha} - 1 \right),$$

where

not the most general one

$q_i^\alpha = 0, 1$ are classical bits

R required precision

D fixed range

- Then

$$x_i \in [-2^D, 2^D].$$

… that brings us to

- QUBO that can be solve on current quantum annealers:

$$f(\mathbf{q}) = \sum_{i,\alpha} a_i^\alpha q_i^r + \sum_{i,j,\alpha,\beta} b_{ij}^{\alpha\beta} q_i^\alpha q_j^\beta + f_0,$$

dense graph!

where for the hermitian case

$$b_{ij}^{\alpha\beta} = \mathcal{A}_{ij} 2^{1-\alpha-\beta+2D},$$

$$a_i^\alpha = \left(2^{-\alpha+D} \mathcal{A}_{ii} - 2^D \sum_j \mathcal{A}_{ij} - \phi_i \right) 2^{1-\alpha+D},$$

$$f_0 = 2^D \left(2^{D-1} \sum_{ij} \mathcal{A}_{ij} + \sum_i \phi_i \right).$$

A technical note #4 …

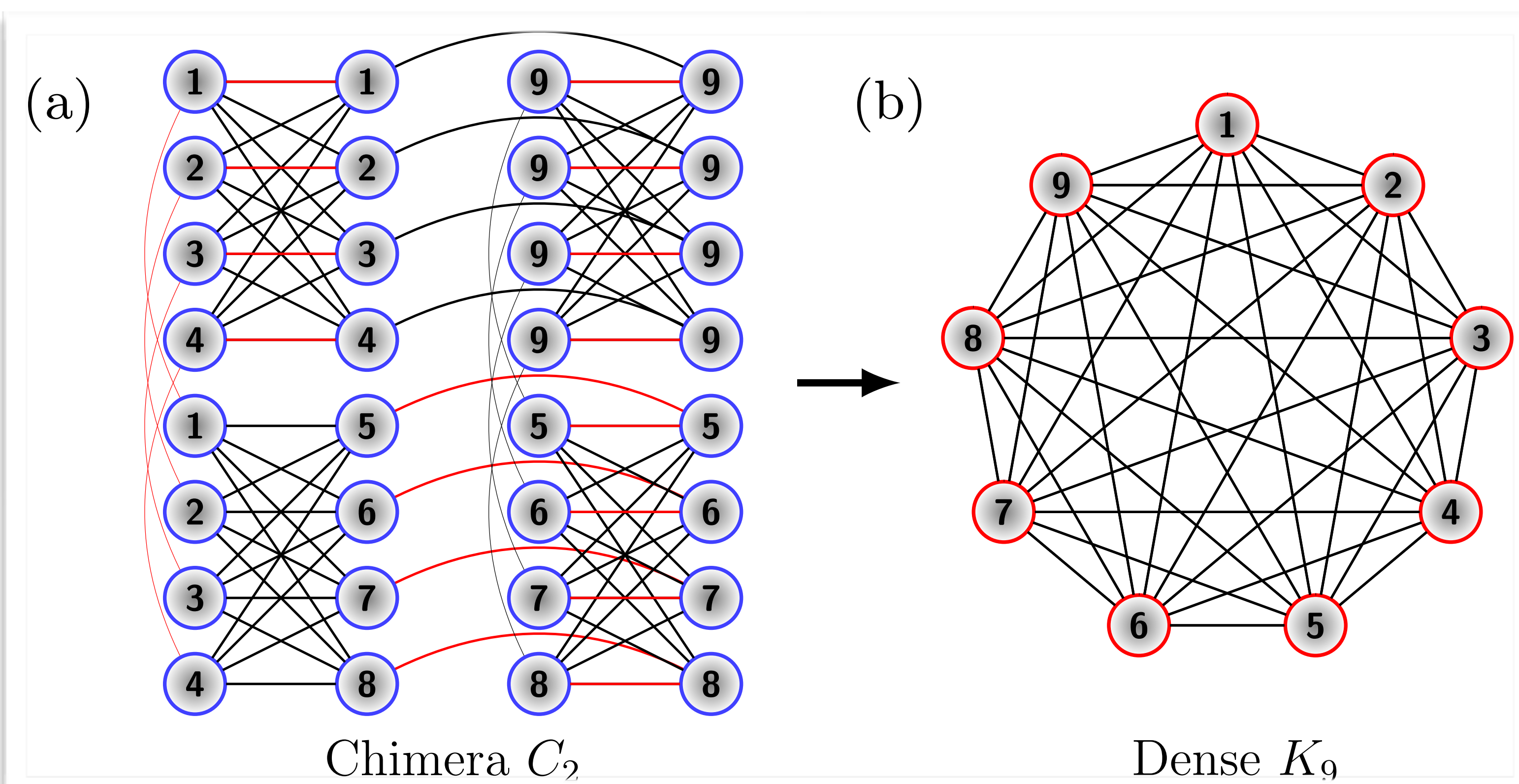
- Complex numbers are possible yet expensive (cost **twice** the amount of qubits)

$$a + bi \mapsto \begin{pmatrix} a & b \\ -b & a \end{pmatrix}$$

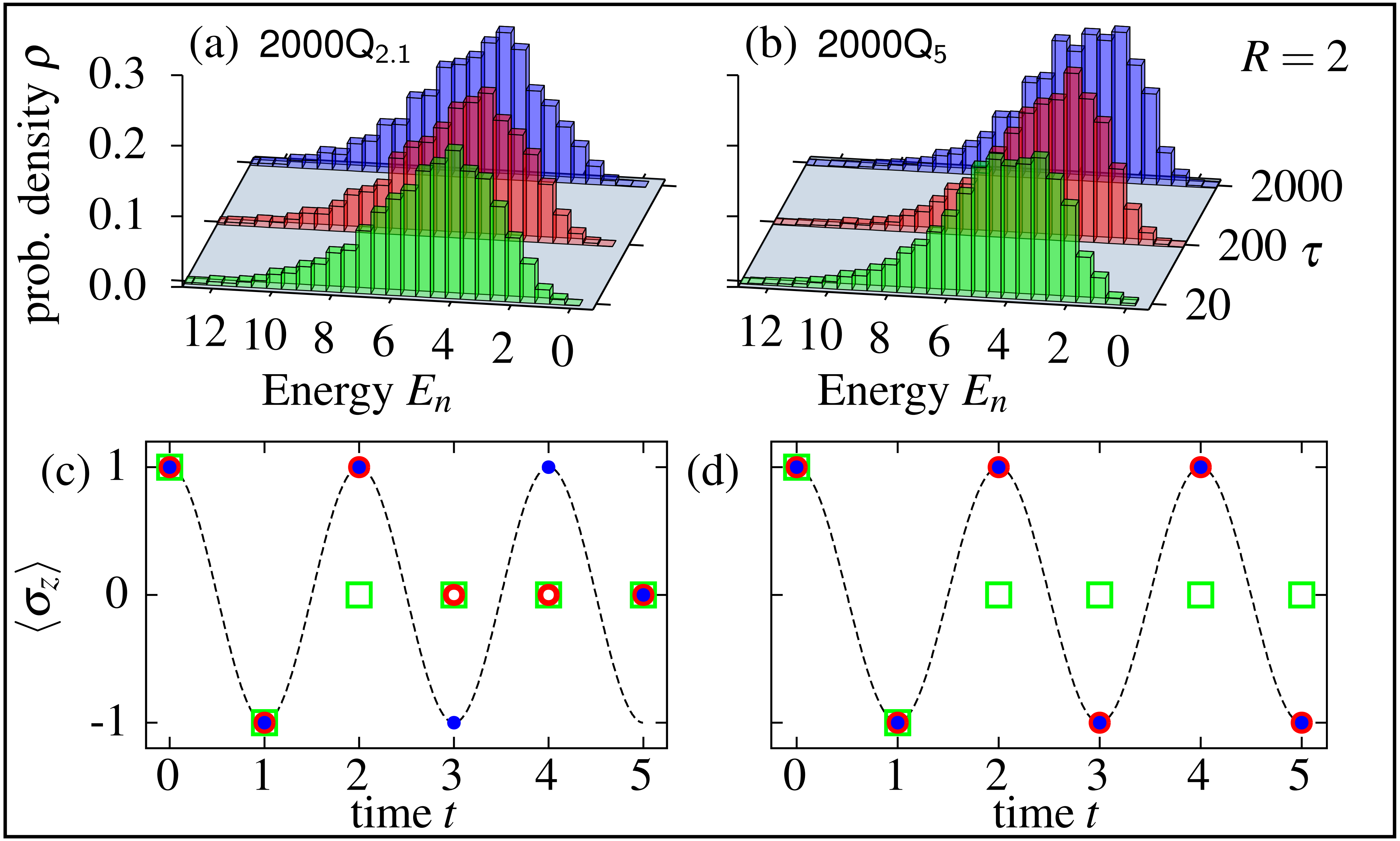
- Only 5 bit precision is possible with D-Wave

- The algorithm requires a complete graph K_{RLT}

- D-Wave: 6 time points and 2 bits precision is possible (for instance)



Recap



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Thank you

Questions/comments/feedback are more than welcome …