Solving hard 2-SAT problems on a D-Wave Two system

Lukas Hobl
Fengping Jin

Hans De Raedt
Kristel Michielsen

Quantum computation

- One qubit ≡ two-level system ≡ one spin-1/2 system

$$\left|\Psi\right\rangle = \alpha\left|0\right\rangle + \beta\left|1\right\rangle \quad ; \quad \left|\alpha\right|^2 + \left|\beta\right|^2 = 1 \quad (\alpha, \beta \in \mathbb{C})$$

- Candidate physical systems for qubits
  - Ensemble of nuclear spins in molecules (NMR quantum computer)
  - Ions in electromagnetic traps
  - Photons in waveguides
  - Quantum dots
  - Dopants in solids
  - Charge, phase or flux in superconductors
  - …

Quantum computation

- Quantum computer hardware can be modeled in terms of qubits that evolve in time (dynamics) according to the time-dependent Schrödinger equation (TDSE)

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = H(t)\left|\psi(t)\right\rangle$$

  - $\left|\psi(t)\right\rangle$: linear combination of all possible qubit states, describes the state of the whole quantum computer at time t
  - $H(t)$: time-dependent Hamiltonian modeling the quantum computer hardware and its control

Quantum computation

- For one spin ½ there is no difference between quantum and classical dynamics

  - *The equation of motion of the expectation value of one spin ½ in a magnetic field is EXACTLY the same as the equation of motion of classical (unit) magnetic moment in a magnetic field*

→ For quantum (&) computation at least two qubits are required

- Simulation of the real dynamics of a quantum computer:
  Solve the time-dependent Schrödinger equation for a given Hamiltonian

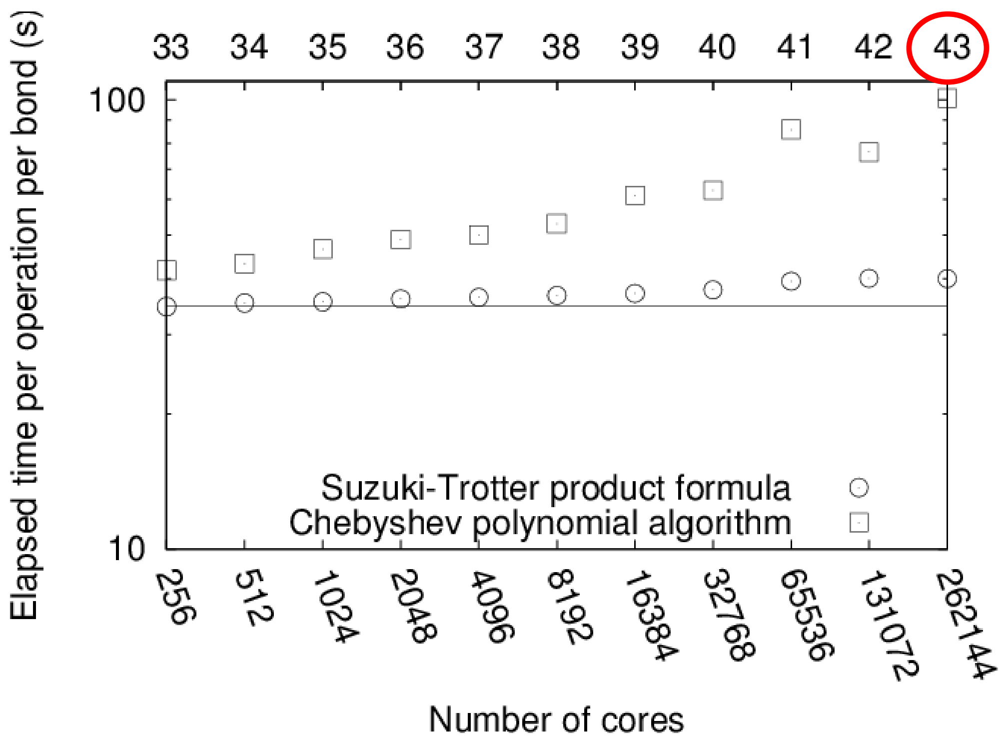
Massively parallel quantum spin dynamics simulator

- MPI/OpenMP FORTRAN 2003 code
- Suzuki-Trotter product formula, Chebyshev polynomials
- Windows, … , IBM BG/Q, Intel-based Linux clusters, …
- Exhibits close to optimal scaling up to 262144 cores (IBM BG/Q)
  - Up to 43 spins (qubits)

Massively parallel quantum spin dynamics simulator

$$i\hbar \frac{\partial \Psi}{\partial t} = H\psi$$

N qubits → ψ is superposition of 2^N quantum states !

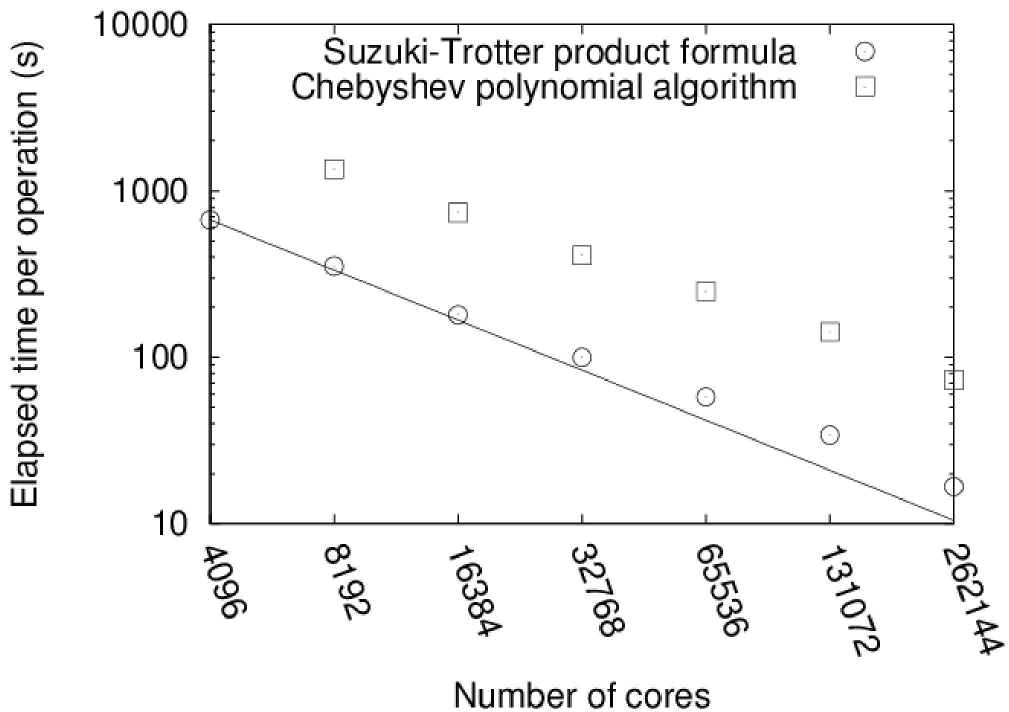


43 qubits: world record

JSC, Jülich

Weak scaling

Massively parallel quantum spin dynamics simulator



Strong scaling

36 spins

Quantum spin dynamics simulator: Applications in quantum computation

- Gate-level quantum computers (single qubit control)
  - PC: Ideal and NMR quantum computer
    - *CNOT gate, TOFFOLI gate, Shor algorithm, Grover algorithm, bit adder, number partitioning*
      - H. De Raedt, A.H. Hams, KM, K. De Raedt, *Quantum computer emulator*, Comp. Phys. Comm. 132, 1 (2000)
      - H. De Raedt, KM, K. De Raedt, S. Miyashita, *Number Partitioning on a Quantum Computer*, Phys. Lett. A 290, 227 (2001)
      - KM, H. De Raedt, K. De Raedt, *A simulator for quantum computer hardware*, NanoTechnology 13, 23 (2002)
      - H. De Raedt, KM, A.H. Hams, S. Miyashita, K. Saito, *Quantum Spin Dynamics as a Model for Quantum Computer Operation*, Eur. Phys. J. B 27, 15 (2002)
      - H. De Raedt and KM, *Computational Methods for Simulating Quantum Computers*, Handbook of Theoretical and Computational Nanotechnology, Vol. 3: Quantum and molecular computing, quantum simulations, Chapter 1, pp. 248, M. Rieth and W. Schommers eds.,American Scientific Publisher, Los Angeles (2006)

  - PC: Superconducting qubits (D. Willsch, master thesis, 2016)

Quantum spin dynamics simulator: Applications in quantum computation

- Gate-level quantum computers (single qubit control)
  - Supercomputer (massively parallel): Ideal and physical quantum computer with nowadays up to 43 qubits
    - *CNOT gate, TOFFOLI gate, Shor algorithm, Grover algorithm, two- and three-integer adder*
      - K. De Raedt, KM, H. De Raedt, B. Trieu, G. Arnold, M. Richter, Th. Lippert, H. Watanabe, N. Ito, *Massively Parallel Quantum Computer Simulator*, Comp. Phys. Comm.176, 121 (2007)
      - H. De Raedt, B. Barbara, S. Miyashita, KM, S. Bertaina, and S. Gambarelli, *Quantum simulations and experiments on Rabi oscillations of spin qubits: Intrinsic vs extrinsic damping*, Phys. Rev. B 85, 014408 (2012)
      - F. Jin, KM, M. Novotny, S. Miyashita, S. Yuan, and H. De Raedt, *Quantum Decoherence Scaling with Bath Size: Importance of Dynamics, Connectivity, and Randomness*, Phys. Rev. A 87, 022117 (2013)
      - M. A. Novotny, F. Jin, S. Yuan, S. Miyashita, H. De Raedt, and KM, *Quantum decoherence and thermalization at finite temperature within the canonical-thermal-state ensemble*, Phys. Rev. A 93, 032110 (2016)

Massively parallel quantum spin dynamics simulator: Applications in quantum computation

- Adiabatic quantum computers (adiabatic evolution of an ensemble of qubits)
  - Supercomputer (massively parallel) and D-Wave Two system:
    - *Random spanning tree problems*
      - L. Hobl, master thesis, 2015
      - M.A. Novotny, L. Hobl, J.S. Hall, KM, *Spanning tree calculations on D-Wave 2 machines*, J. Phys.: Conf. Ser. 681, 012005 (2016)
    - *2-SAT problems*
      - L. Hobl, master thesis 2015
      - Publication in preparation

D-Wave Two system: System 13

- D-Wave system = programmable artificial spin system manufactured as an integrated circuit that performs quantum annealing **???**

- Our comparison test:
  - Solve small but hard 2-SAT problems, characterized by a **KNOWN** unique ground state and highly degenerate first excited state, on a D-Wave Two system
  - Solve the same 2-SAT problems with **IDEAL** quantum annealing by solving the time-dependent Schrödinger equation (TDSE)

Quantum annealing

- The classical optimization problem can be written in terms of an Ising spin Hamiltonian

$$H_P = -\sum_{i=1}^{N} h_i \sigma_i^z + \sum_{\langle ij \rangle} J_{ij} \sigma_i^z \sigma_j^z$$ where $\sigma_i^z = \pm 1$ (spin up or down)

J_{ij} : spin-spin interaction

h_i : external magnetic field

- A transverse field is added to induce quantum transitions between the spin-up and spin-down states

$$H_I = -\sum_{i=1}^{N} \sigma_i^x$$

Quantum annealing

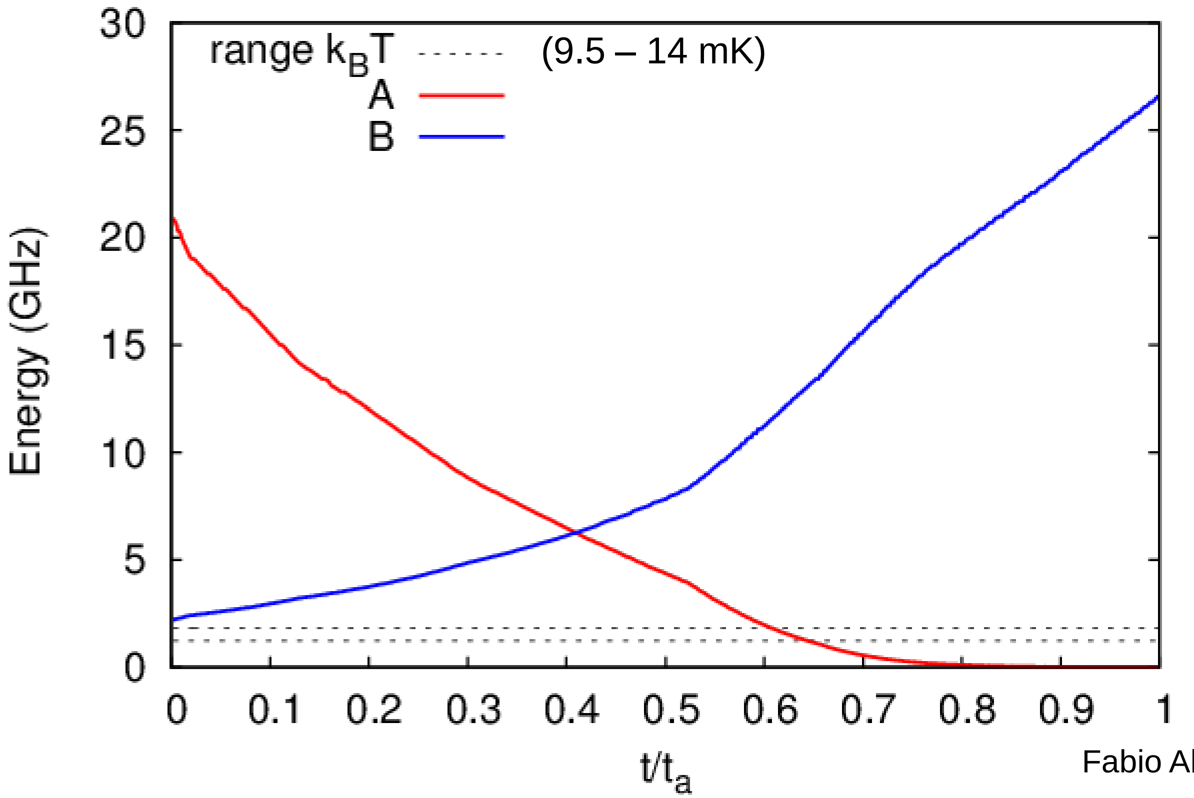
- Total Hamiltonian for quantum annealing

$$H(t) = A(t)H_I + B(t)H_P$$

where $0 \leq t \leq t_a$, $A(0)/B(0) \gg 1$ and $A(t_a)/B(t_a) \ll 1$

  - The total Hamiltonian changes from H_I at $t = 0$ to H_P at $t = t_a$
  - If $A(0)$ is much larger than all other energy scales, then the system will start in the ground state of H_I with a probability of 1
  - If the time evolution is adiabatic, then at $t = t_a$ the system is in the ground state of H_P

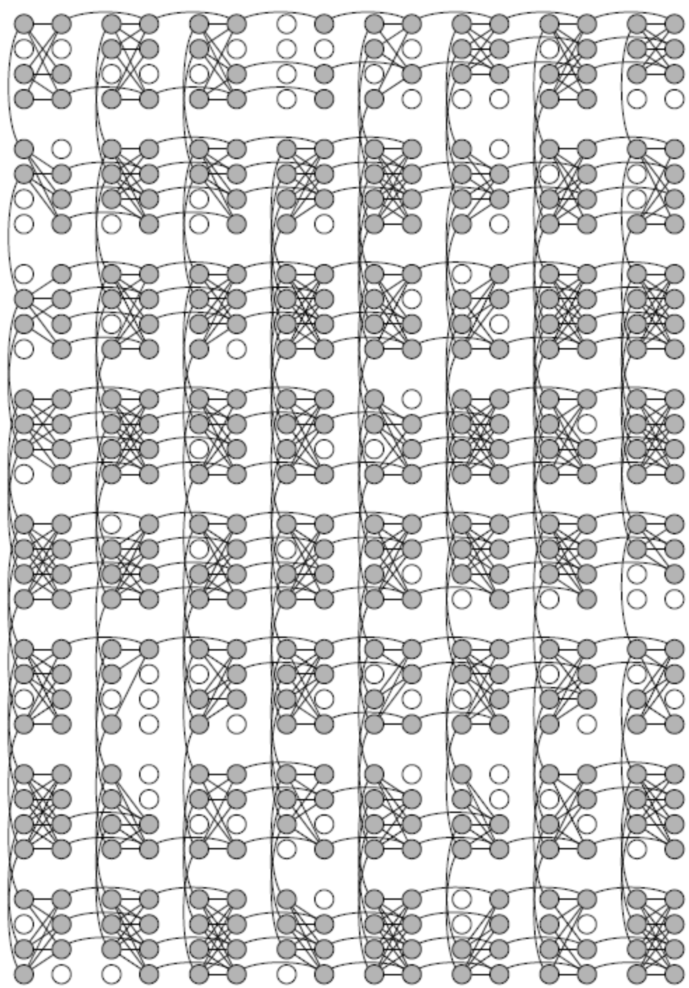
System 13: Annealing schedule (in units $\hbar = 1$)



Fabio Altomare, D-Wave Systems

annealing time: $t_a = 20\mu s$

D-Wave System 13: Chimera graph



: operable qubits
: inoperable qubits
: qubit-qubit interactions

Hard 2-SAT problems

- 2-SAT problems with $i = 1, \ldots, N$ Boolean variables $x_i = 0,1$ and M clauses
- Hard problems are designed to hide the **unique** ground state from a large number of first excited states
- Clause-to-variable ratio $\alpha = M / N = (N+1) / N$
- We consider hard 2-SAT problems for $N = 8,12,18$
  - Example for $N = 8$:

$$\left(x_6 \vee x_3\right) \wedge \left(x_5 \vee \overline{x_6}\right) \wedge \left(x_8 \vee \overline{x_4}\right) \wedge \left(x_8 \vee \overline{x_7}\right) \wedge \left(x_1 \vee \overline{x_3}\right) \wedge$$

$$\left(\overline{x_5} \vee \overline{x_1}\right) \wedge \left(x_6 \vee \overline{x_3}\right) \wedge \left(x_3 \vee \overline{x_8}\right) \wedge \left(\overline{x_2} \vee \overline{x_5}\right)$$

Hard 2-SAT problems

- 2-SAT problems can be mapped to the Ising model H_P
  - Example for $N = 8$
  - Consider the clauses $(x_6 \vee x_3)$ and $(x_5 \vee \overline{x_6})$

OR	T	T	T	F
x_6	1	1	0	0
x_3	1	0	1	0

OR	T	T	T	F
σ_6	1	1	-1	-1
σ_3	1	-1	1	-1
m = $\sigma_6 + \sigma_3$	2	0	0	-2

OR	T	T	T	F
x_5	1	1	0	0
$\overline{x_6}$	0	1	0	1

OR	T	T	T	F
σ_5	1	1	-1	-1
σ_6	-1	1	-1	1
m = $\sigma_5 - \sigma_6$	2	0	-0	-2

Hard 2-SAT problems

- For one clause, an Ising Hamiltonian can be constructed with a magnetization $m = \sigma_i + \sigma_j$ so that the solution of the 2-SAT problem is the ground state of this Ising Hamiltonian

$$
\begin{aligned}
H &= m(m-2) \\
&= \sigma_i^2 + \sigma_j^2 + 2\sigma_i\sigma_j - 2\sigma_i - 2\sigma_j \\
&= 2 + 2\sigma_i\sigma_j - 2\sigma_i - 2\sigma_j
\end{aligned}
$$

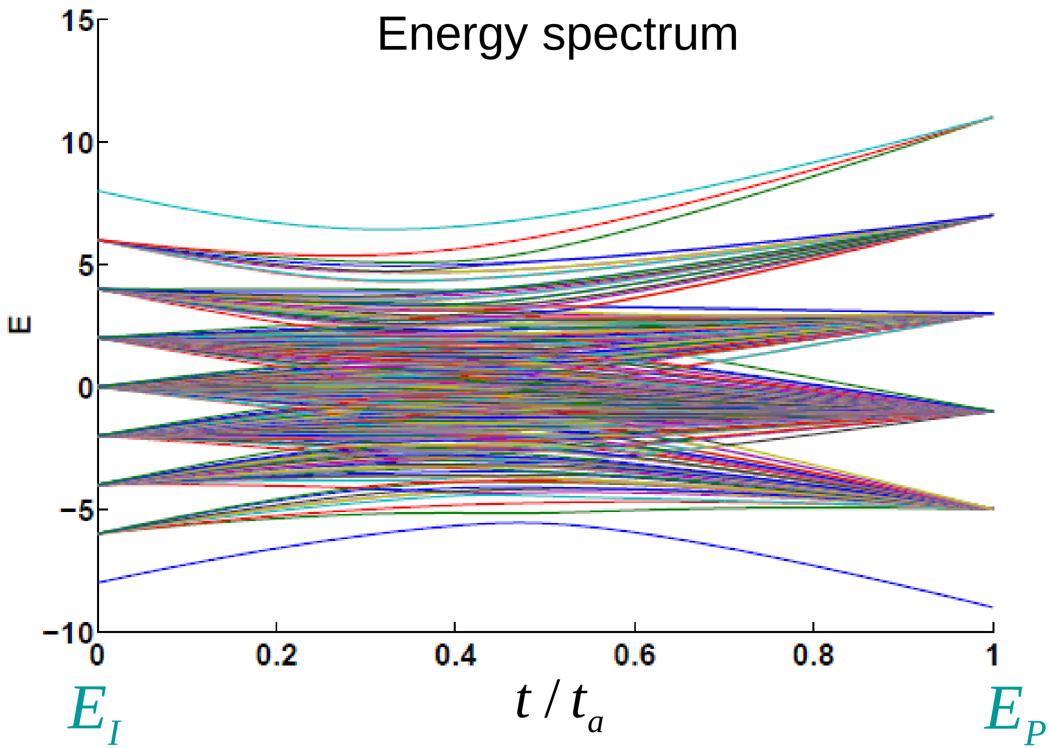
- Comparison with $H_P = -\sum_{i=1}^{N} h_i\sigma_i^z + \sum_{\langle ij\rangle} J_{ij}\sigma_i^z\sigma_j^z$ gives

$$h_i = 2, h_j = 2, J_{ij} = -2$$

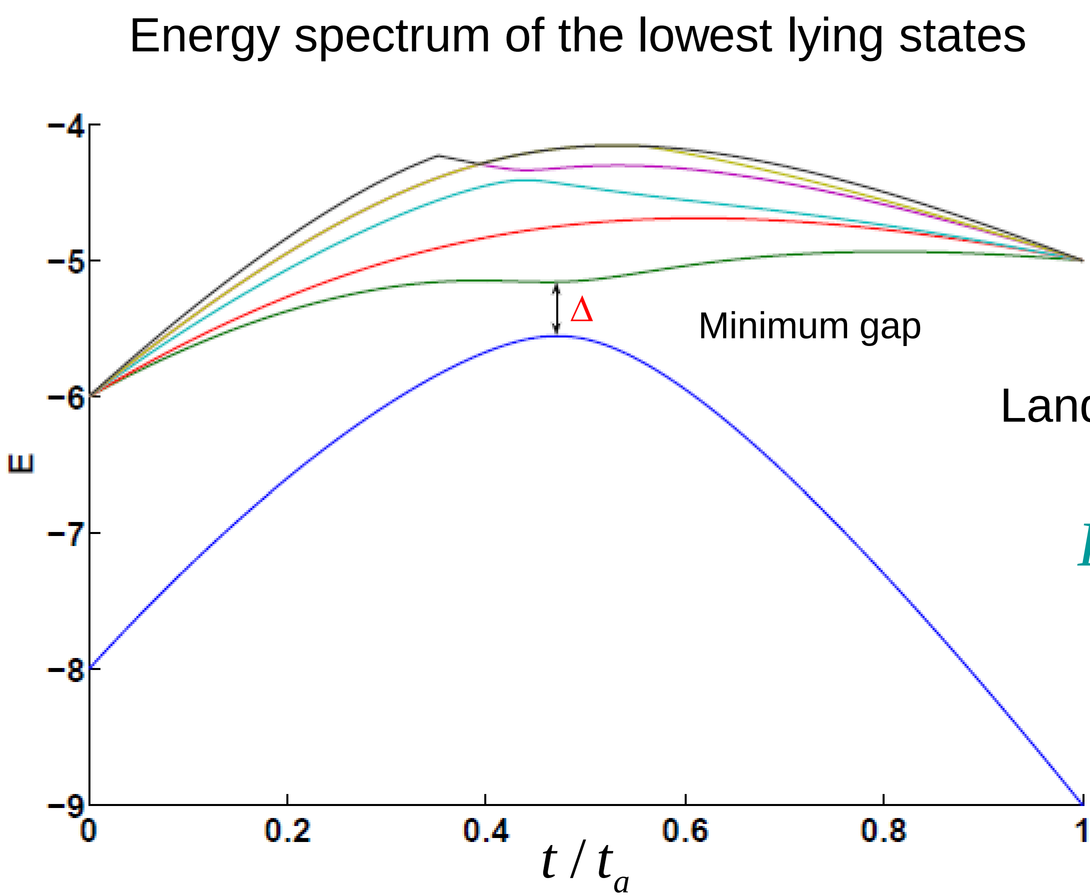
- This procedure is repeated for all clauses

Hard 2-SAT problem for $N = 8$

"Quantum annealing" hardness of the problem is determined by the gap between the ground state and the first excited state



Hard 2-SAT problem for $N = 8$



Landau-Zener formula:

$$P = 1 - e^{-\frac{\pi \Delta^2}{2v}}$$

P : probability to remain in the ground state during annealing

v : sweep velocity

$v \to 0 : P = 1$

$v \to \infty : P = 0$

Procedure for the comparison test

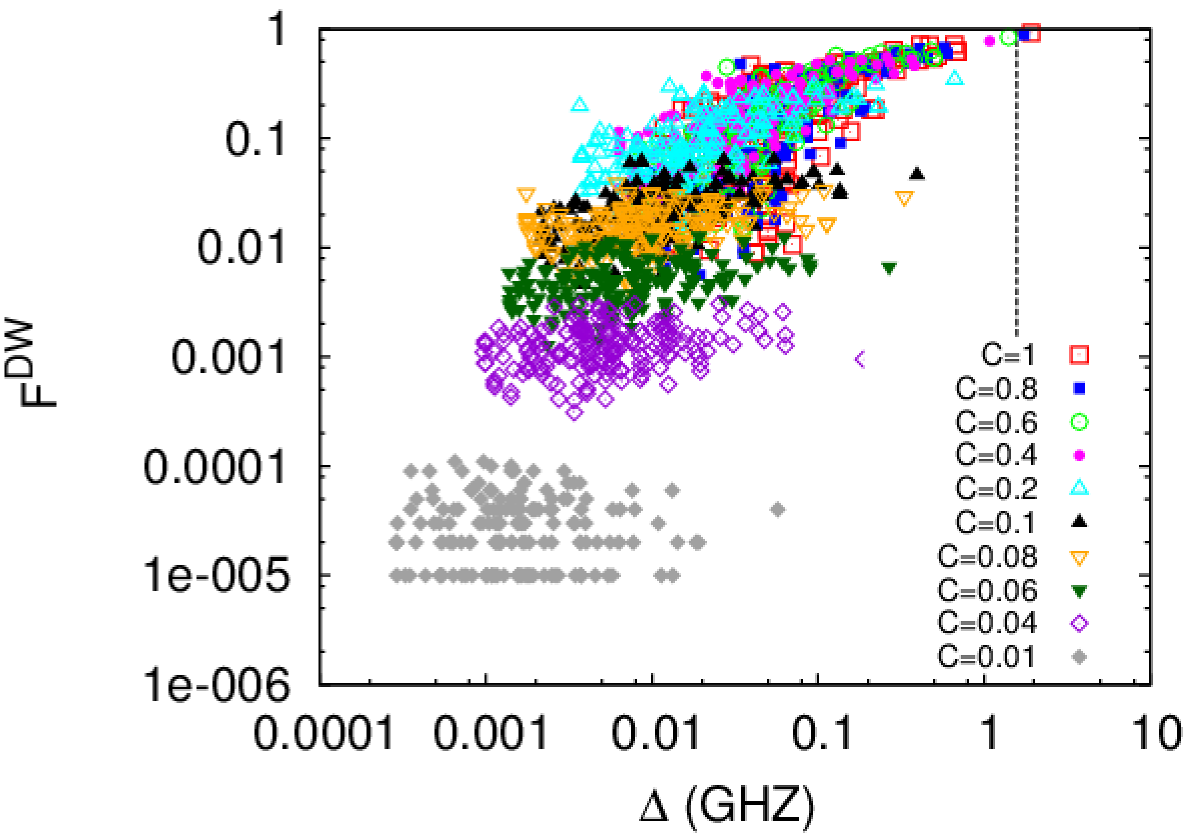
- Consider those hard 2-SAT problems that can be mapped on the Chimera graph of the D-Wave processor (direct embedding, no logical qubits)
- Calculate the minimum gap Δ
- Enlarge the collection of 2-SAT problems by rescaling H_P : CH_P with $0.01 < C \leq 1$ → problems with smaller Δ
- Use the D-Wave system to determine the frequency F^{DW} to find the **KNOWN** ground state
- Use the TDSE solver with the D-Wave system parameters to determine the probability P to find the **KNOWN** ground state
- Plot P and F^{DW} as a function of Δ and compare the results

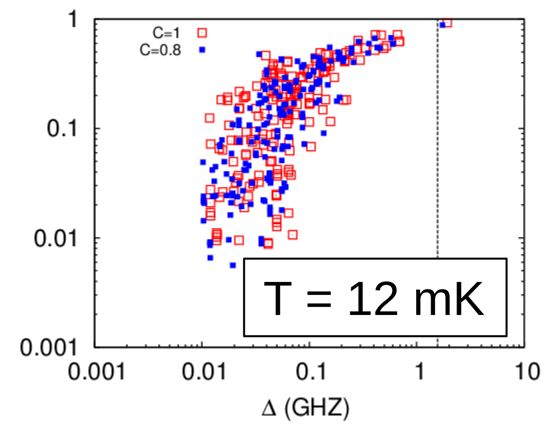
Notes

- By default, the smallest annealing time for one run is 20 μs
- By default, the D-Wave system performs 1000 annealing runs for one problem solving request → the system returns 1000 “solutions” for every problem submitted
- For each problem, 1000 solving requests were submitted resulting in one million “solutions” per problem → the frequency of finding the correct solution for each 2SAT problem is based on one million trials

Results for $N = 18$ obtained with D-Wave System 13

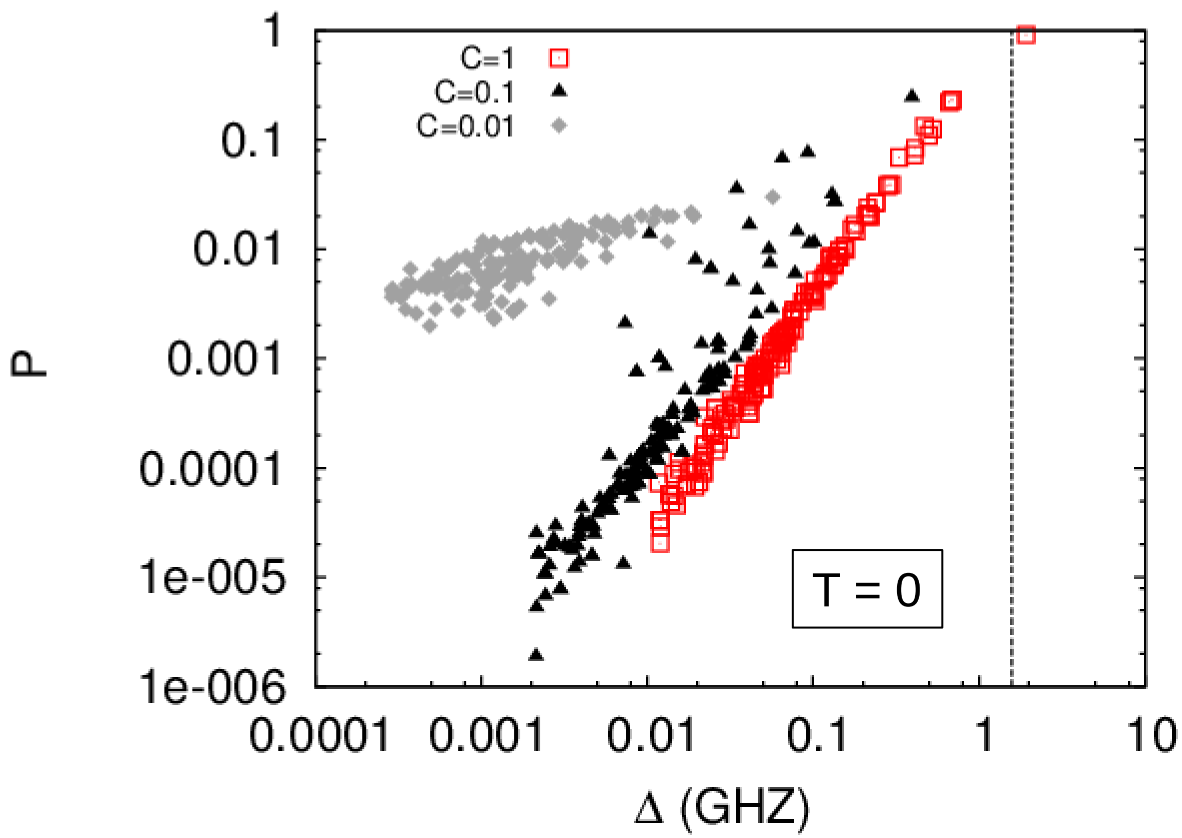
$t_a = 20\mu s$





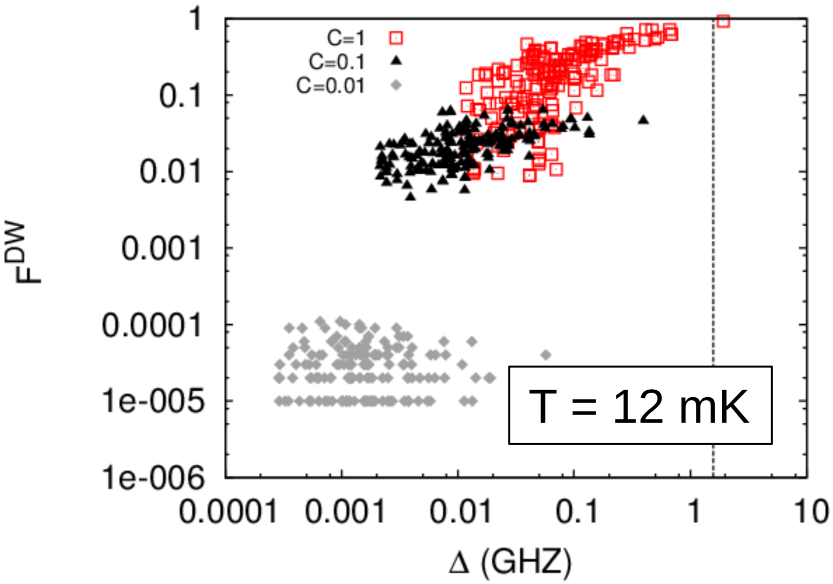
Results for $N = 18$ obtained with TDSE solver

$$t_a = 0.05\mu s$$



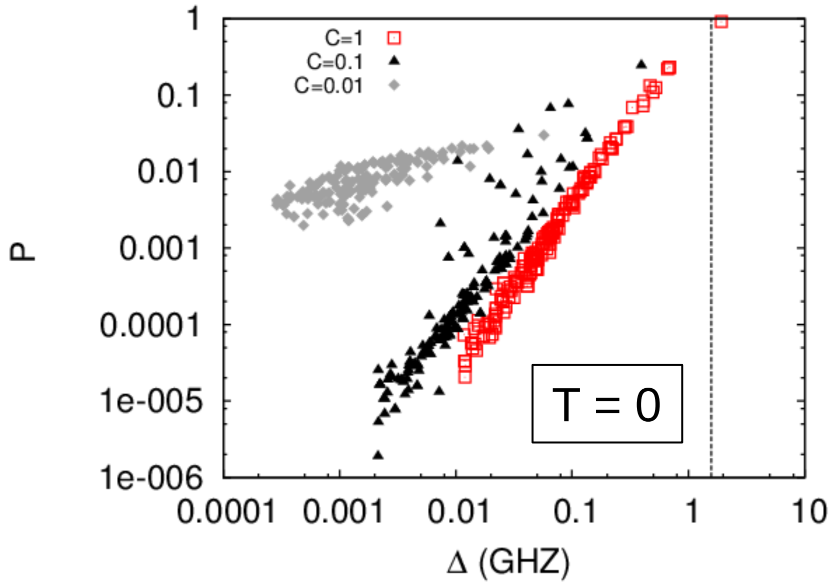
Comparison System 13 – TDSE solver for $N = 18$

$t_a = 20 \mu s$



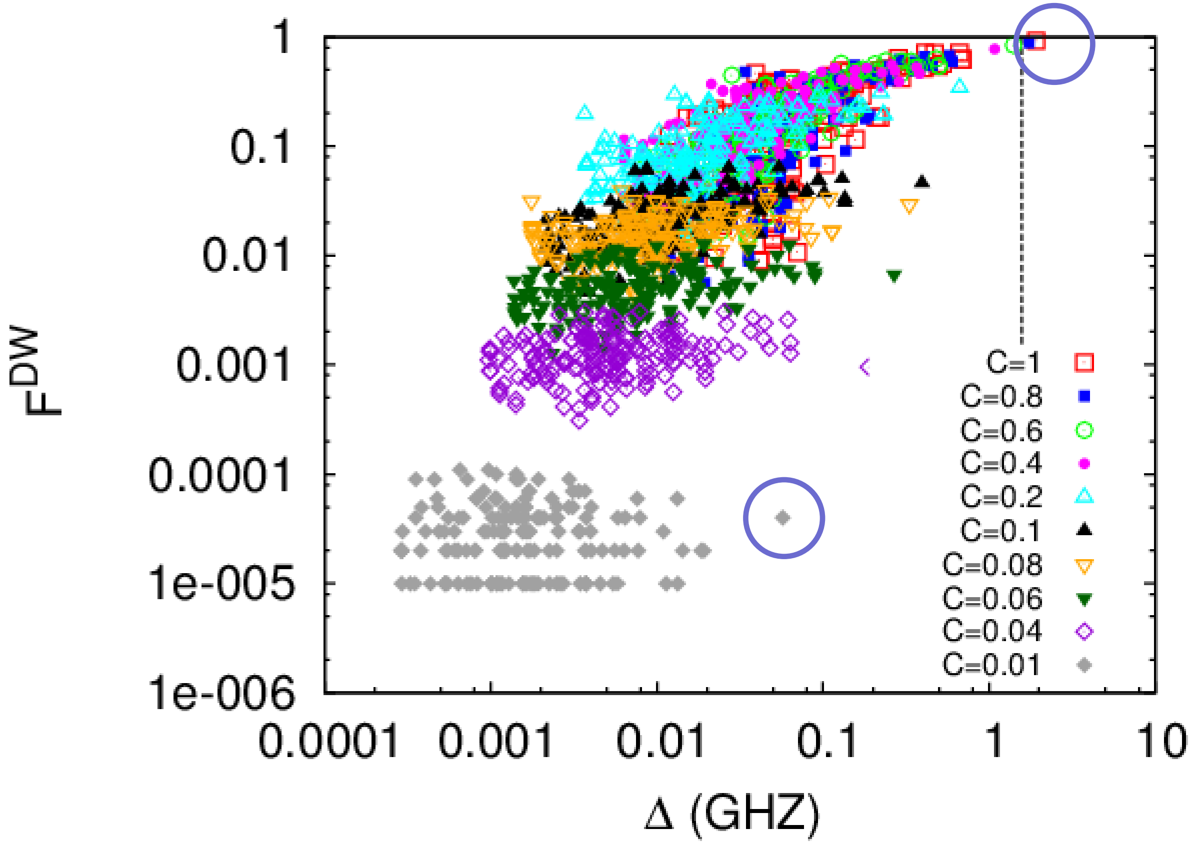
D-Wave System 13

$t_a = 0.05 \mu s$

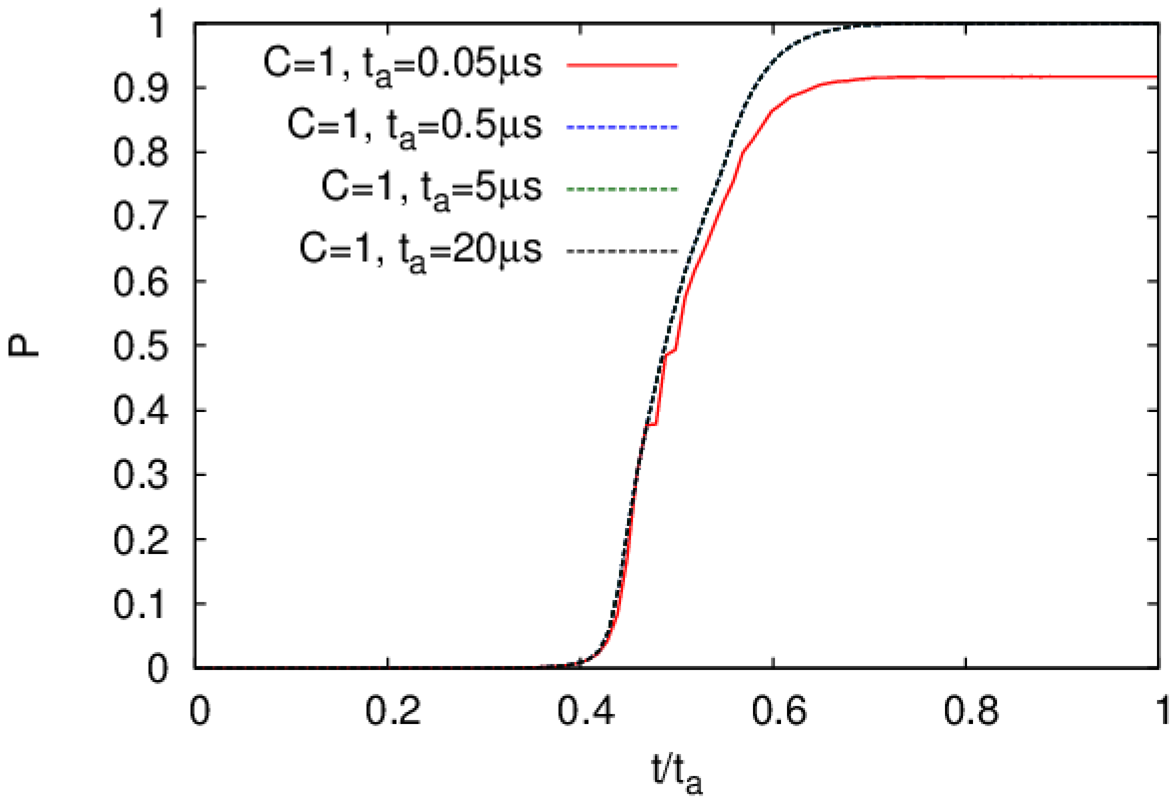


TDSE solver

One example: “Problem 332” with $C = 1, C = 0.01$

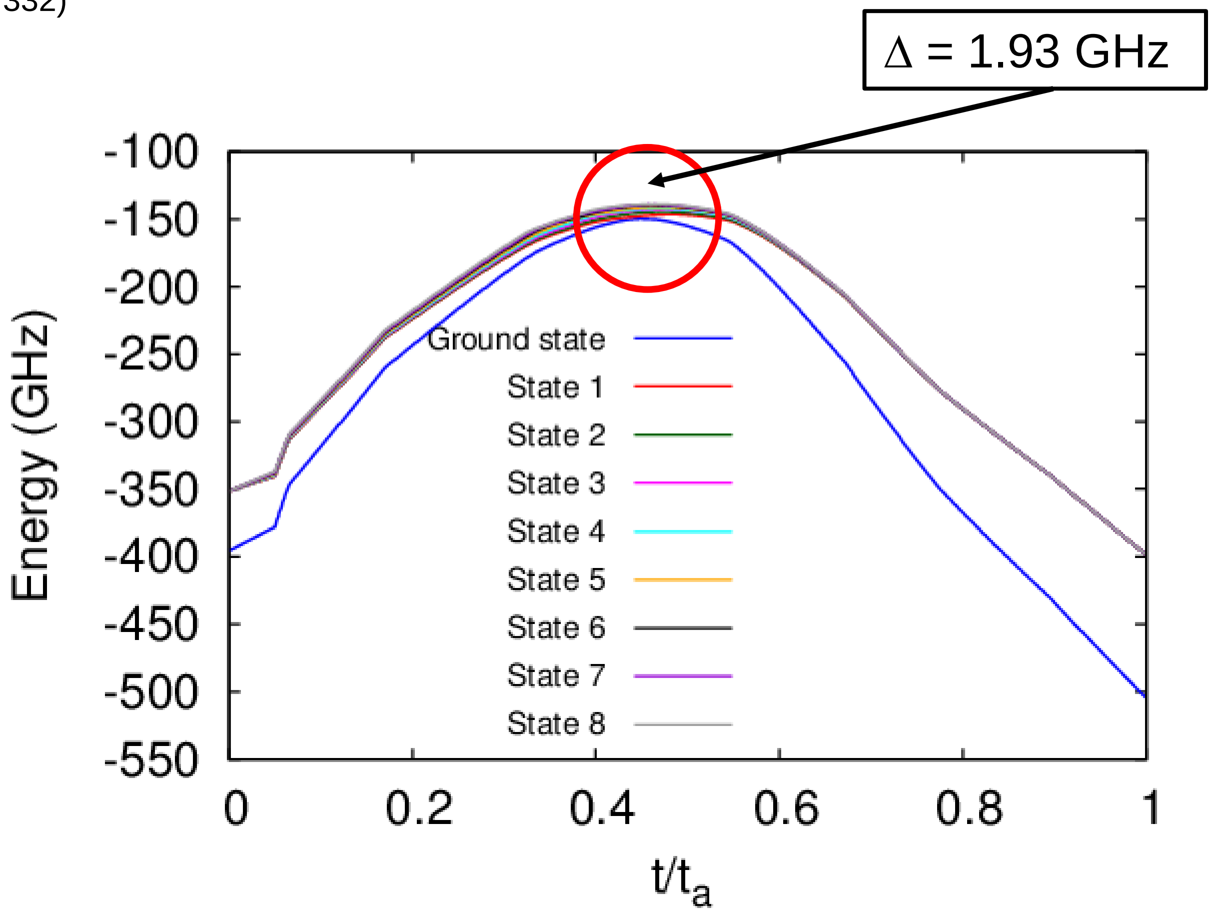


Success probability for one example with $N = 18, C = 1$ (Problem 332)



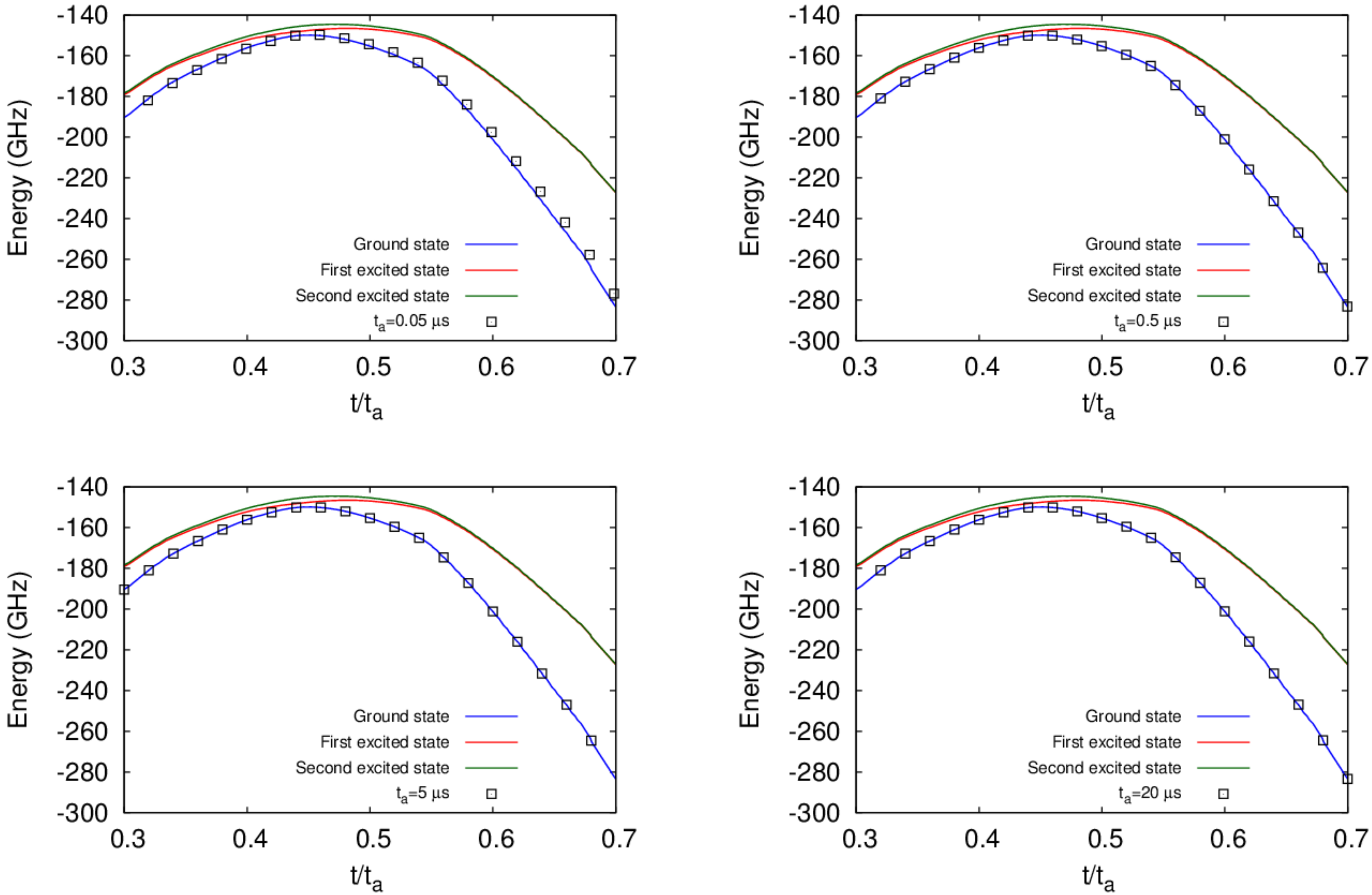
Spectrum for one example with $N = 18, C = 1$

(Problem 332)

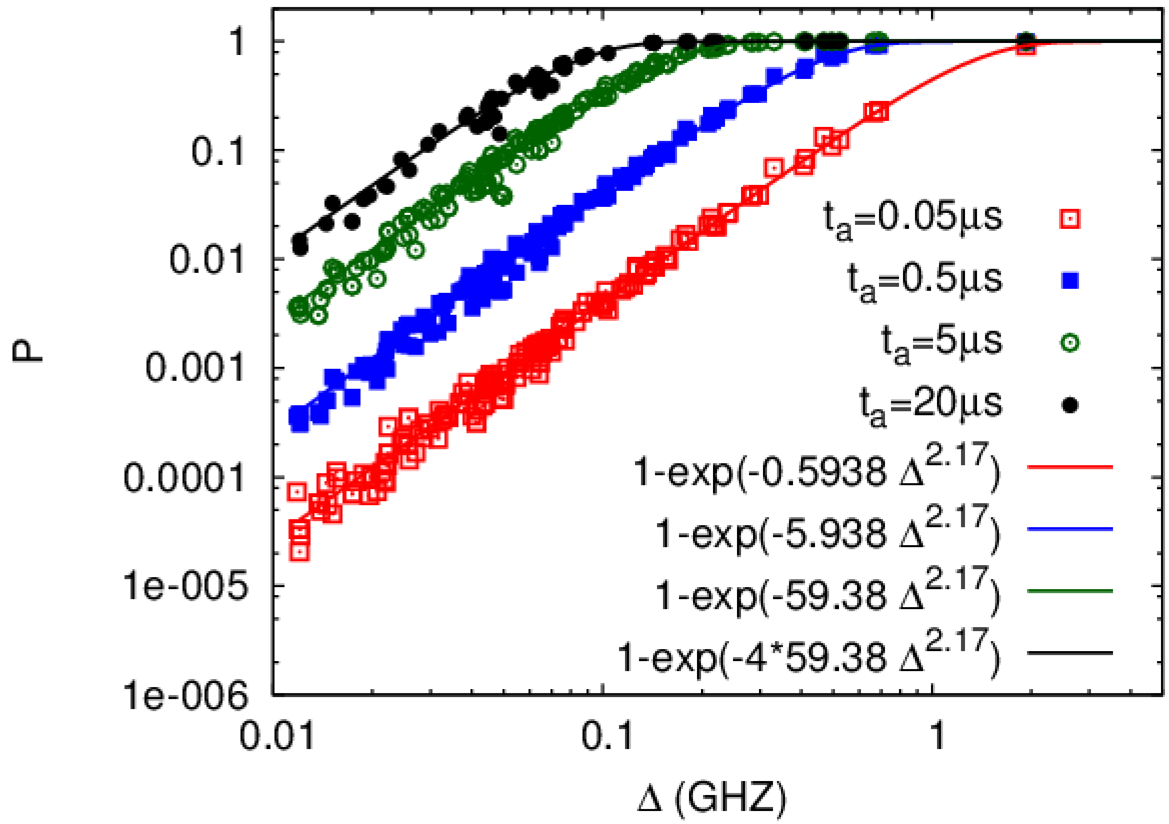


System energy for one example with $N = 18, C = 1$

(Problem 332)



Landau-Zener behavior for problems with $N = 18, C = 1$



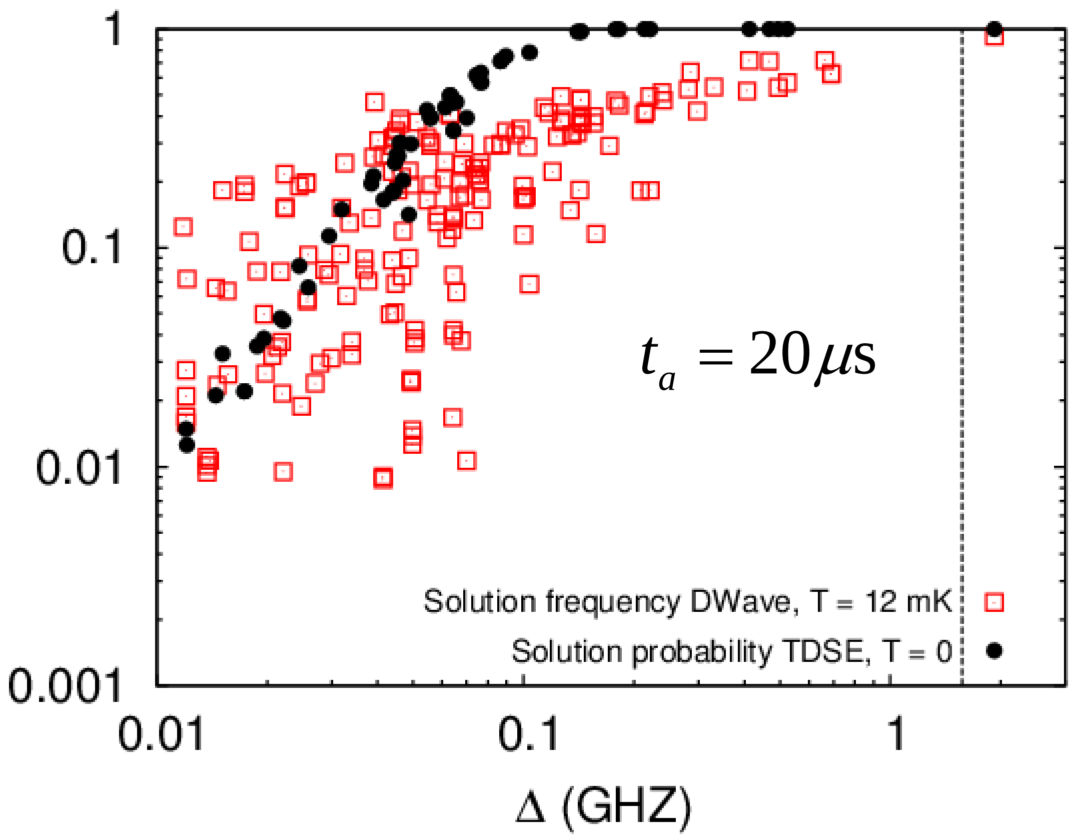
Landau-Zener formula:

$$P = 1 - \exp\left(-\frac{\pi}{2v}\Delta^2\right)$$

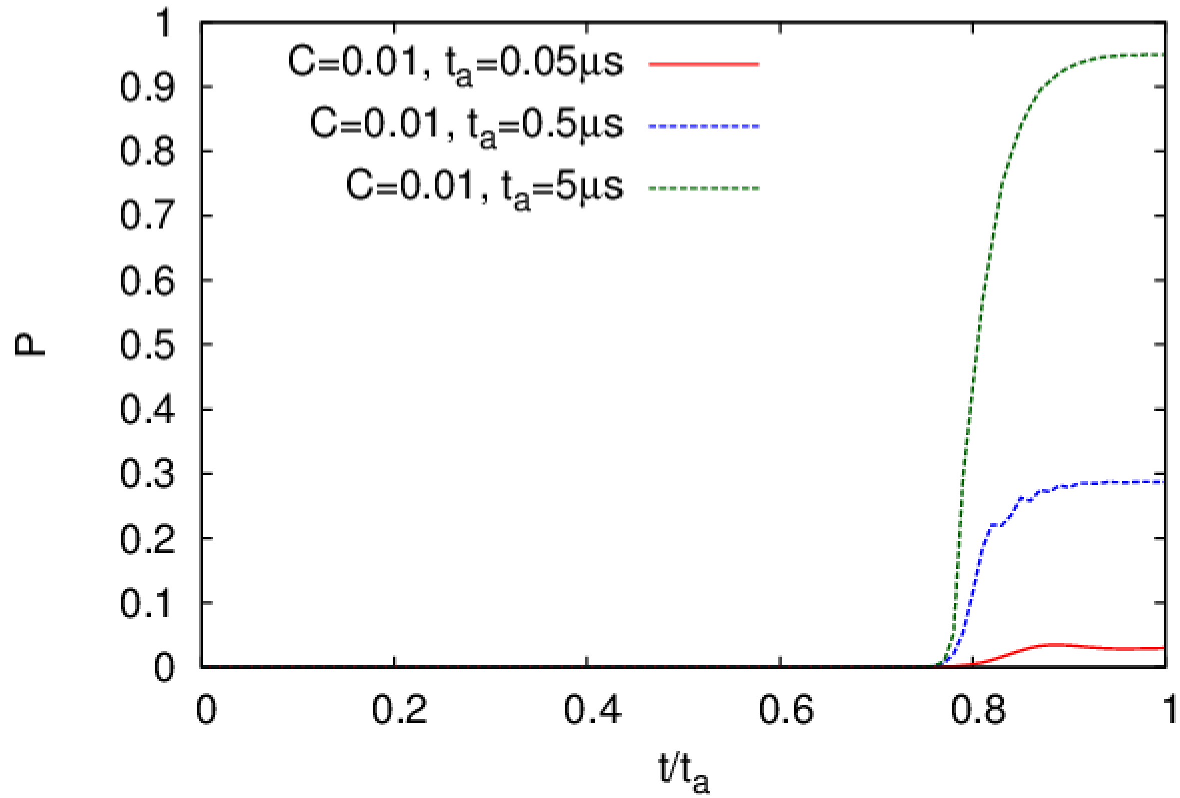
$$= 1 - \exp\left(-\alpha t_a \Delta^2\right)$$

TDSE solver

Landau-Zener behavior for problems with $N = 18, C = 1$



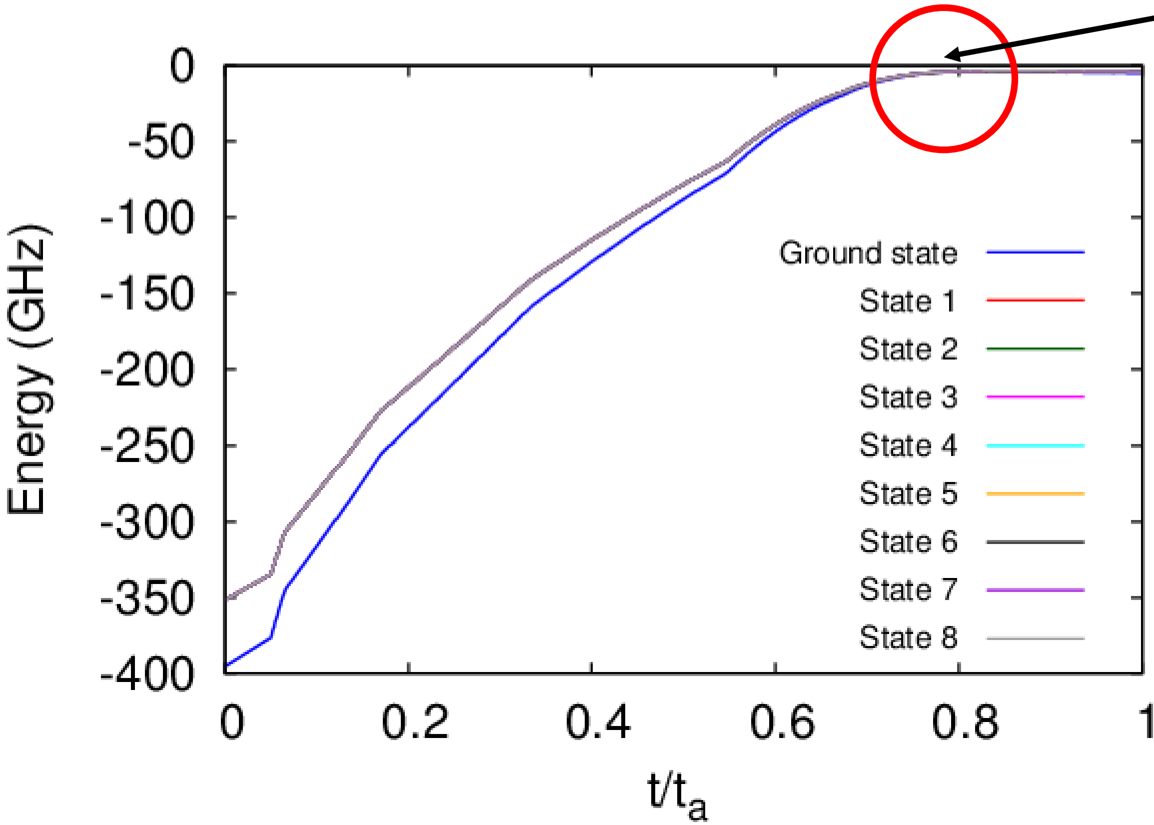
Success probability for one example with $N = 18, C = 0.01$ (Problem 332)



Spectrum for one example with $N = 18, C = 0.01$

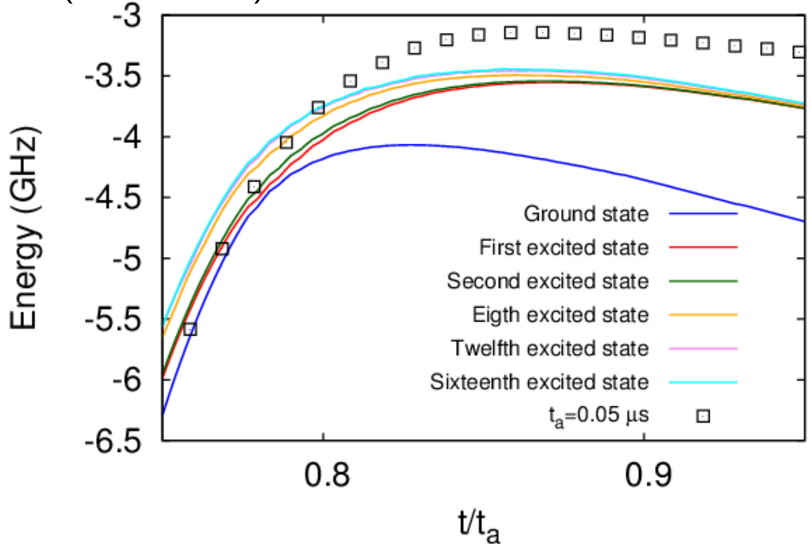
(Problem 332)

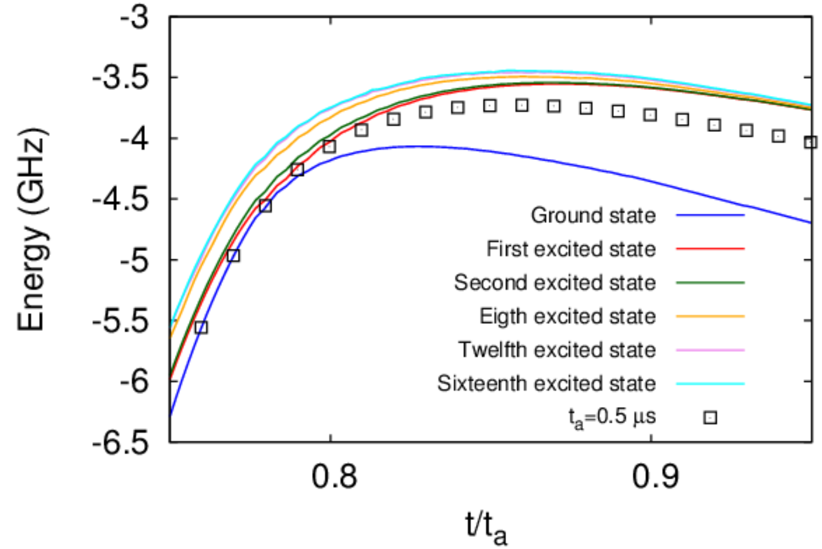
Δ = 0.057 GHz

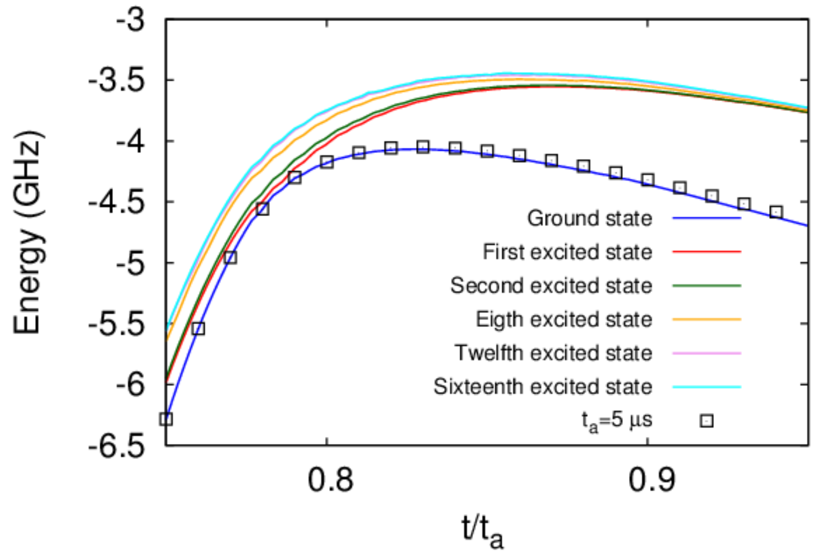


System energy for one example with $N = 18, C = 0.01$

(Problem 332)







Preliminary conclusions

- Is the D-Wave Two system performing quantum annealing?
  - For problems with $\Delta > k_B T$: probably
  - For problems with $\Delta \leq k_B T$ (very hard 2SAT problems): very likely not
- Temperature effects?
  - For problems with $\Delta \leq k_B T$: very probable
  - For problems with $\Delta > k_B T$ and long annealing times ?
- Future work:
  - Couple the 8-spin system to a finite-temperature spin bath with up to 20 spins
  - Study the effects of temperature on the success probability for finding the solution of the 2SAT problems

Conclusion

- Simulating quantum annealing on supercomputers and performing quantum annealing on D-Wave machines sheds light on the physical processes involved