

# Simulation of a Quantum Annealer for Solving the 2-Satisfiability Problem at Zero and Finite Temperature

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# Introduction of the Quantum Annealing

- ▶ The goal of the quantum annealing is to find the ground state of a given Hamiltonian.
- ▶ The Hamiltonian used by a quantum annealing process can be written as follow

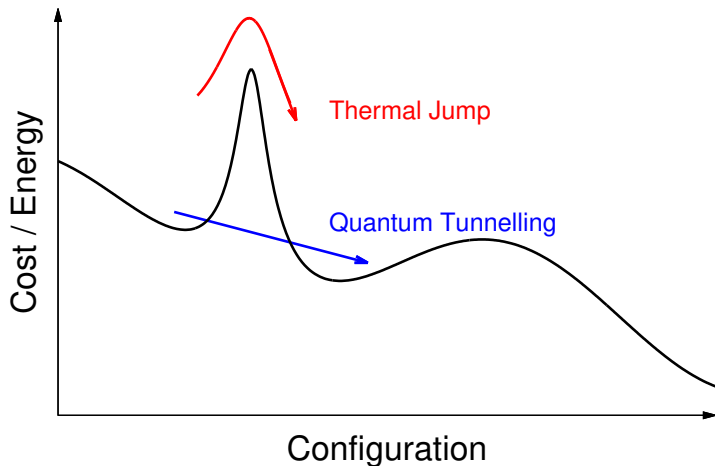
$$H(t) = (1 - \frac{t}{T})H_{init} + (\frac{t}{T})H_{problem}$$

$$H_{init} = - \sum_{i=1}^N h_i^x \sigma_i^x$$

$$H_{problem} = - \sum_{i,j}^N J_{ij}^z \sigma_i^z \sigma_j^z - \sum_i^N h_i^z \sigma_i^z,$$

where  $t$  is the current time step and  $T$  is the total annealing time.

# The Difference between the Quantum Annealing and the Simulated Annealing



# Adiabatic Theorem

If a quantum system stays in an eigenstate of a slowly varying Hamiltonian at one time, it will remain in an eigenstate at later times, while its eigenenergy evolves continuously.

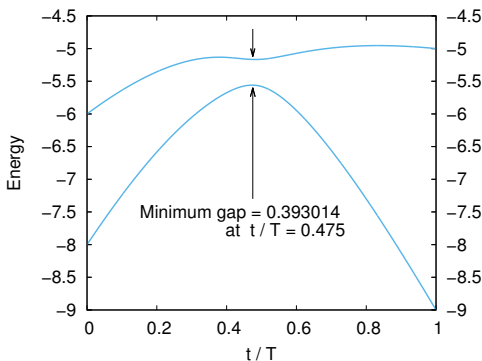
# Landau-Zener Transition

- The Landau-Zener formula gives out the probability of a diabatic transition from a lower energy eigenstate to a higher energy eigenstate.

The probability of a diabatic transition,  $P_{\text{diabatic}}$ , can be described by

$$P_{\text{adiabatic}}(T) = 1 - P_{\text{diabatic}}(T)$$

$$P_{\text{diabatic}}(T) = \exp(-c \cdot \Delta_{\min}^2).$$



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# The 2-Satisfiability Problem

A  $k$ -SAT problem is a problem with  $k$  as the upper limit of the number of variables in one clause.

An example 2-SAT problem with 8 boolean variables is shown below:

## Example

$$(x_1 \vee x_2) \wedge (x_3 \vee \neg x_4) \wedge (\neg x_5 \vee x_4) \wedge (\neg x_6 \vee \neg x_7) \wedge (\neg x_3 \vee \neg x_8),$$

where  $\wedge$ ,  $\vee$ , and  $\neg$  state for logical and, logical or, and logical not respectively.

# The 2-Satisfiability Problem

$$(x_1 \vee x_2) \wedge (x_3 \vee \neg x_4) \wedge (\neg x_5 \vee x_4) \wedge (\neg x_6 \vee \neg x_7) \wedge (\neg x_3 \vee \neg x_8)$$

A key question is how to map a given problem into the Hamiltonian. For example, a possible mapping is as follows :

2-SAT Variables

	T	T	T	F
$x_1$	1	1	0	0
$x_2$	1	0	1	0

$\Rightarrow$

Ising variables

	T	T	T	F
$\sigma_1$	1	1	-1	-1
$\sigma_2$	1	-1	1	-1
$m = \sigma_1 + \sigma_2$	2	0	0	-2

	T	T	T	F
$x_3$	1	1	0	0
$x_4$	0	1	0	1

$\Rightarrow$

	T	T	T	F
$\sigma_3$	1	1	-1	-1
$\sigma_4$	-1	1	-1	1
$m = \sigma_3 - \sigma_4$	2	0	0	-2

## The 2-Satisfiability Problem

To encode the solution of the 2-SAT problem, the Hamiltonian can be designed for the first clause as

	T	T	T	F
$m = \sigma_1 + \sigma_2$	2	0	0	-2

$$\begin{aligned}H &= m \cdot (m - 2) \\&= \sigma_1^2 + \sigma_2^2 + 2\sigma_1\sigma_2 - 2\sigma_1 - 2\sigma_2 \\&= 2\sigma_1\sigma_2 - 2\sigma_1 - 2\sigma_2 + \text{const.}\end{aligned}$$

Then one can correspond  $h_1^z$ ,  $h_2^z$ , and  $J_{12}$  in  $H_{problem}$  to 2, 2, and -2 respectively, and repeat this procedure for all clauses.

$$H_{problem} = - \sum_{i,j}^N J_{ij}^z \sigma_i^z \sigma_j^z - \sum_i^N h_i^z \sigma_i^z$$

# The Quantum Annealing Algorithm

## Quantum Annealing Algorithm

Set up  $H_{problem}$  according to a given problem. Combine  $H_{init}$  and  $H_{problem}$  to build  $H(t)$ .

1. Initialise the system to the ground state of  $H_{init}$ .
2. Evolve the system by computing time-dependent Schrödinger equation for time  $t$  according to a given time scheme.
3. The system will end up in the ground state of the  $H_{problem}$ , if the total annealing  $T$  is long enough.

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# Time-Dependent Schrödinger Equation

- ▶ The quantum annealing process can be described by time-dependent Schrödinger equation with the Hamiltonian given as

$$H(t) = \left(1 - \frac{t}{T}\right)H_{init} + \left(\frac{t}{T}\right)H_{problem}$$

- ▶ The solution of this is

$$\begin{aligned}\Psi(t + \tau) &= U(t + \tau, t)\Psi(t) \\ &= \exp\left(-i \int_t^{t+\tau} H\left(\frac{t+\tau}{2}\right)d\tau\right)\Psi(t),\end{aligned}$$

where  $\tau$  is the time step, and  $U(t + \tau)$  is a unitary matrix that transform system from  $t$  to  $t + \tau$ .

- ▶ The time step should be small enough to keep  $H(t)$  piecewise constant, and the solution can be rewritten as

$$\Psi(t + \tau) = \exp\left(-iH\left(\frac{t+\tau}{2}\right)\tau\right)\Psi(t).$$

# The Suzuki-Trotter Product Formula Approach

$$H(t) = \left(1 - \frac{t}{T}\right)H_{init} + \left(\frac{t}{T}\right)H_{problem}$$

$$H_{init} = -\sum_{i=1}^N h_i^x \sigma_i^x, \quad H_{problem} = -\sum_i^N h_i^z \sigma_i^z - \sum_{i,j}^N J_{ij}^z \sigma_i^z \sigma_j^z$$

Based on the Hamiltonian used above, one way to construct the approximation is

$$\Psi(t + \tau) = \tilde{U}(t)\Psi(t)$$

$$\tilde{U}(t) = \exp\left(\frac{-i\tau H_{\sigma^x,z}}{2}\right) \exp(-i\tau H_{\sigma_z \sigma_z}) \exp\left(\frac{-i\tau H_{\sigma^x,z}}{2}\right).$$

## Simulation Result: Ground State Energy

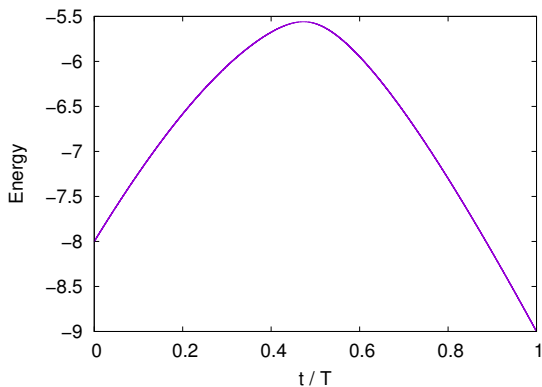


Figure: An result with total annealing time = 1000



# Simulation Result: Success Probability

Annealing time = 1000

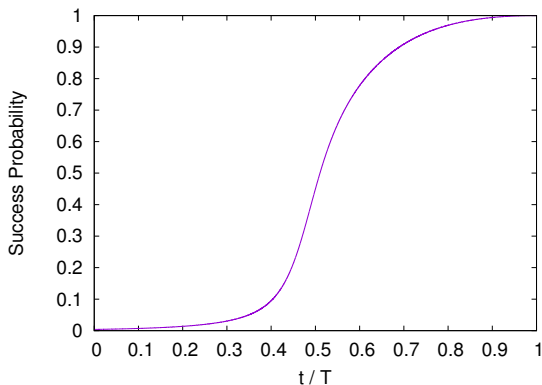
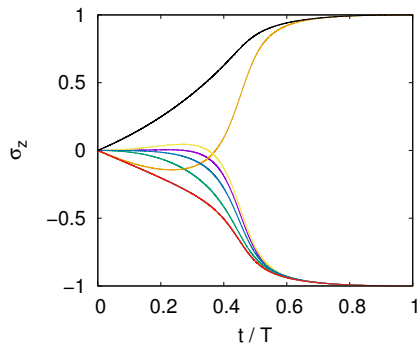
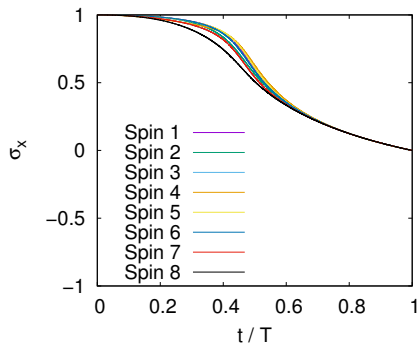


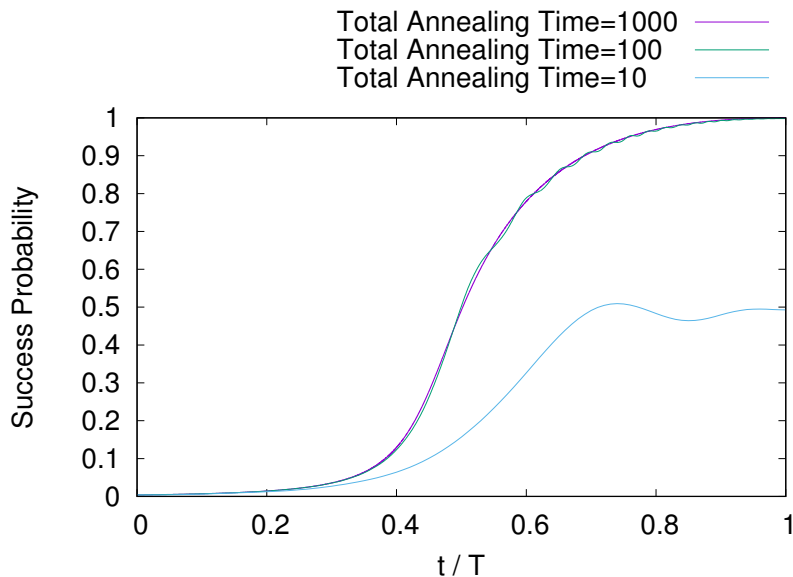
Figure: An result with total annealing time = 1000

# Simulation Result: Spin Value

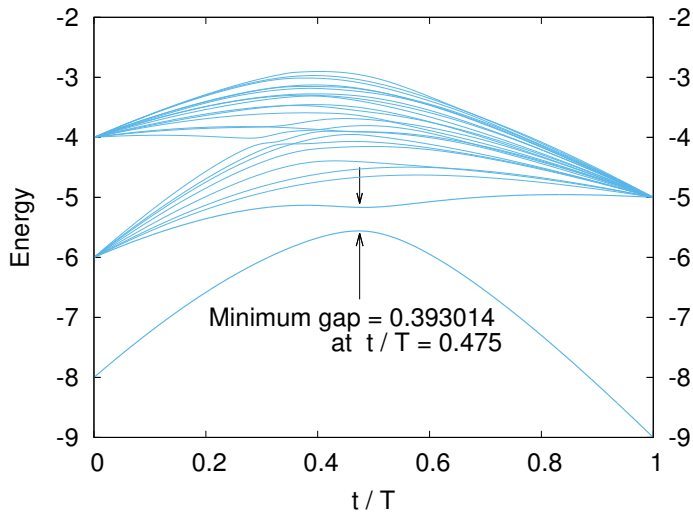
$$H_{init} = - \sum_{i=1}^N h_i^x \sigma_i^x, \quad H_{problem} = - \sum_i h_i^z \sigma_i^z - \sum_{i,j} J_{ij}^z \sigma_i^z \sigma_j^z$$



## Effect of Total Annealing Time



# The Energy Spectrum and the Minimum Gap



# Effect of Minimum Gap

$$P_{\text{adiabatic}}(T) = 1 - P_{\text{diabatic}}(T)$$

$$P_{\text{diabatic}}(T) = \exp(-c \cdot \Delta_{\min}^2).$$

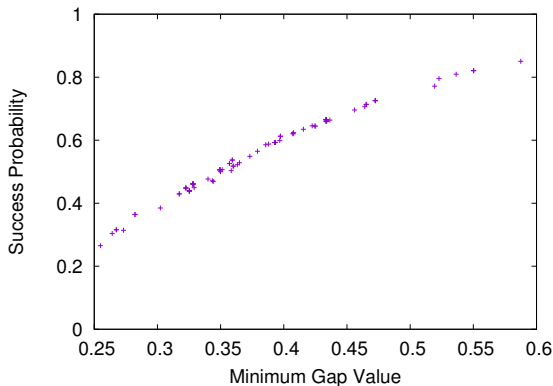


Figure: A plot with 100 different 2-SAT problems.

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# Hamiltonian for a System at Finite Temperature

In order to simulate a system at finite temperature, the quantum system  $S$  is coupled to a heat bath  $B$  and the Hamiltonian of the entire system (i.e.  $S+B$ ) is defined as

$$H = H_S + H_B + gH_{SB},$$

where  $H_S$  is the Hamiltonian of the system,  $H_B$  is the Hamiltonian of the heat bath, and  $H_{SB}$  is the interaction between the subsystem  $S$  and the heat bath  $B$  with  $g$  indicates the global coupling strength between  $S$  and  $B$ .

# Effect of Total Annealing Time at different Temperature

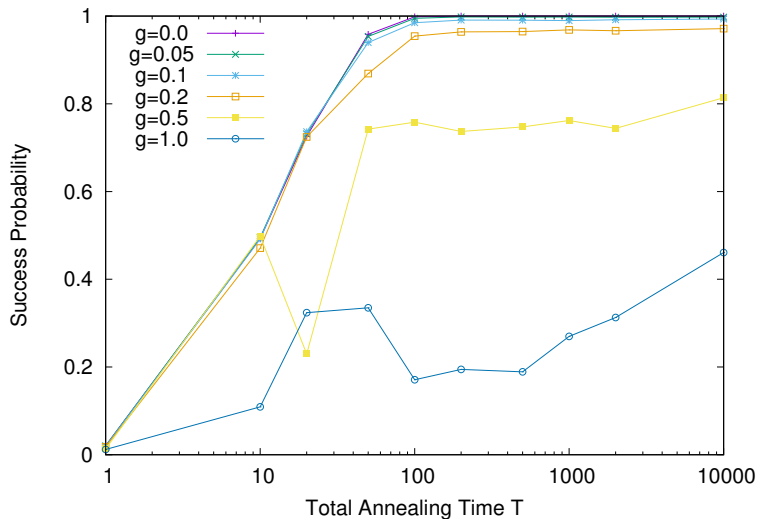


Figure: A result at Temperature = 0.02



# Effect of Total Annealing Time at different Temperature

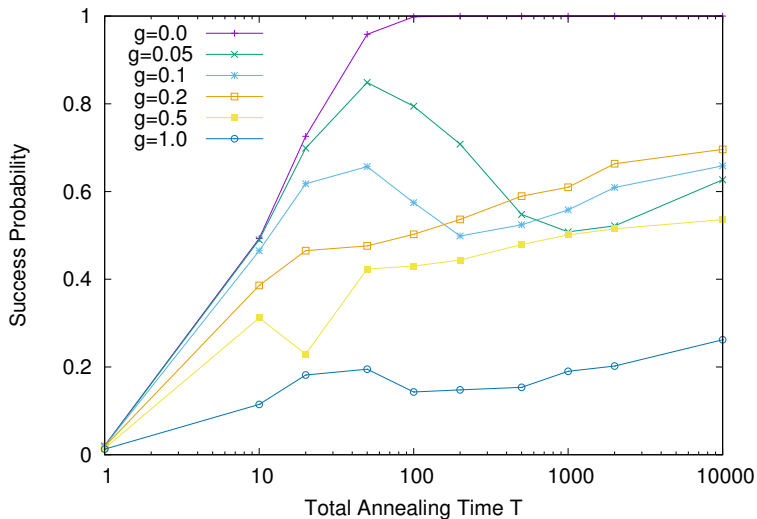


Figure: A result at Temperature = 1

# Effect of Total Annealing Time at different Temperature

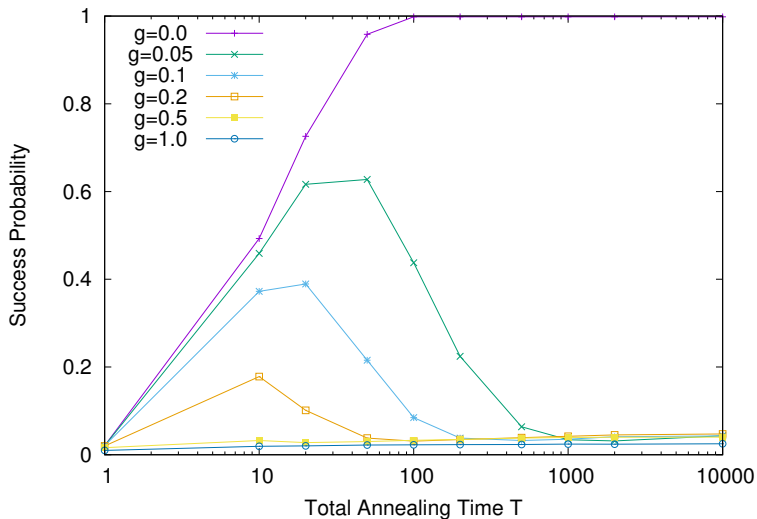
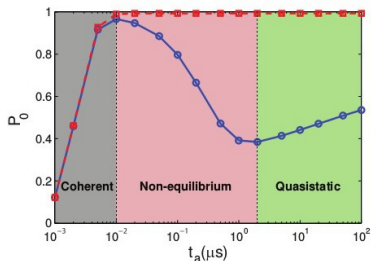
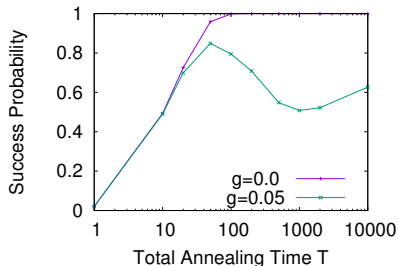


Figure: A result at Temperature = 1000

# Effect of Total Annealing Time at different Temperature

Temperature = 1

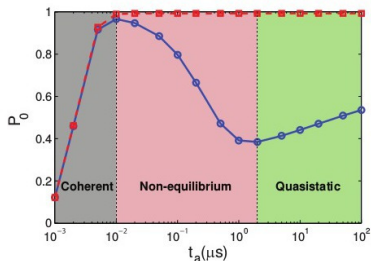
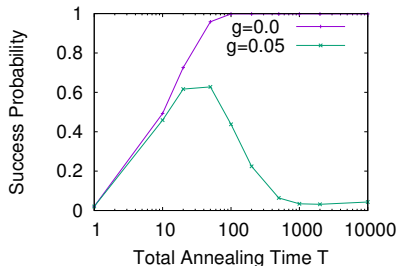


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\* Amin, M. H. (2015). Searching for quantum speedup in quasistatic quantum annealers. Physical Review A - Atomic, Molecular, and Optical Physics, 92(5), 1–5. <https://doi.org/10.1103/PhysRevA.92.052323>

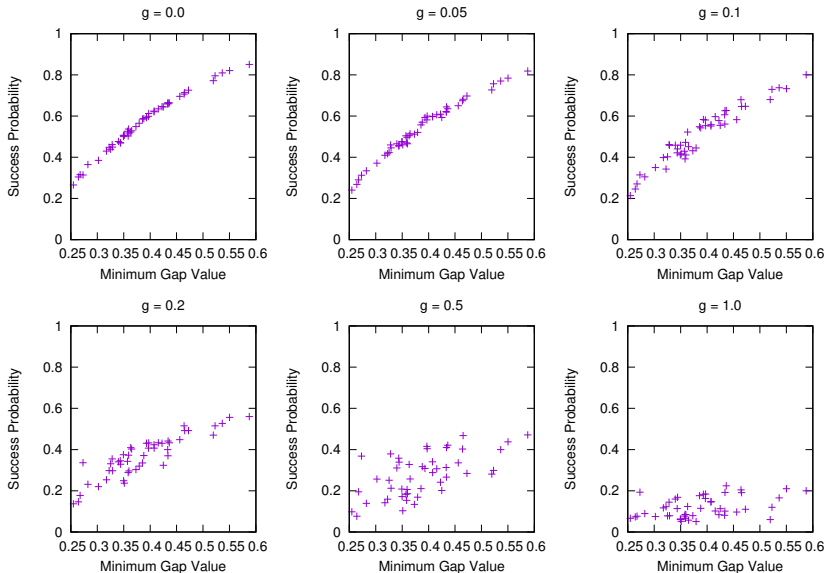
# Effect of Total Annealing Time at different Temperature

Temperature = 1000

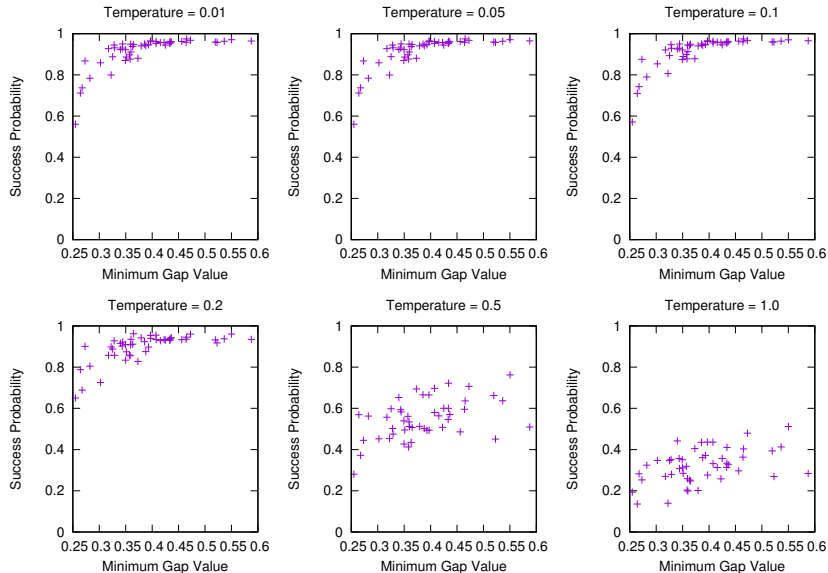


\* Amin, M. H. (2015). Searching for quantum speedup in quasistatic quantum annealers. Physical Review A - Atomic, Molecular, and Optical Physics, 92(5), 1–5. <https://doi.org/10.1103/PhysRevA.92.052323>

# Effect of Minimum Gap under different Coupling Strength



# Effect of Minimum Gap under different Temperature



# Conclusion

- ▶ The quantum annealing does provide a different approach to solve 2-SAT problem.
- ▶ A quantum annealing process at finite temperature will go through a coherent state, non-equilibrium state, and finally a quasistatic state as mentioned in a previous paper.
- ▶ The quantum annealing process can be influenced not only by the total annealing time, minimum gap, but also the temperature.
- ▶ The simulation done in this study can be tested on a D-Wave annealer and provide explanation for some behaviour of it.





## Appendix

## Appendix: Computational Basis

- ▶  $\Psi$  is defined as a direct product state of the  $N$  single spin states in  $z$ -basis.
- ▶ Each single spin has two possible states,  $|\uparrow\rangle$  or  $|\downarrow\rangle$ , which, for convenience, are corresponded to  $|0\rangle$  or  $|1\rangle$ . The relation is defined as

$$|\uparrow\rangle \equiv |0\rangle, |\downarrow\rangle \equiv |1\rangle$$

- ▶ Thus, the single spin state can be written as a linear superposition of these two basis state,

$$|\psi\rangle = a(0)|0\rangle + a(1)|1\rangle,$$

where  $a(0)$  and  $a(1)$  are the coefficient of the amplitude of each state.

- ▶ Furthermore, a  $N$ -spin system is made up of  $2^N$  state vectors and it can be written as

$$|\Psi\rangle = a(00\dots 0)|00\dots 0\rangle + a(00\dots 1)|00\dots 1\rangle \cdots + a(11\dots 1)|11\dots 1\rangle$$

## Appendix: The Full Diagonalisation method

$$\Psi(t + \tau) = \exp\left(-iH\left(\frac{t + \tau}{2}\right)\tau\right)\Psi(t).$$

- ▶ By diagonalisation, the time evolution can be calculated as

$$U(\tau) = \exp(-i\tau H) = V \exp(-i\tau \Lambda) V^\dagger.$$

- ▶ The main limitation comes from the size of the quantum system.
- ▶ This approach serves mostly as a tool to validate the correctness of other algorithm when solving a time-dependent Schrödinger equation.

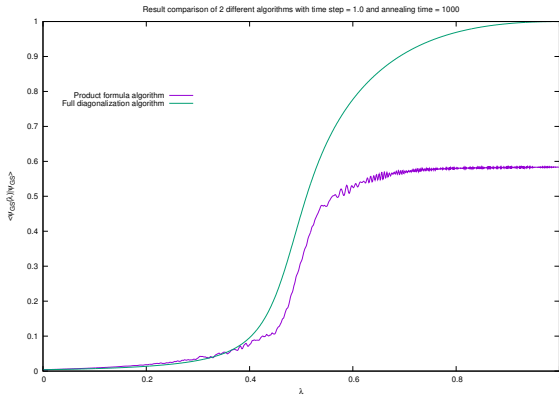
## Appendix: The Suzuki-Trotter Product Formula Approach

- ▶ The Suzuki-Trotter product formula approach can handle a larger quantum system than the full diagonalisation method does.
- ▶ Suzuki-Trotter product formula approximate a unitary matrix exponentials by decomposing the matrix properly, that is

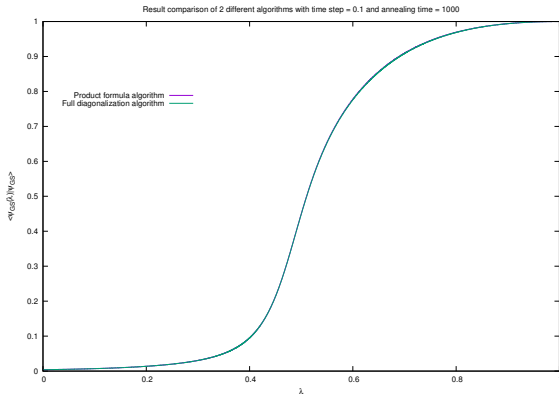
$$\begin{aligned}U(t) &= \exp(-itH) \\&= \exp(-it(H_1 + H_2 + \cdots + H_K)) \\&= \lim_{m \rightarrow \infty} \left( \prod_{k=1}^K \exp(-itH_k/m) \right)^m\end{aligned}$$

- ▶ The crucial step of this approach is to choose  $H_k$  properly in a way that it is easy enough to calculate there matrix exponential efficiently.

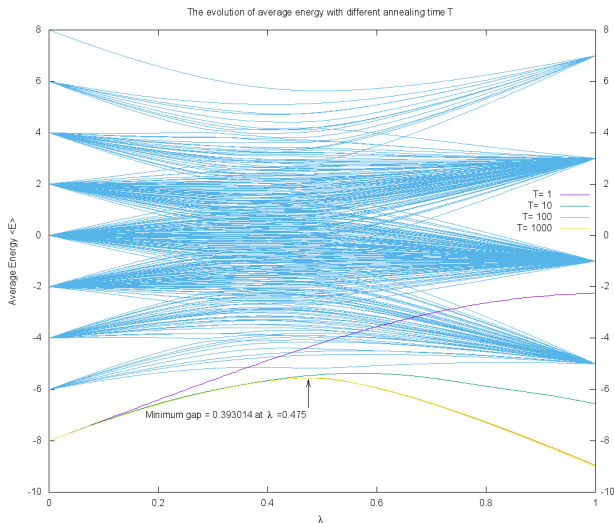
# Appendix: The Suzuki-Trotter Product Formula Approach and The Full Diagonalisation Method



# Appendix: The Suzuki-Trotter Product Formula Approach and the Full Diagonalisation Method



# Appendix: The Energy Spectrum and the Effect of Minimum Gap



## Appendix: Canonical Ensemble

An observable  $A$  can be calculated by going through all energy eigenstate of the heat bath as following:

$$|\Psi(t)\rangle = e^{-iHt} |E_B\rangle |S'\rangle$$

$$\langle A(t) \rangle = \text{Tr} A(t) \rho_B \rho_S = \sum_B \frac{e^{\beta E_B}}{Z} \langle \Psi(t) | A | \Psi(t) \rangle$$



## Appendix: The Random Sampling Method

Based on the hypothesis that with random sampling one can approximate the solution of a time-dependent Schrödinger Equation by solving a sample of randomly chosen initial state.

$$\text{Tr}A = \sum_{n=1}^D \langle \Psi_n | A | \Psi_n \rangle$$

Then a random vector  $|\phi\rangle$  can be constructed by choosing  $D$  complex random numbers with which mean is 0.

$$|\phi\rangle = \sum_{n=1}^D c_n |\Psi_n\rangle, \text{ with } c_n \equiv f_n + ig_n$$

## Appendix: The Random Sampling Method

It follows that

$$\langle \phi | A | \phi \rangle = \sum_{m,n=1}^D c_m^* c_n \langle \psi_m | A | \psi_n \rangle$$

It is possible to increase the accuracy by generate several samplings. If  $S$  realisations are sampled and then averaged out, it yields

$$\frac{1}{S} \sum_{p=1}^S \langle \phi_p | A | \phi_p \rangle = \frac{1}{S} \sum_{p=1}^S \sum_{m,n=1}^D c_{m,p}^* c_{n,p} \langle \psi_{m,p} | A | \psi_{n,p} \rangle$$

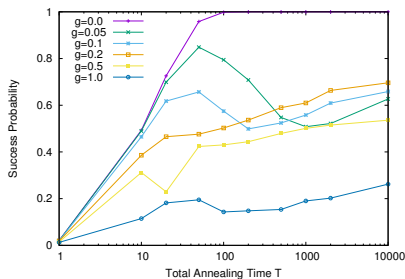
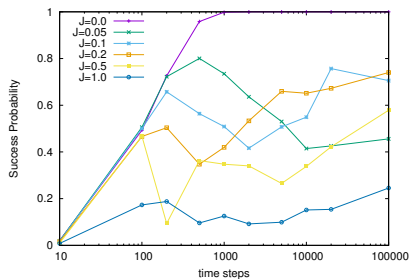
## Appendix: The Random Sampling Method

If there is no correlation between the random numbers in different realisation, and the random number  $f_n$  and  $g_n$  are drawn from an even and symmetric probability distribution, the argument can further be made as

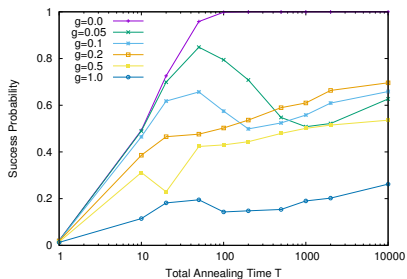
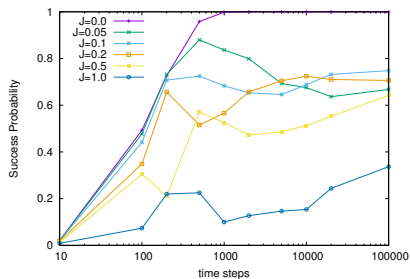
$$\begin{aligned}\lim_{S \rightarrow \infty} \frac{1}{S} \sum_{p=1}^S \langle \phi_p | A | \phi_p \rangle &= E(|c|^2) \sum_{n=1}^D \langle \psi_n | A | \psi_n \rangle \\ &= E(|c|^2) \text{Tr} A,\end{aligned}$$

where  $E(\cdot)$  is the expectation value based on the probability distribution used to draw  $c_n$ .

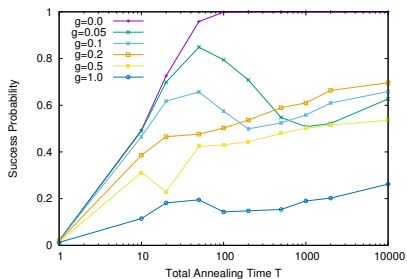
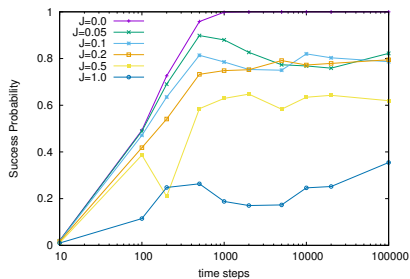
# Appendix: Results of the Random Sampling Method



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