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

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Table of Contents

Table of Contents

Introdution 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

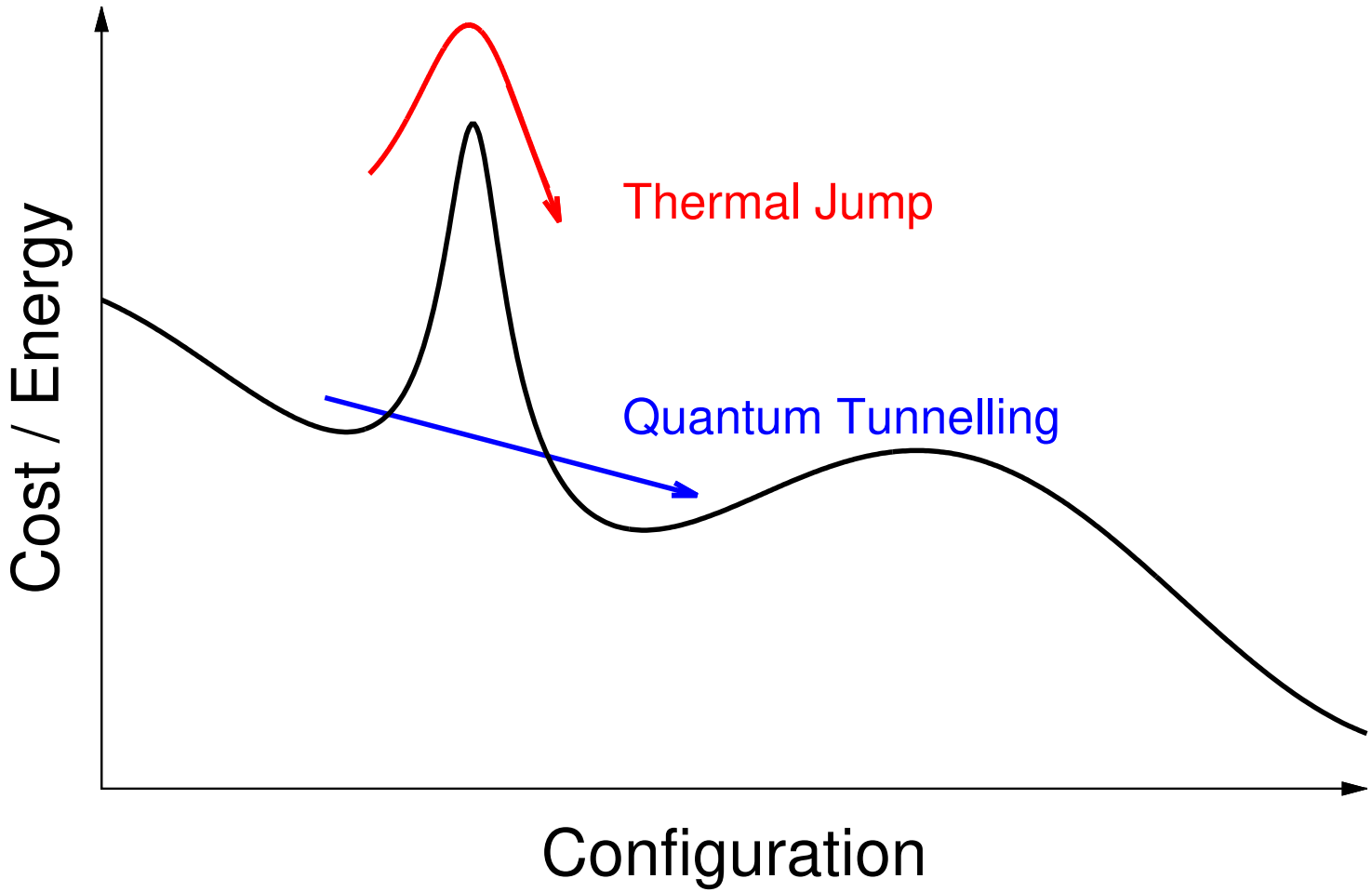
$$H(t) = (1 - \frac{t}{T})H_{init} + (\frac{t}{T})H_{problem}$$

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

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

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 an adiabatic transition, $P_{adiabatic}$, can be described by

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

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

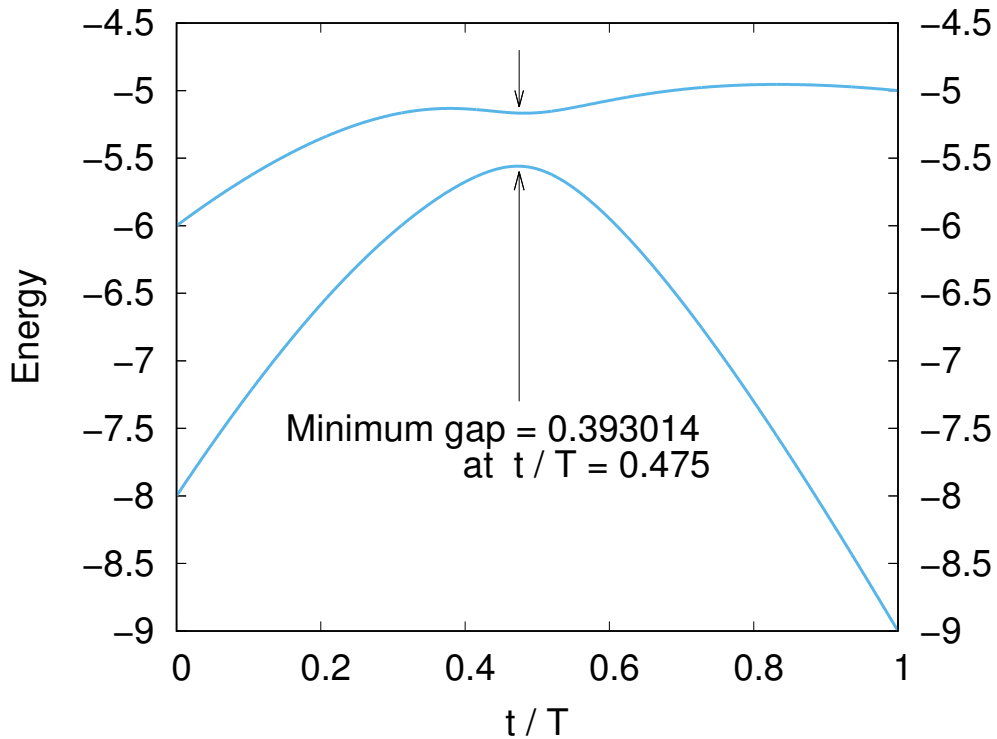


Table of Contents

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
σ_1	1	1	-1	-1
σ_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
σ_3	1	1	-1	-1
σ_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

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

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 $H_{problem}$, if the total annealing time T is long enough.

Table of Contents

Time-Dependent Schrödinger Equation

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

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

- The solution of this is

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

where τ 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

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

The Suzuki-Trotter Product Formula Approach

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

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

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

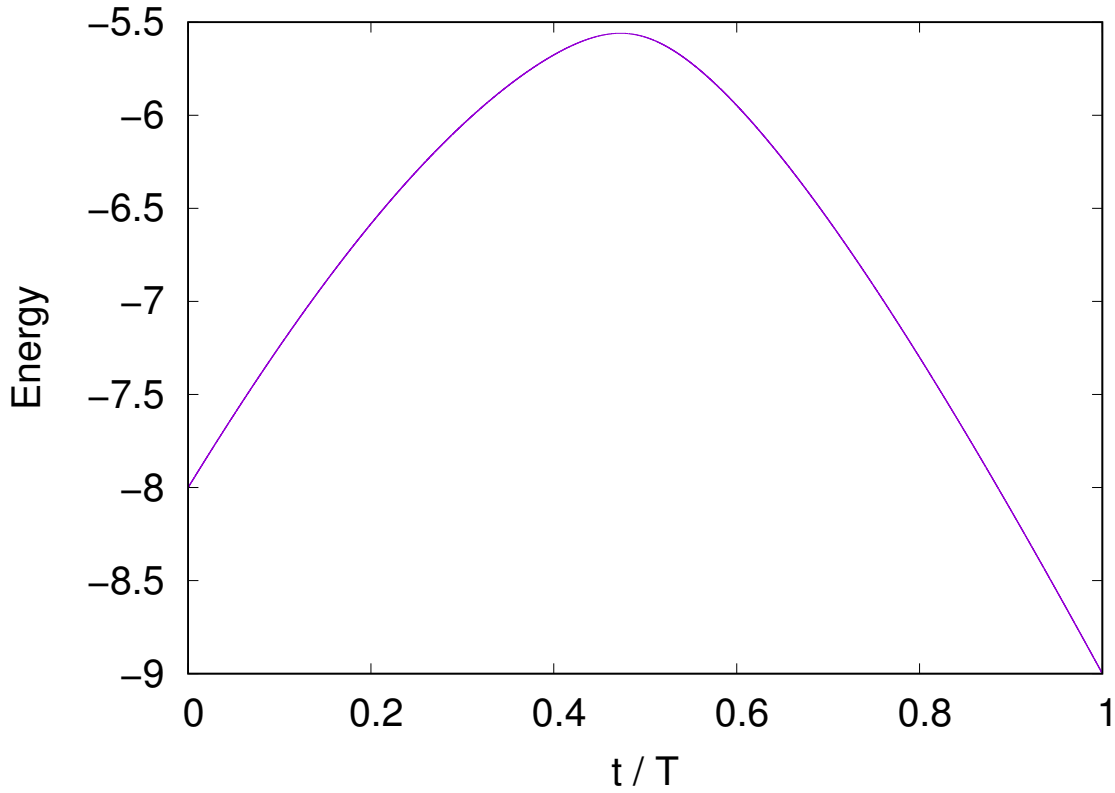


Figure: A result with total annealing time = 1000

Simulation Result: Success Probability

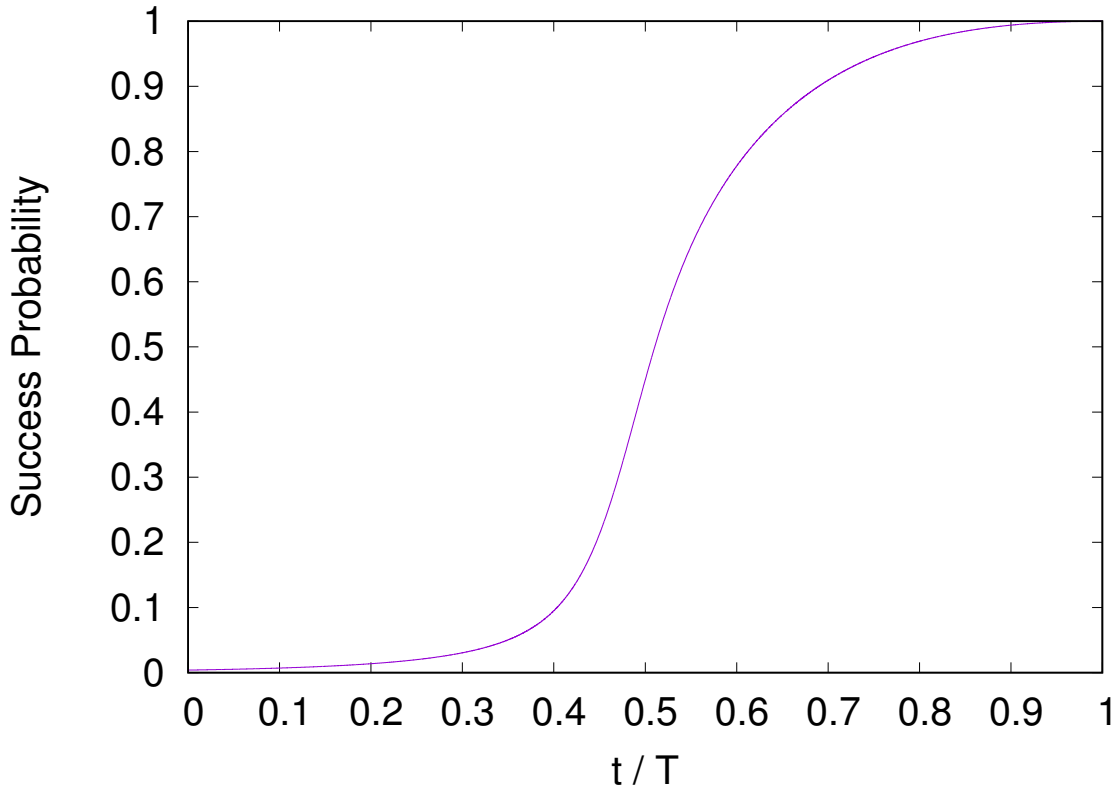
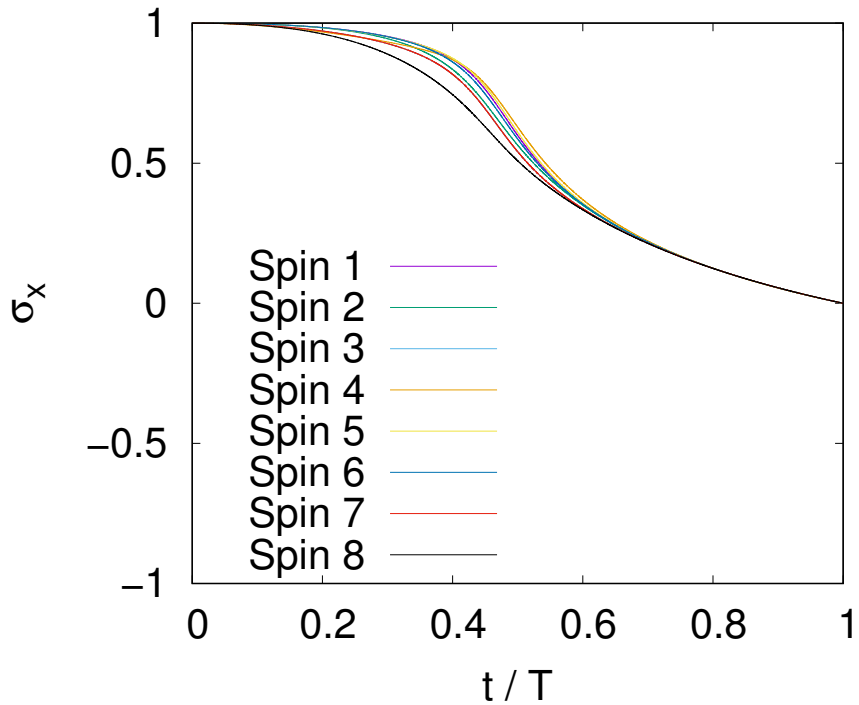
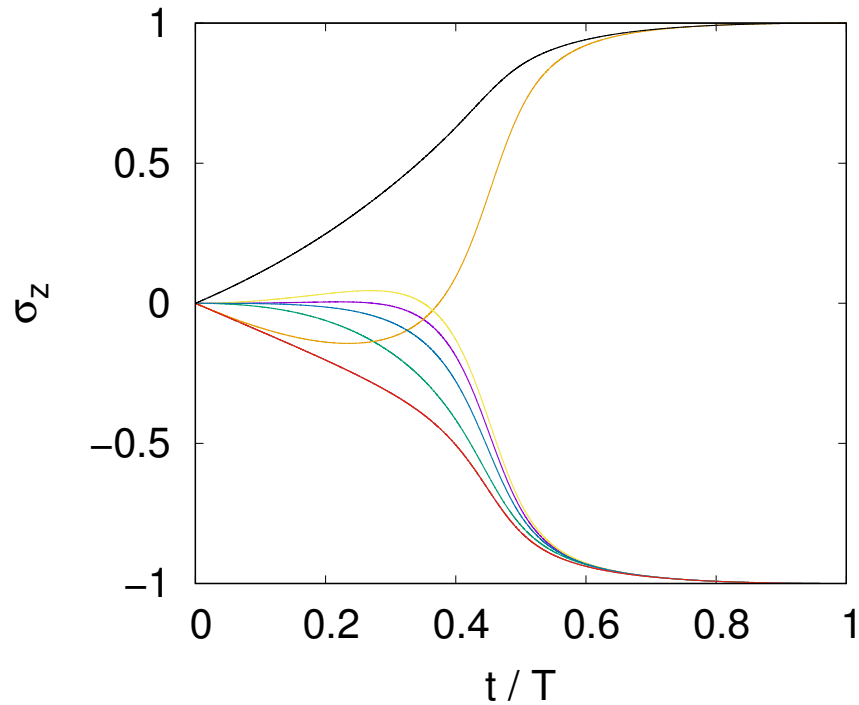


Figure: A result with total annealing time = 1000

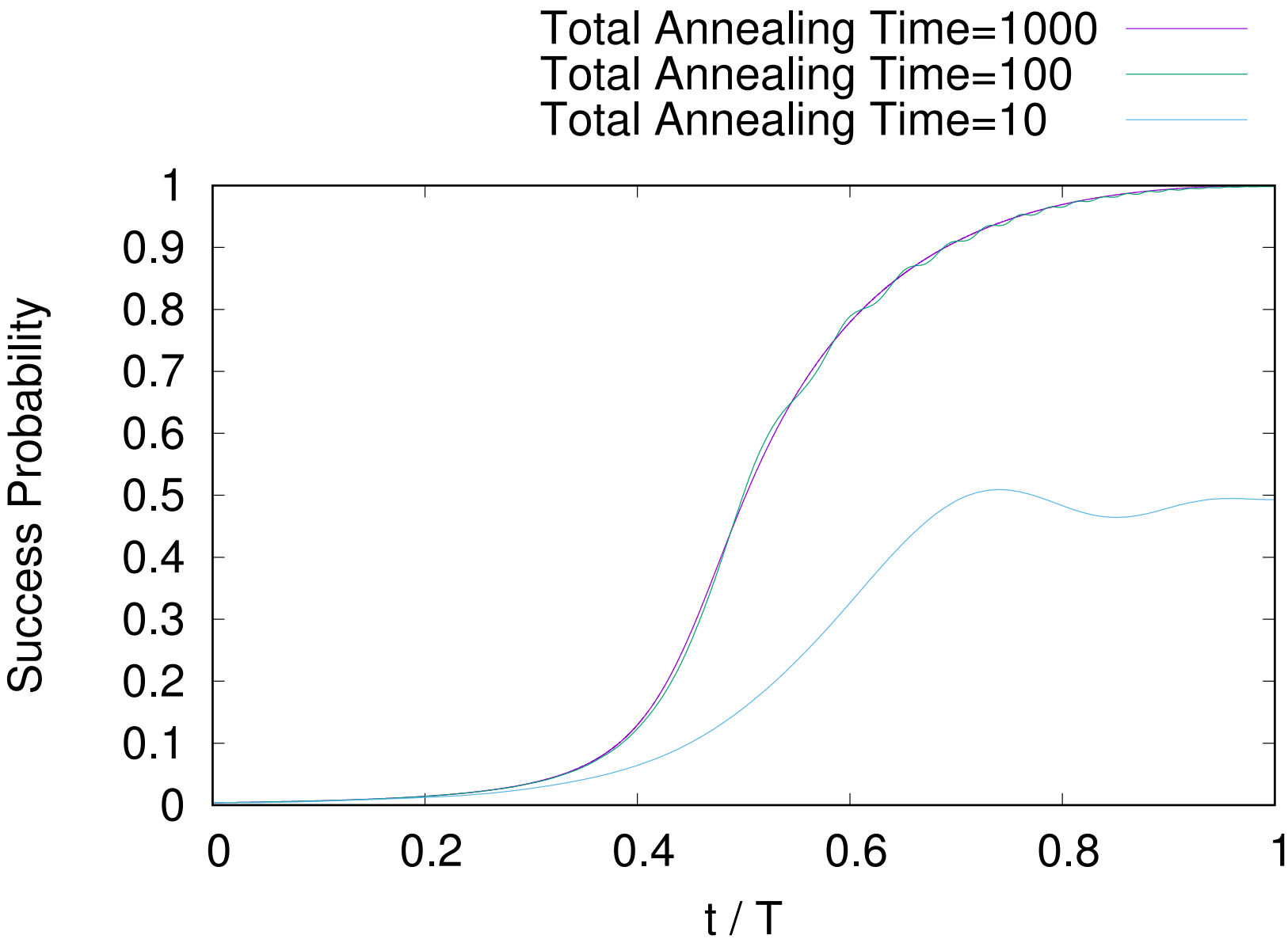
Simulation Result: Spin Value

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

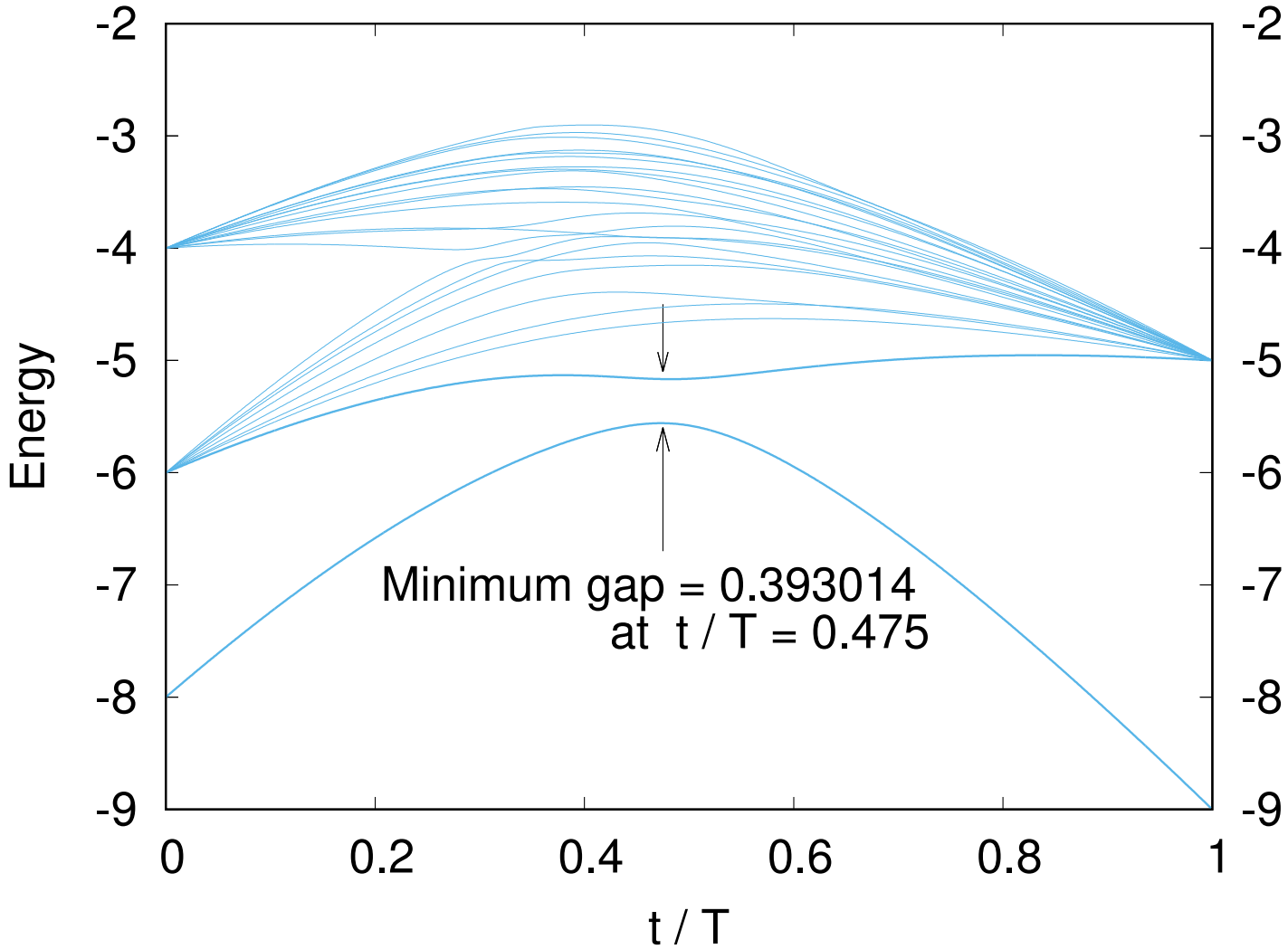




Effect of Total Annealing Time



The Energy Spectrum and the Minimum Gap



Effect of Minimum Gap

$$P_{adiabatic}(T) = 1 - P_{diabatic}(T)$$
$$P_{diabatic}(T) = \exp\left(-c \cdot \Delta_{min}^2\right)$$

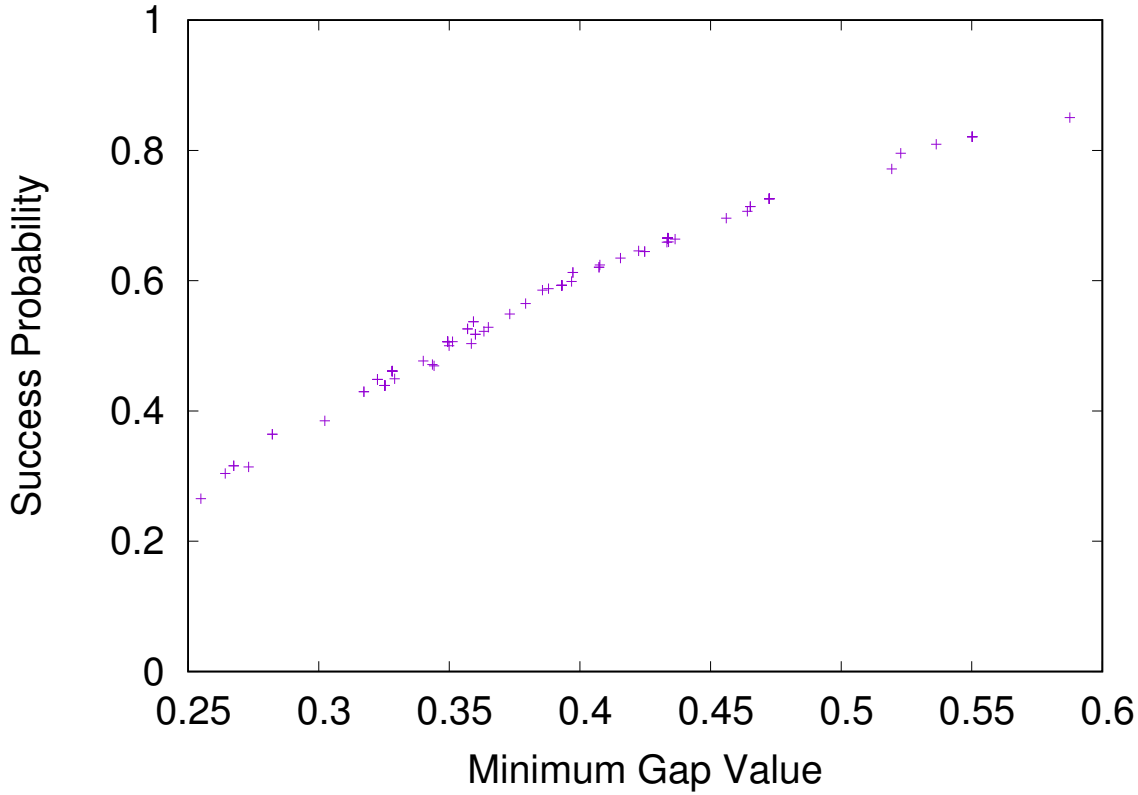


Figure: A plot with 100 different 2-SAT problems.

Table of Contents

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

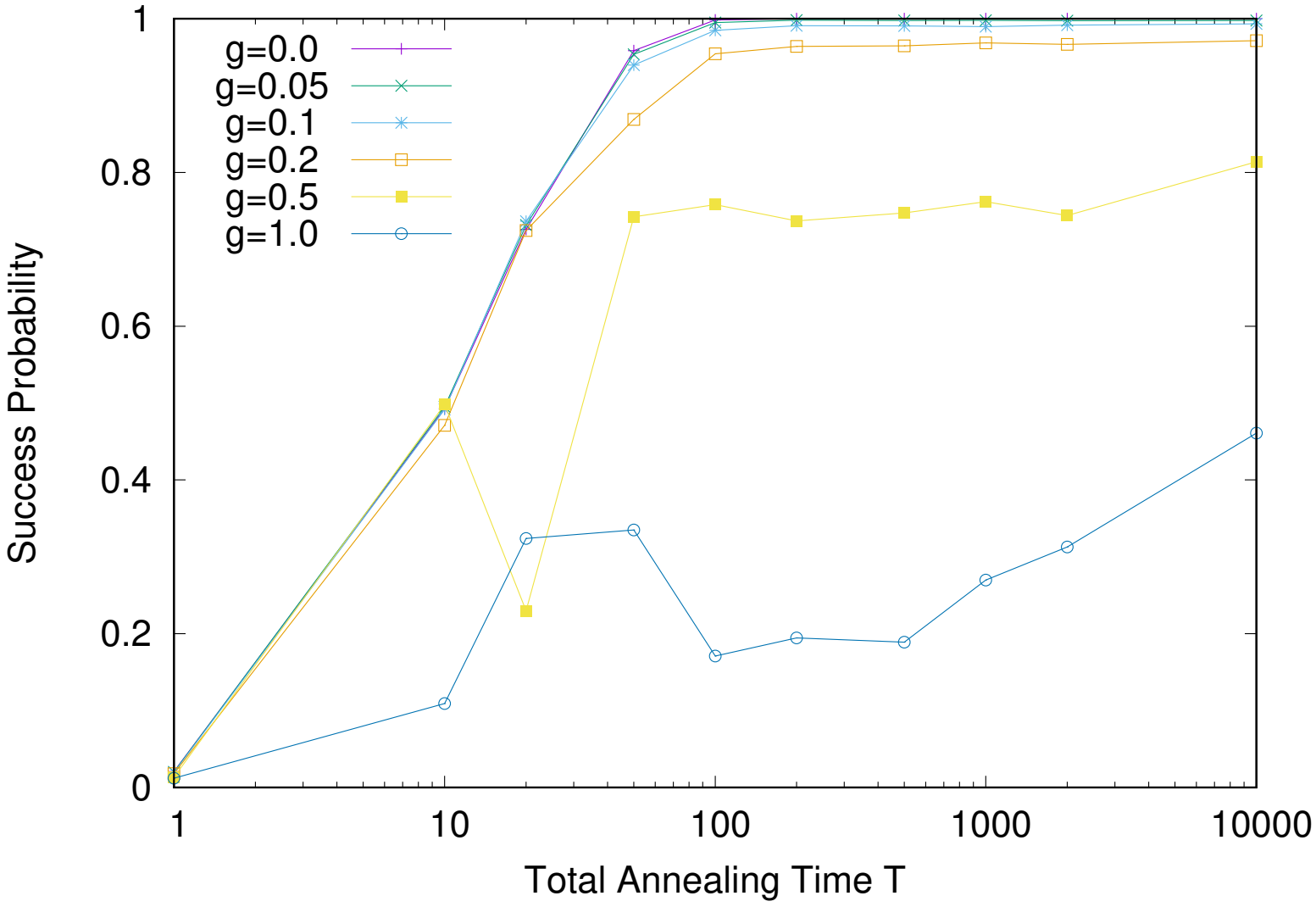


Figure: A result at Temperature = 0.02

Effect of Total Annealing Time at different Temperature

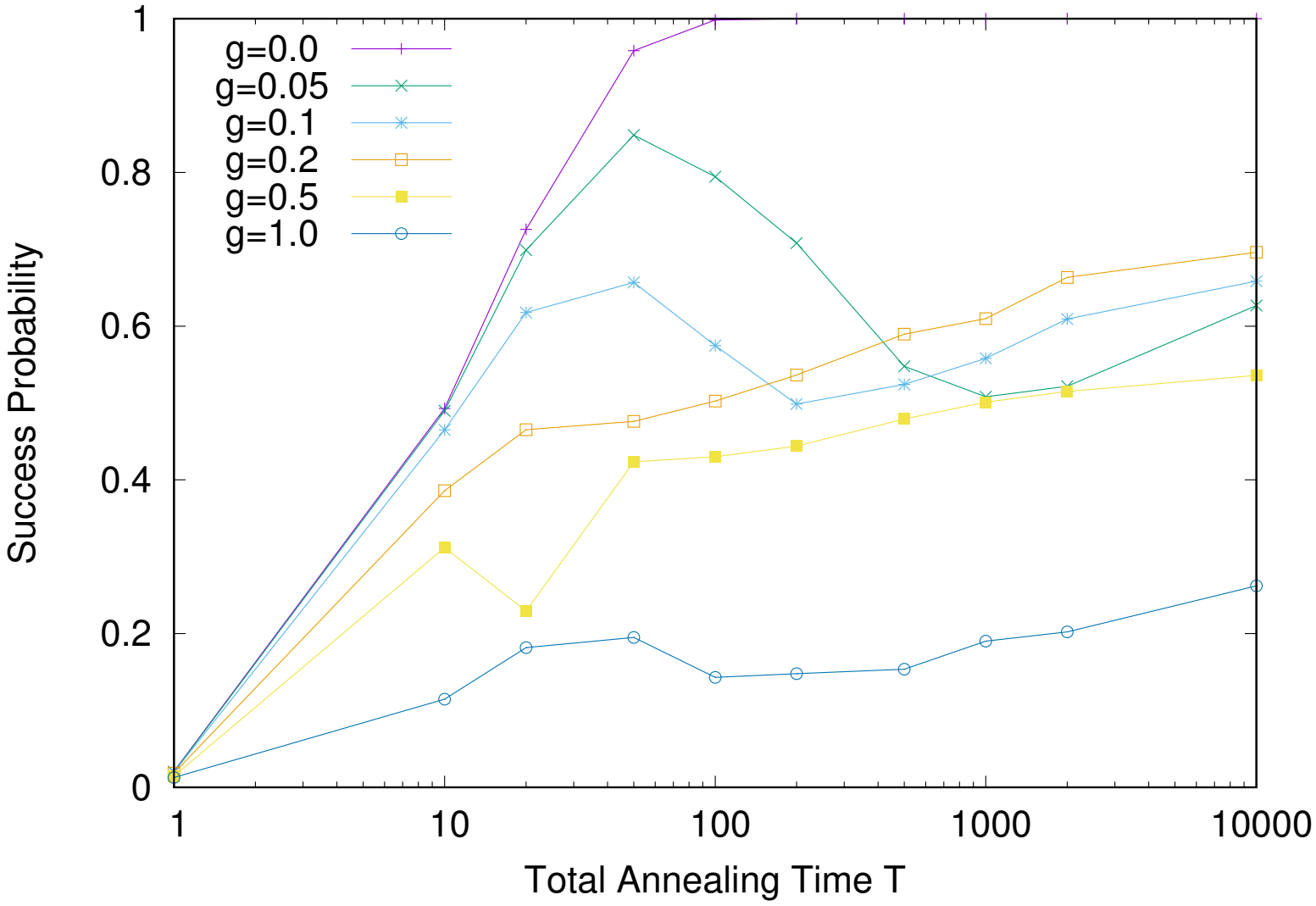


Figure: A result at Temperature = 1

Effect of Total Annealing Time at different Temperature

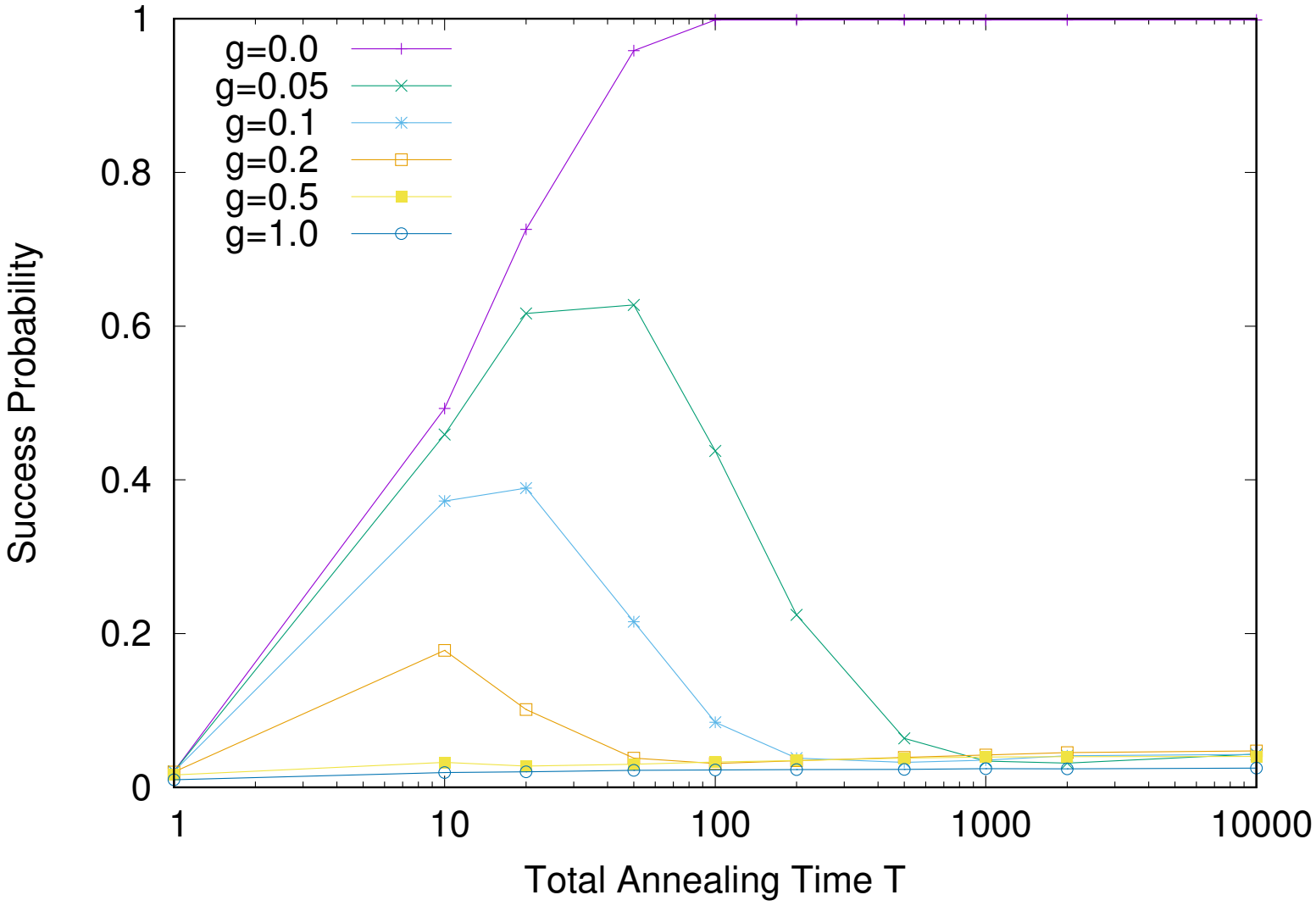
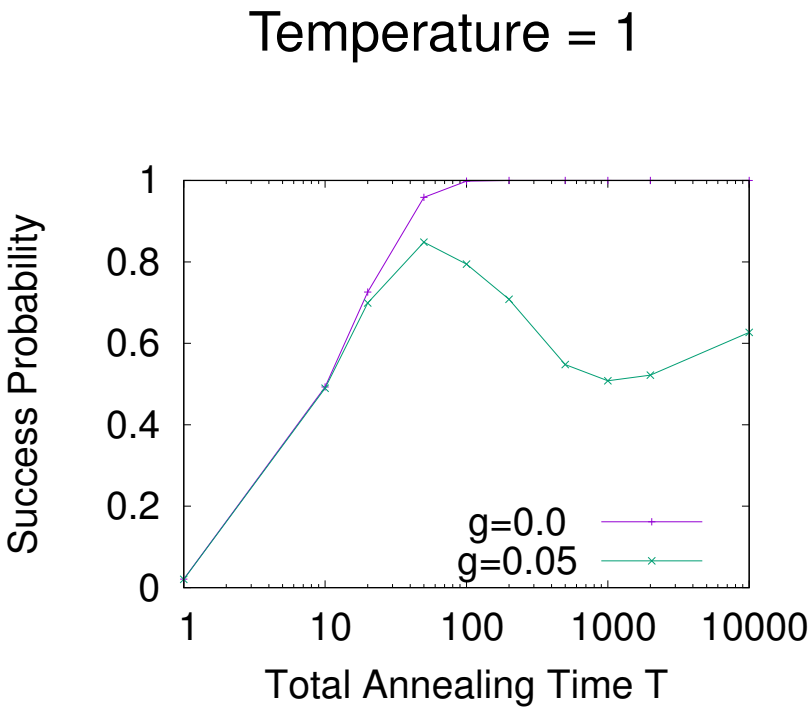
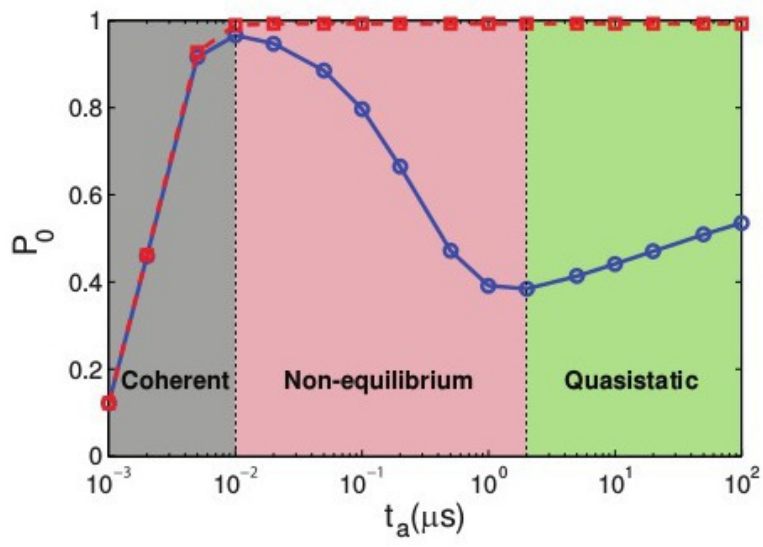


Figure: A result at Temperature = 1000

Effect of Total Annealing Time at different Temperature





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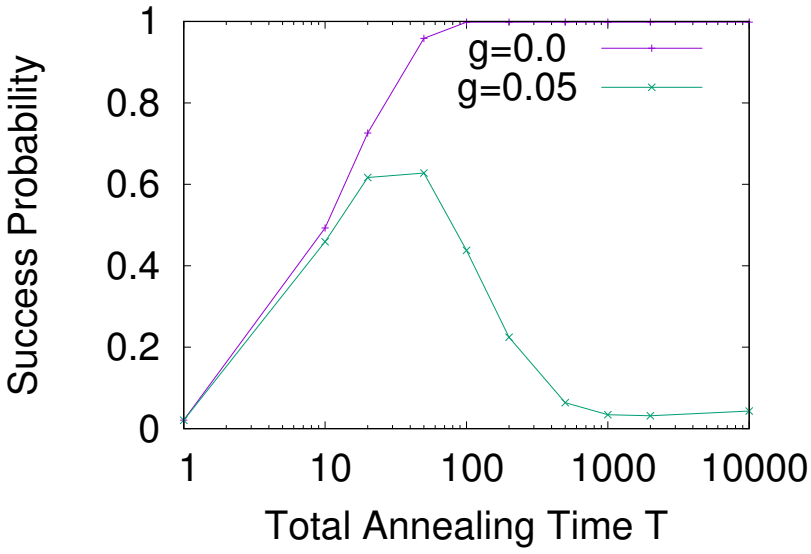
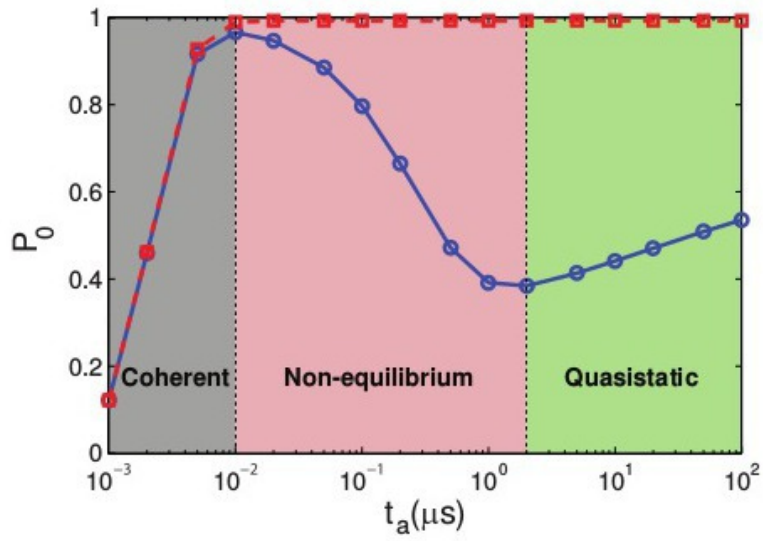
*Amin, M. H. (2015). Searching for quantum speedup in quasistatic quantum annealers. Physical Review A - Atomic, Molecular, and Optical Physics, 92(5), 1–5. https://doi.org/10.1103/PhysRevA.92.052323

Effect of Total Annealing Time at different Temperature

Temperature = 1000





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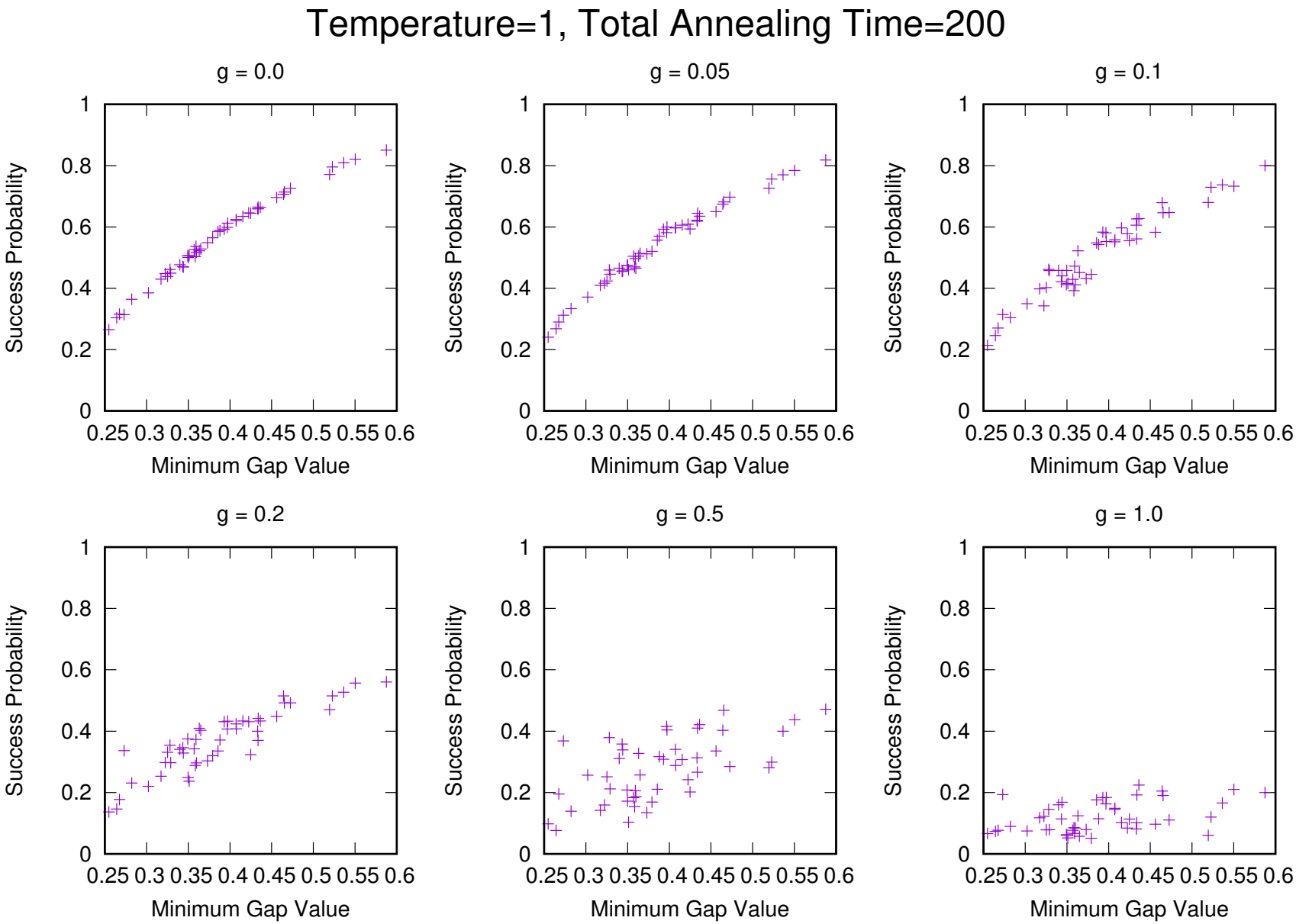
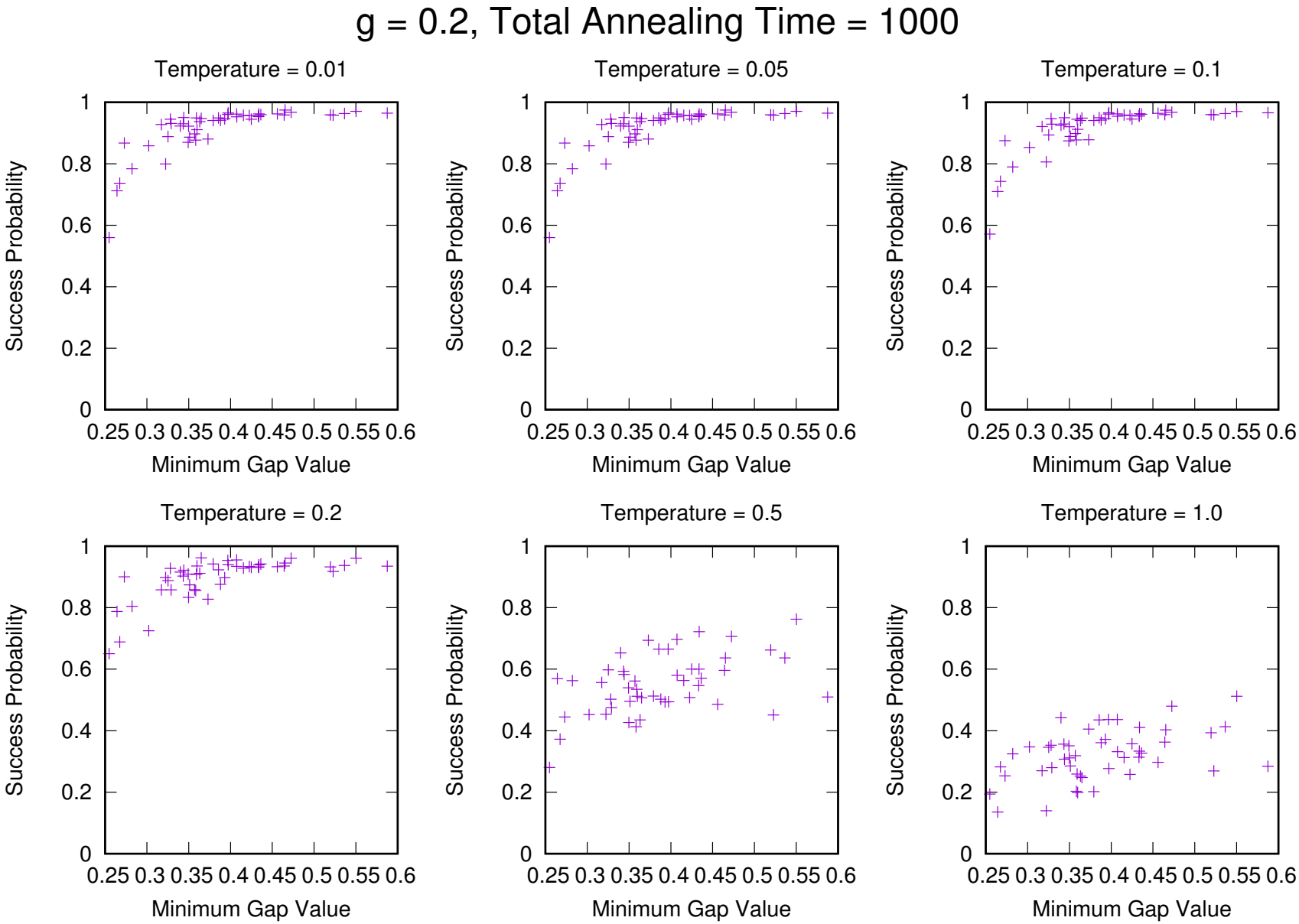
Effect of Minimum Gap under different Coupling Strength



Effect of Minimum Gap under different Temperature



Conclusion

- The quantum annealing does provide a different approach to solve the 2-SAT problem.
- A quantum annealing process at finite temperature will go through a coherent state, non-equlibrium 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, the minimum gap value, but also the temperature.
- The simulation done in this study can be tested on a D-Wave quantum annealer.

Appendix

Appendix: Computational Basis

- Ψ 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 theses 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

$$|\Psi\rangle = a(00\ldots0)\,|00\ldots0\rangle + a(00\ldots1)\,|00\ldots1\rangle \cdots + a(11\ldots1)\,|11\ldots1\rangle$$

Appendix: The Full Diagonalisation method

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

- By diagonalisation, the time evolution can be calculated as

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

- 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.

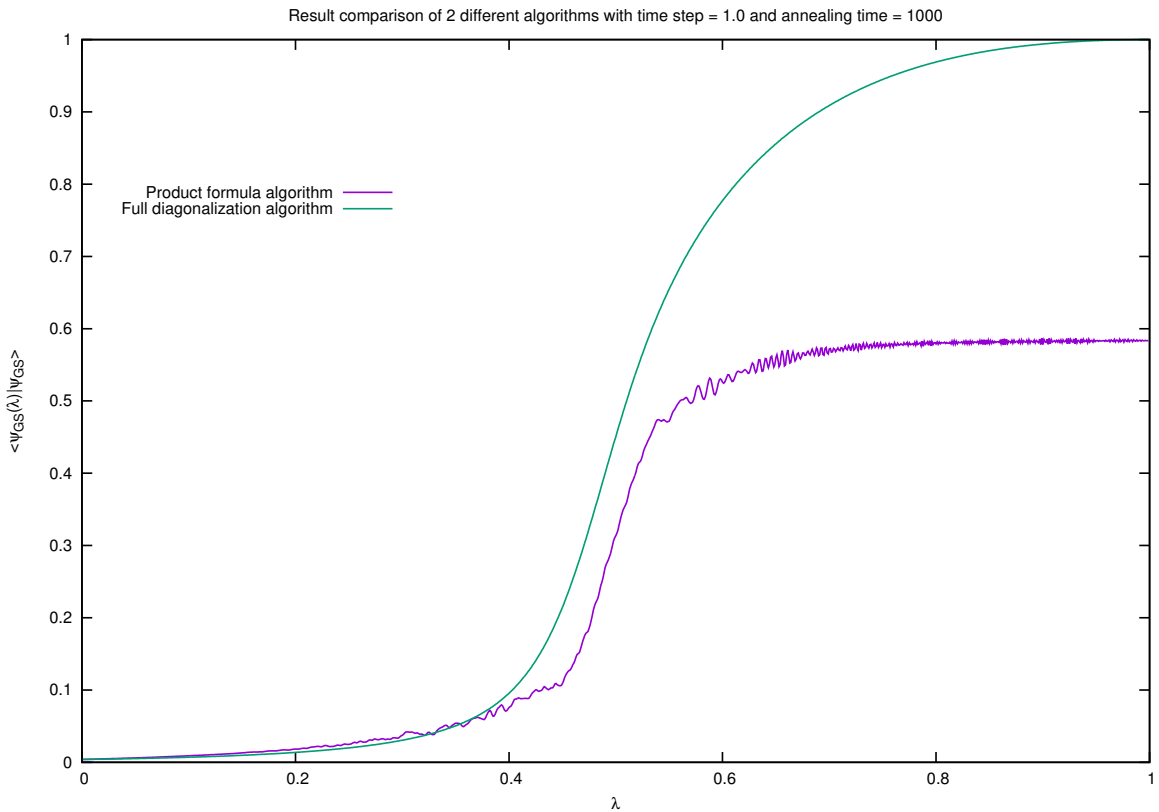
Appendix: The Suzuki-Trotter Product Formula Approach

- 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

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

- 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 Diaganolisation Method



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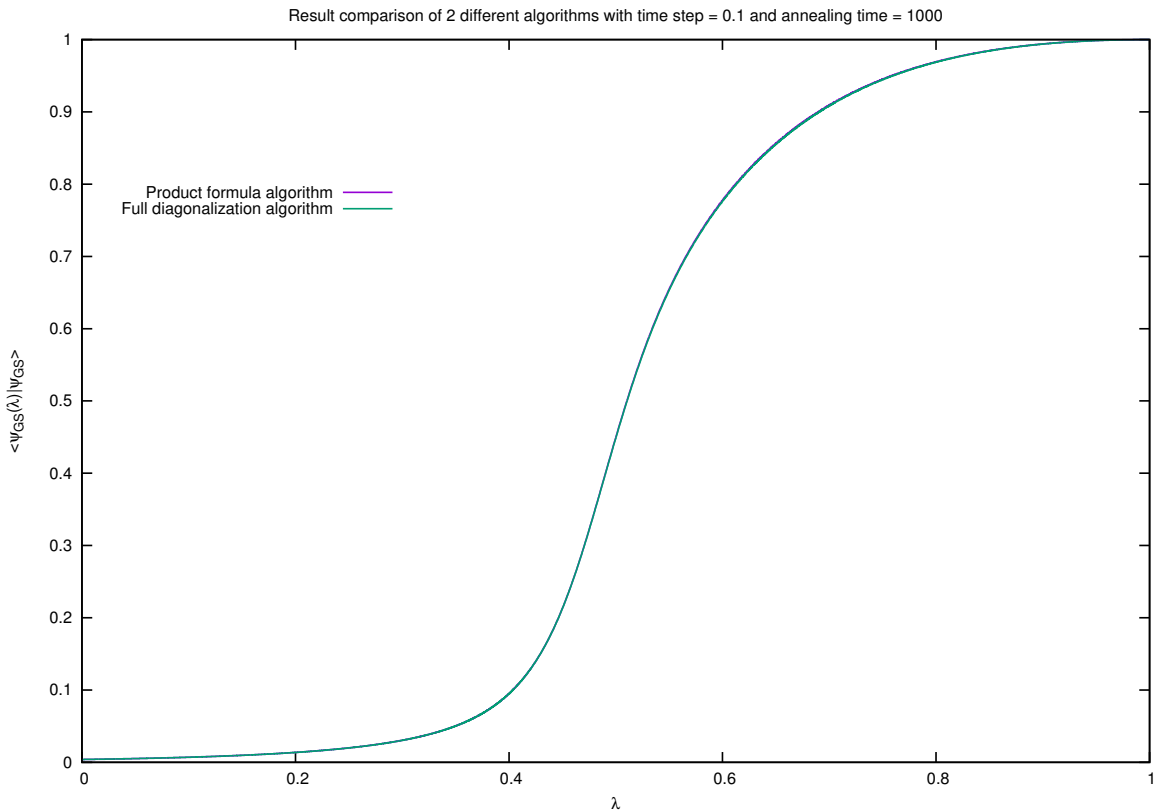
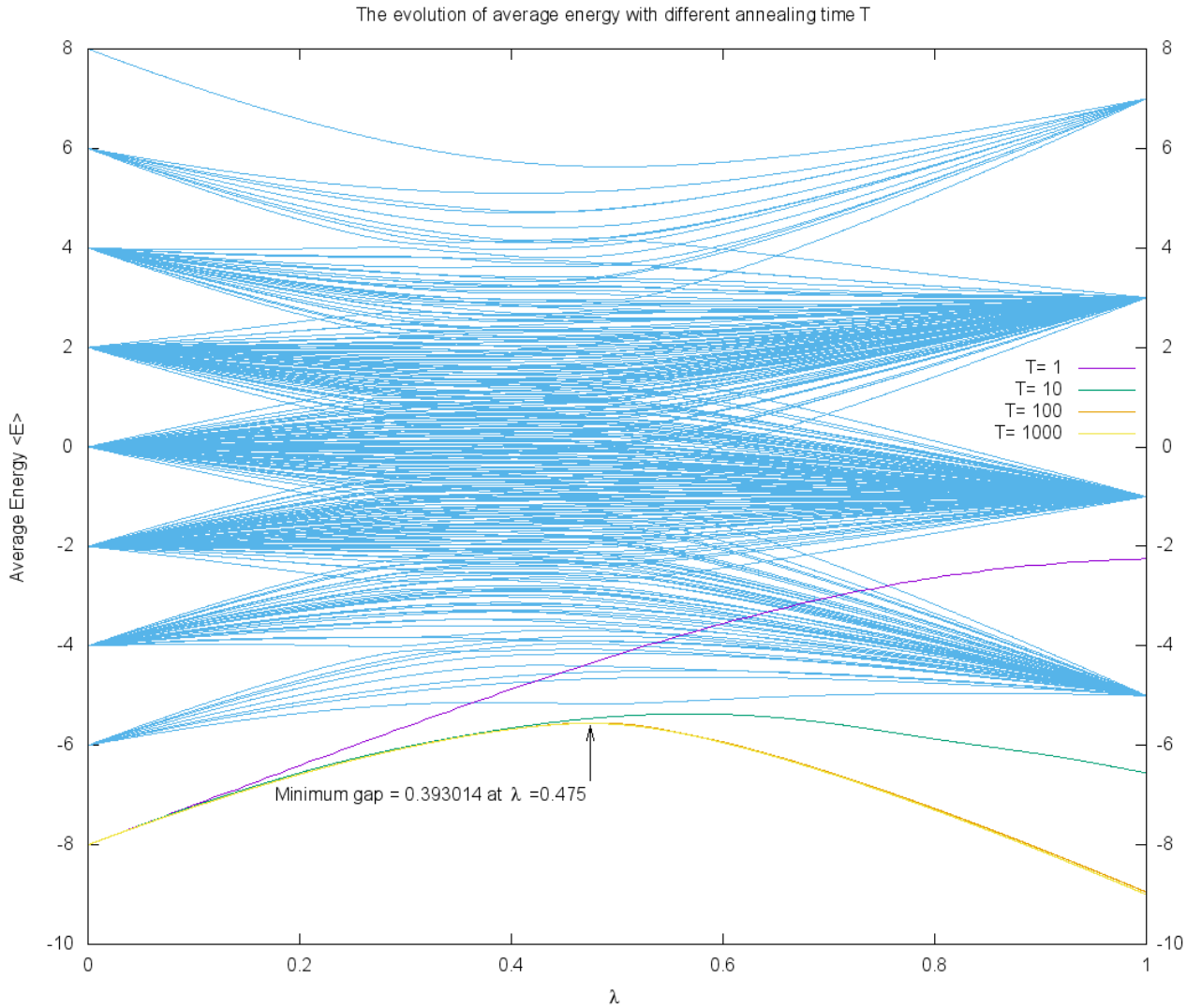


Appendix: The Energy Spectrum and the Effect of Minimum Gap



Appendix: Canonical Ensemble

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

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

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

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.

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

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

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

Appendix: The Random Sampling Method

It follows that

$$\langle \phi | A | \phi \rangle = \sum_{m,n=1}^{D} c_m^\star c_n \langle \Psi_m | A | \Psi_n \rangle$$

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

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

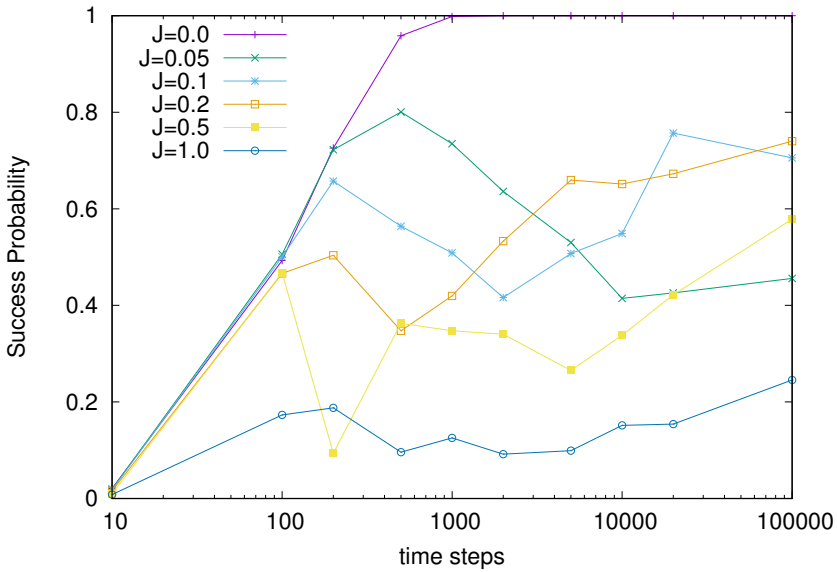
Appendix: The Random Sampling Method

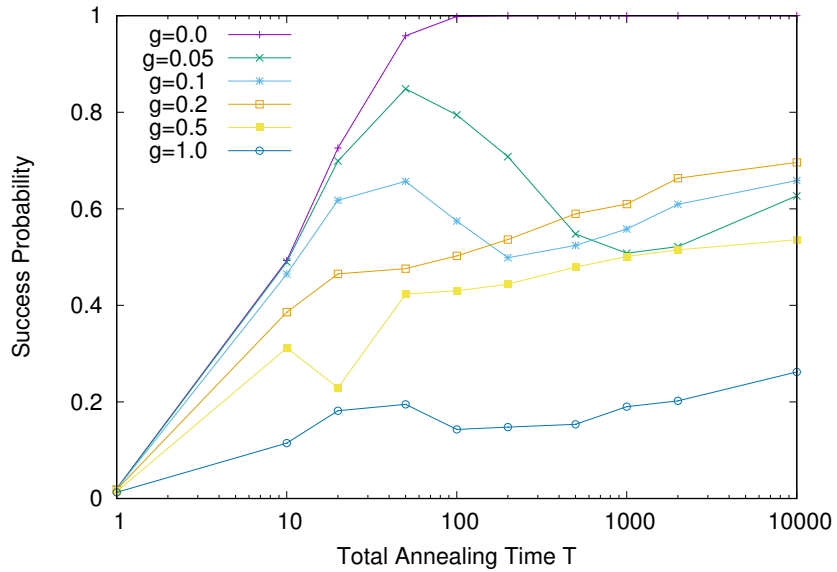
If there is no correlation between the random numbers in different realisation, and the random number f_n and g_n are drawn from an even and symmetric probability distribution, the argument can further be made as

$$\lim_{S\to\infty} \frac{1}{S} \sum_{p=1}^{S} \langle \phi_p | A | \phi_p \rangle = E(|c|^2) \sum_{n=1}^{D} \langle \Psi_n | A | \Psi_n \rangle$$
$$= E(|c|^2) TrA,$$

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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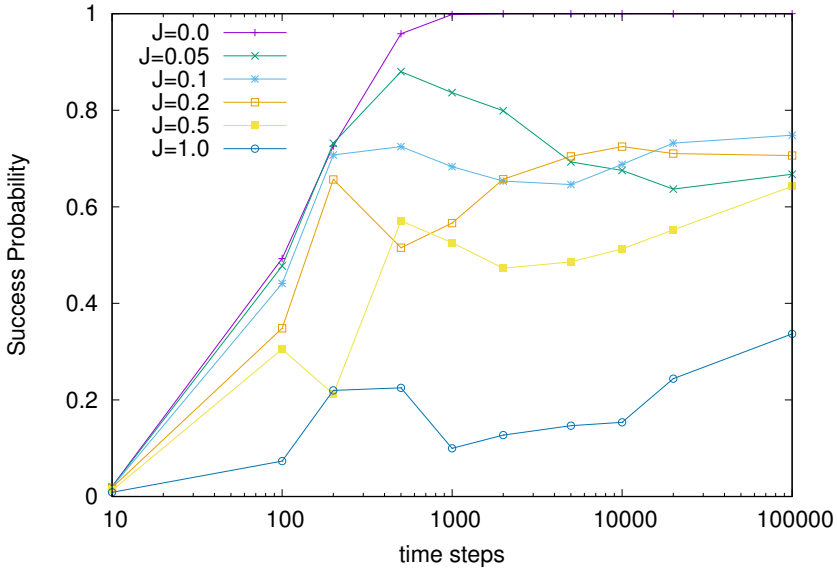

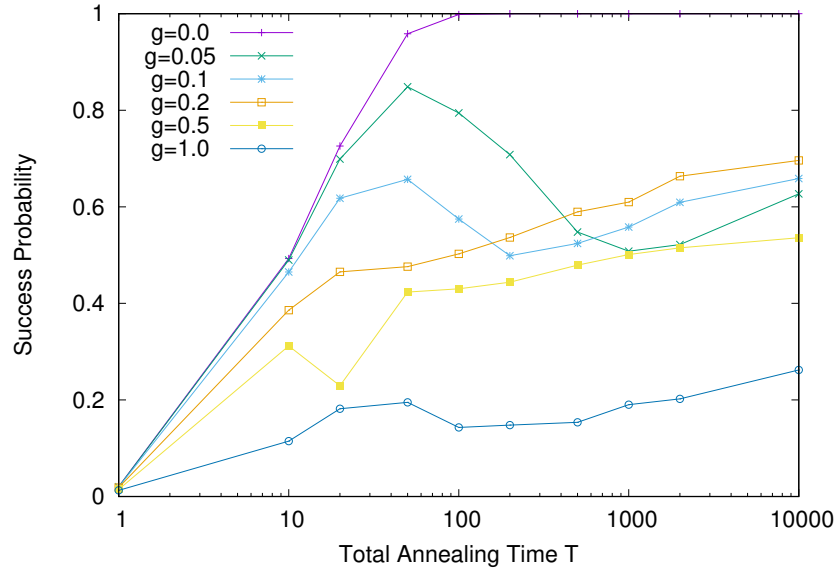

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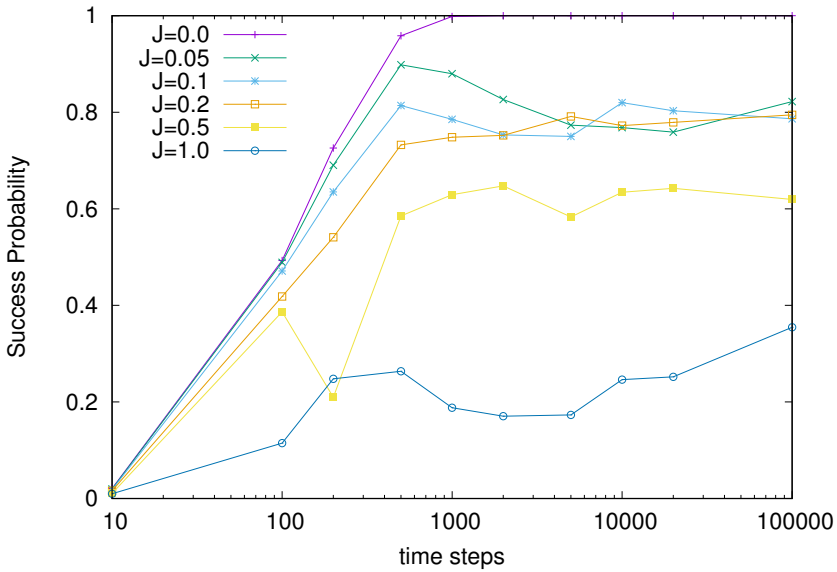

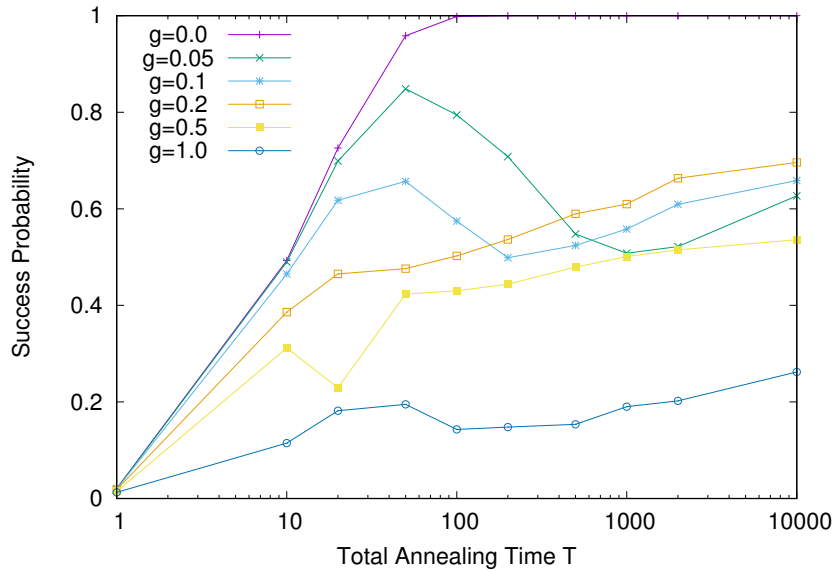

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