Non-Stoquastic Hamiltonians and Quantum Annealing of Ising Spin Glass

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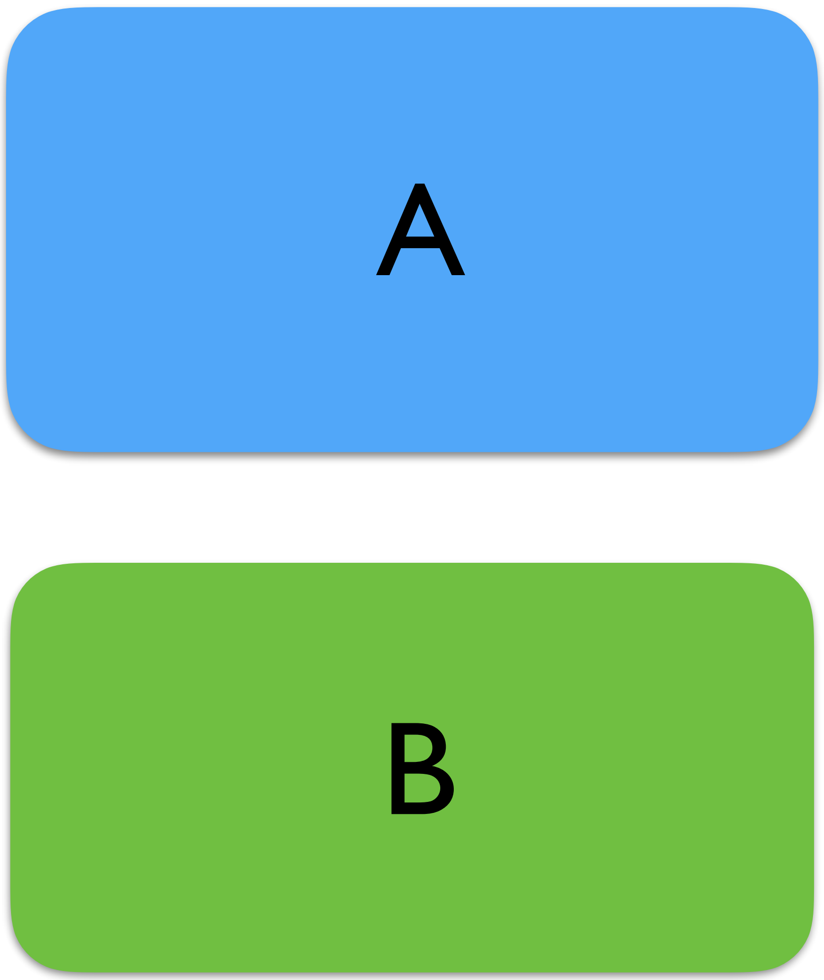
The Basic Idea



1. A and B are both ‘quantum optimization machines.’

2. A can be simulated efficiently using a classical computer.

3. B cannot be simulated efficiently using a classical computer.

Is there a difference between the performance of A and B in solving optimization problems?

Quantum Annealing

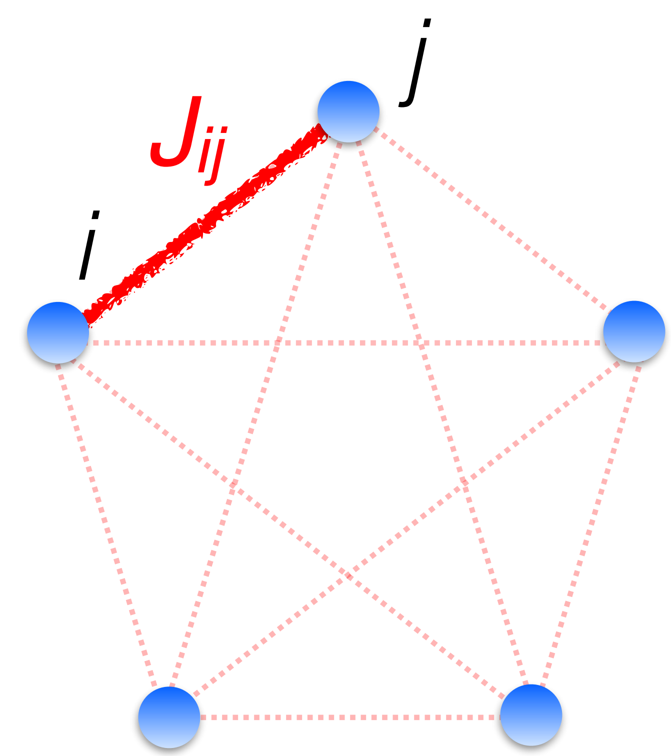
Kadowaki & Nishimori, '98
Farhi et al., '00

1. Encode a potentially hard optimization problem into parameters of a disordered Ising Hamiltonian: → **Problem Hamiltonian**

$$H_p = \sum_{i<j} J_{ij} Z_i Z_j + \sum_i h_i Z_i$$

Lucas, '14

Traveling Salesman Problem



Goal: Find the shortest path.

Quantum Annealing

Kadowaki & Nishimori, '98
Farhi et al., '00

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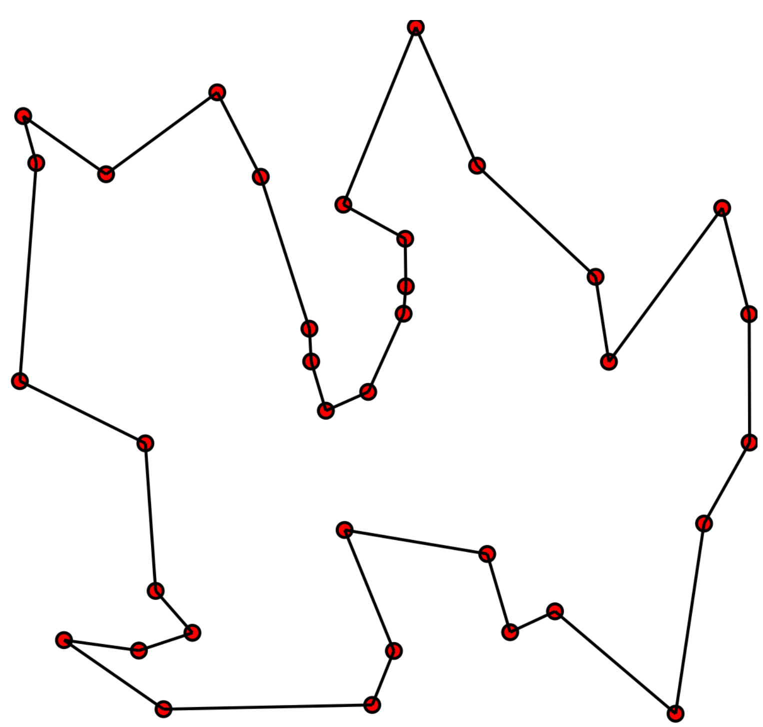
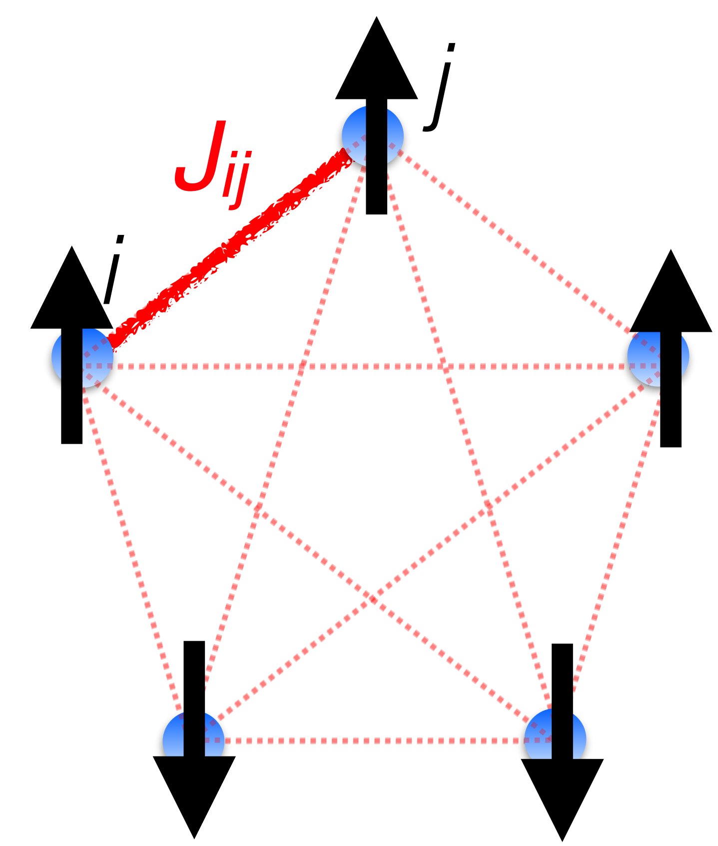
Lucas, '14

Traveling Salesman Problem





Solution: The shortest path

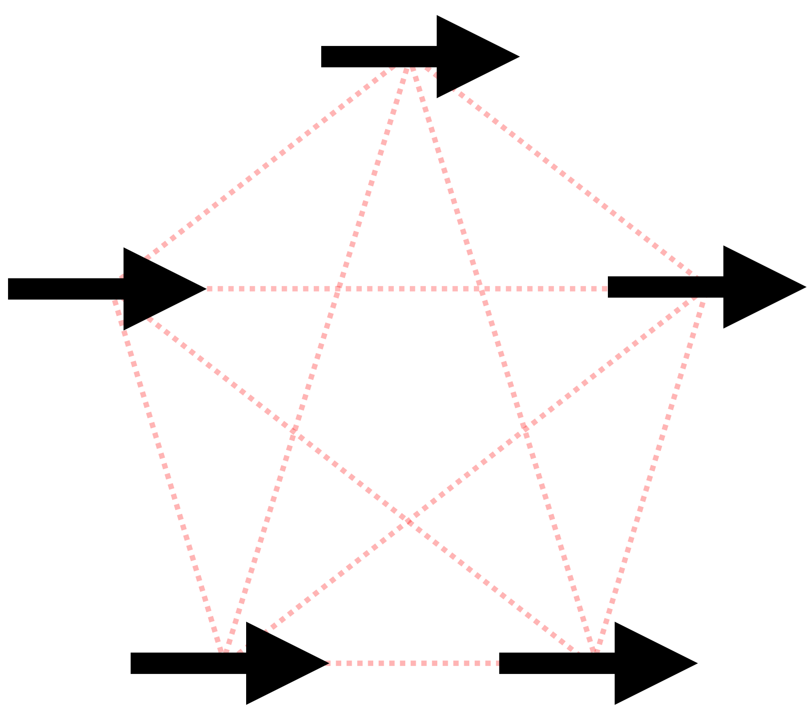
Groundstate configuration

Quantum Annealing

Kadowaki & Nishimori, '98
Farhi et al., '00

2. Initialize the system into the groundstate of an 'easy' Hamiltonian, traditionally a uniform transverse field: → **Initial/Driver Hamiltonian**

$$H_0 = \sum_i X_i$$



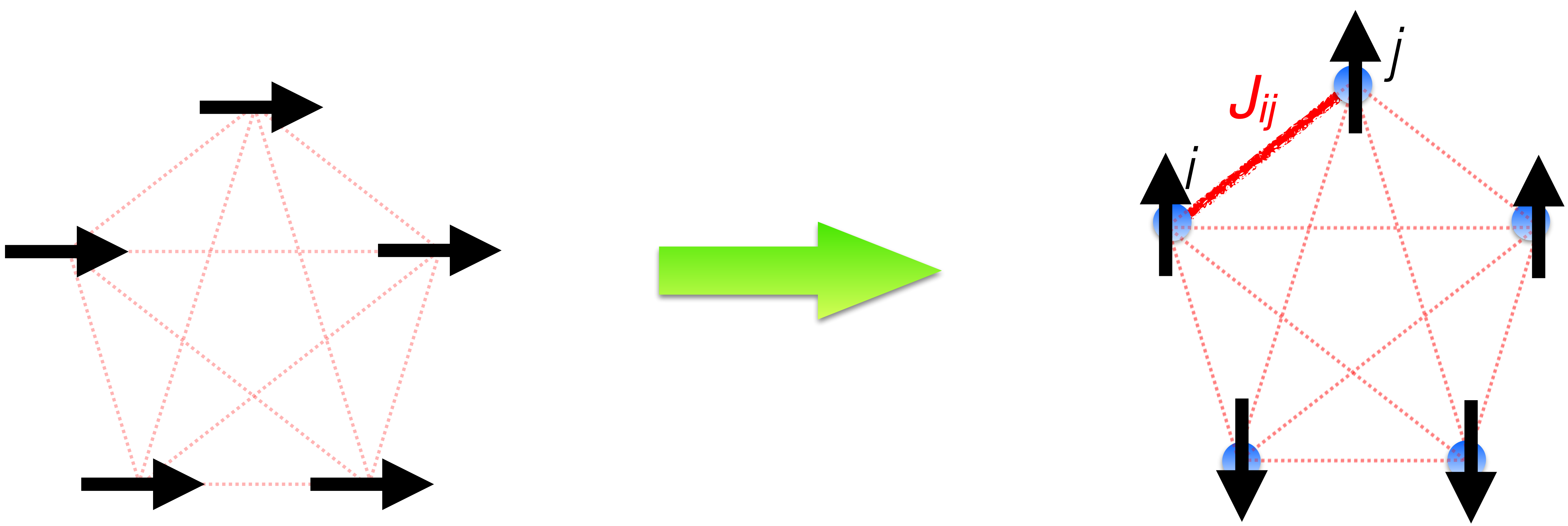
Quantum Annealing

Kadowaki & Nishimori, ‘98
Farhi et al., ‘00

3. Evolve the the total Hamiltonian <u>slowly</u> into the groundstate of the problem Hamiltonian: $\rightarrow$ Annealing Schedule

$$H_0 = \sum_i X_i$$

$$H_p = \sum_{i<j} J_{ij} Z_i Z_j + \sum_i h_i Z_i$$



$$H(s) = (1-s)H_0 + sH_P \qquad s = t/\tau$$

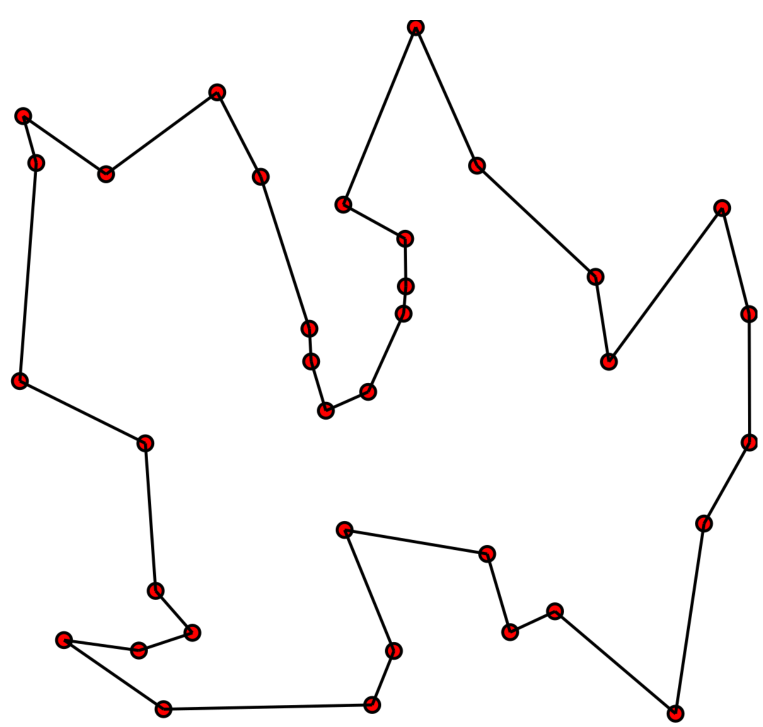
Quantum Annealing

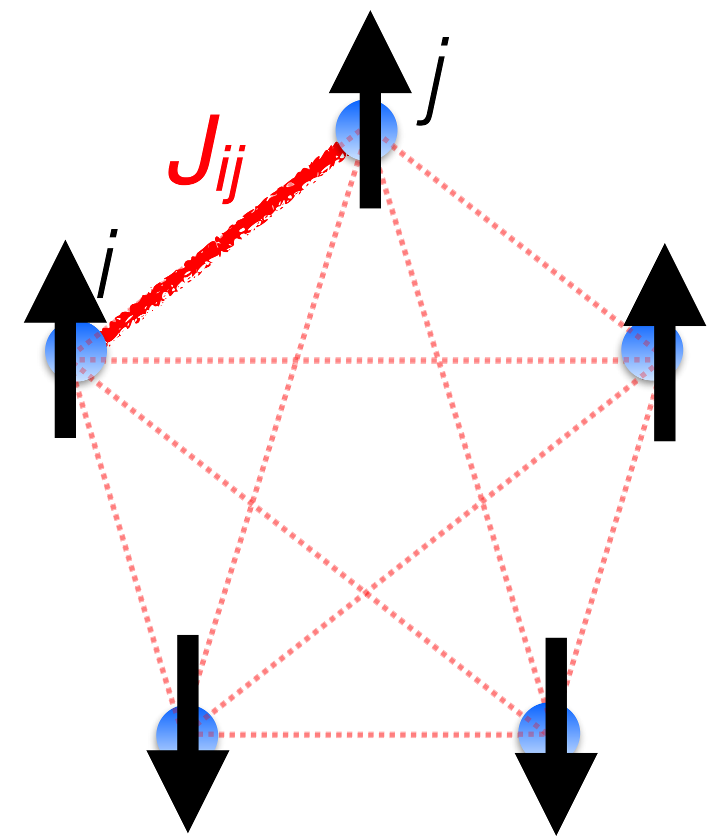
Kadowaki & Nishimori, '98
Farhi et al., '00

4. Measure the final spin configuration. This will (hopefully) be an answer to the optimization problem.

$$H_0 = \sum_i X_i$$

$$H_p = \sum_{i<j} J_{ij} Z_i Z_j + \sum_i h_i Z_i$$

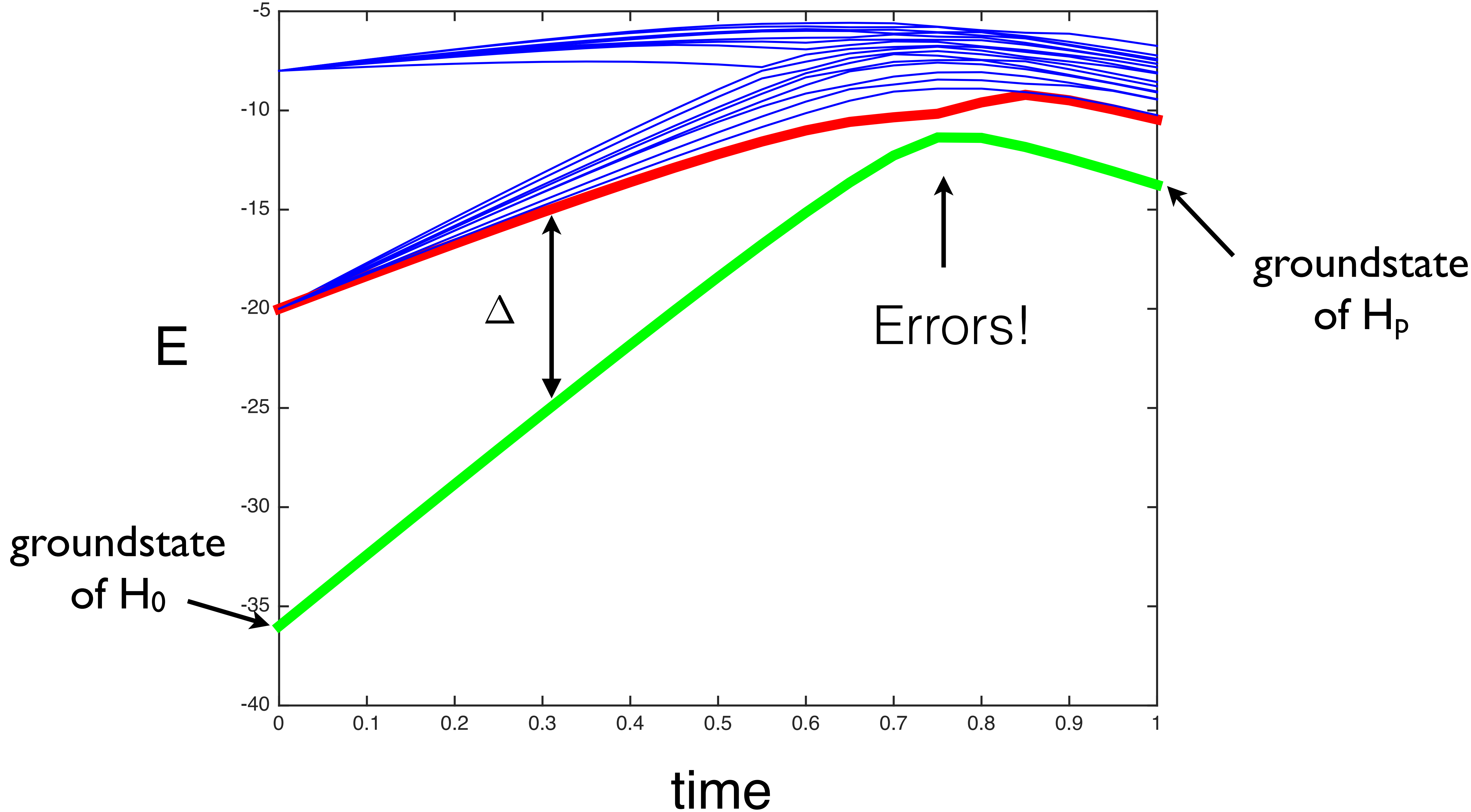




Solution: The shortest path

Groundstate configuration

Sources of Error



The smaller the gap, the higher are the chances of errors.

Stoquastic Hamiltonians and QMC

Stoquastic '=' stochastic + quantum!

Bennet
Bravyi et al, '06

Stochastic sampling of the system's configurations in the ***Quantum Monte Carlo*** Algorithm can be done efficiently.

Stoquastic Hamiltonians: Real and non-positive off-diagonal matrix elements in the computational basis.

This includes all **bosonic systems**, **non-frustrated** magnets and those fermionic systems which **do not suffer** from **"sign problem."**

Loh et al, '90

Numerically, Quantum Monte Carlo and Quantum Annealing show the same scaling for tunneling problems.

Isakov et al, '15
Denchev et al, '16
Jiang et al, '17

Conjecture:

If a problem is inefficient for QMC, then probably it is also inefficient for QA with a **stoquastic** Hamiltonian.

Non-Stoquastic Hamiltonians

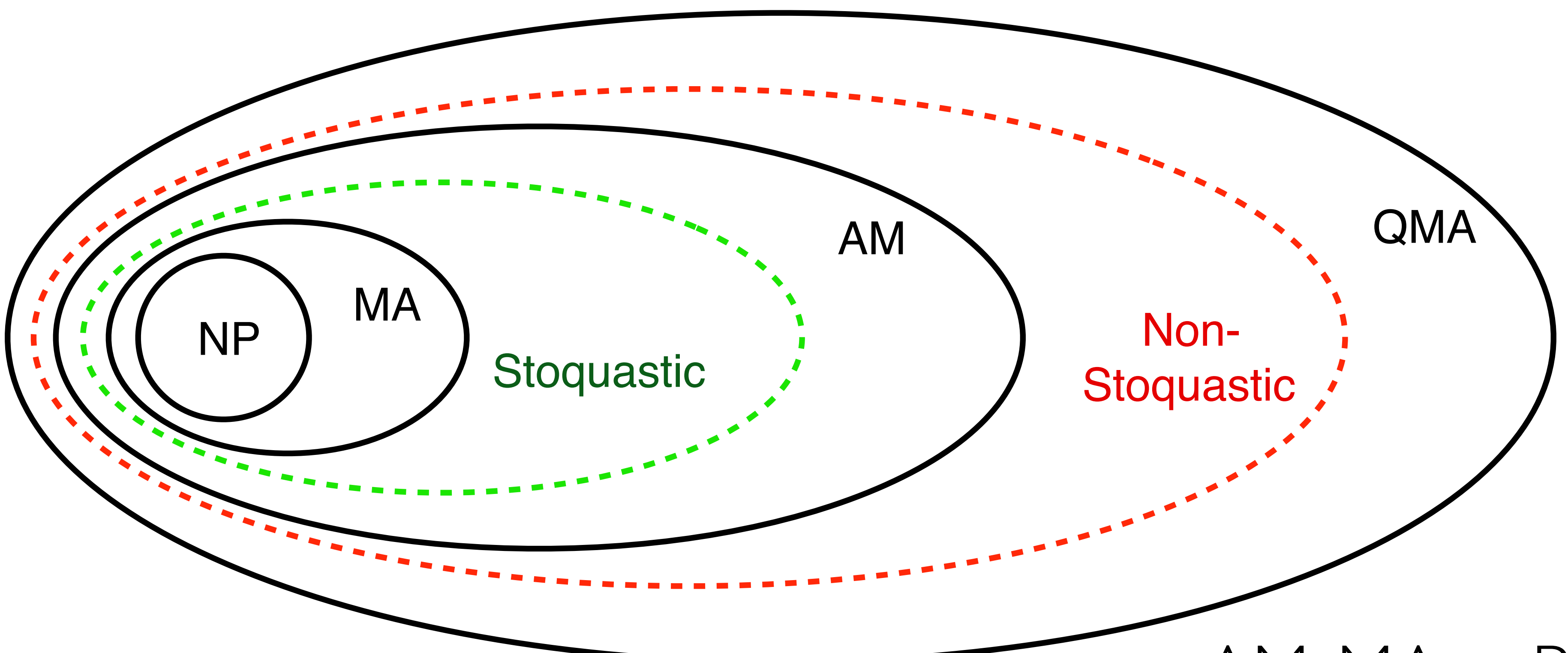
Non-Stoquastic Hamiltonians: those that suffer from the **"sign problem"** i.e. most **fermionic systems**, **frustrated** magnets, etc.

Bravyi et al, '06

Troyer & Wiese, '04

→ **Quantum Monte Carlo is inefficient.**

Non-stoquastic Hamiltonians are more complex and cannot be efficiently simulated with classical computers.



AM, MA ~ Probabilistic version of NP

QMA ~ Quantum version of NP

Non-Stoquastic Hamiltonians

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Bravyi et al, '06

→ Quantum Monte Carlo is inefficient.

Troyer & Wiese, '04

Non-stoquastic Hamiltonians are more complex and cannot be efficiently simulated with classical computers.

Universal adiabatic quantum computing is possible for non-stoquastic Hamiltonians.

Aharonov et al, '04

→ Can this additional complexity help solving hard optimization problems in the context of quantum annealing?

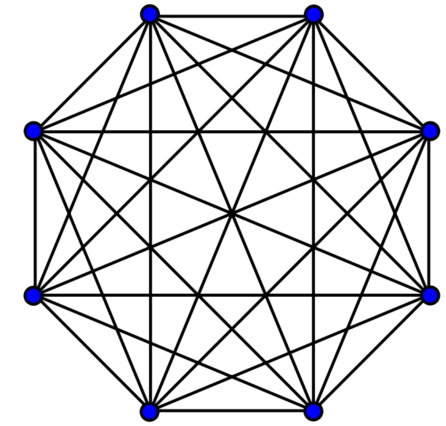
$$\text{Non-Stoquastic} \longrightarrow H = \alpha(s)\, \underbrace{H_i}_{\text{Additional Terms}} + \beta(s)\, H_p \longleftarrow \text{Stoquastic but hard}$$

The Ising Spin Glass as H_p

Problem Hamiltonian: Similar to the Sherrington-Kirkpatrick model of Ising spin glass

$$H_p = \sum_{i<j} J_{ij} Z_i Z_j + \sum_i h_i Z_i$$

Random from a Gaussian distribution Zero



Fully connected graphs

- Infinite-dimensional
- Worst cases are NP-hard

Barahona, '82

Additional Terms:

$$H = \alpha \sum_{i<j} X_i X_j + \beta H_p \qquad \alpha > 0$$

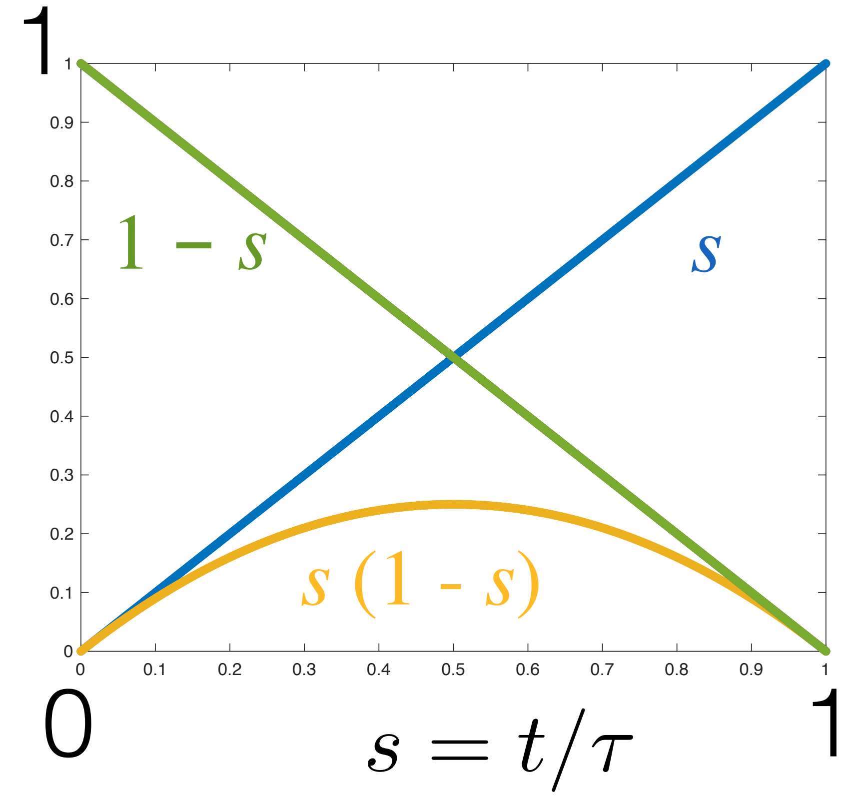
Intrinsic non-stoquastic Hamiltonian

frustration → groundstate degeneracy → $H_0 \neq \sum_{i<j} X_i X_j$

Annealing Schedules

Farhi et al, '02
Crosson et al, '14

$$H = (1-s)H_0 + s(1-s)H_i + sH_p$$



$$H_0 = \sum_i X_i$$

$H_i = 0$ → Uncoupled

$H_i = -\sum_{i<j} X_i X_j$ → Ferromagnetic → Stoquastic

$H_i = +\sum_{i<j} X_i X_j$ → Anti-ferromagnetic

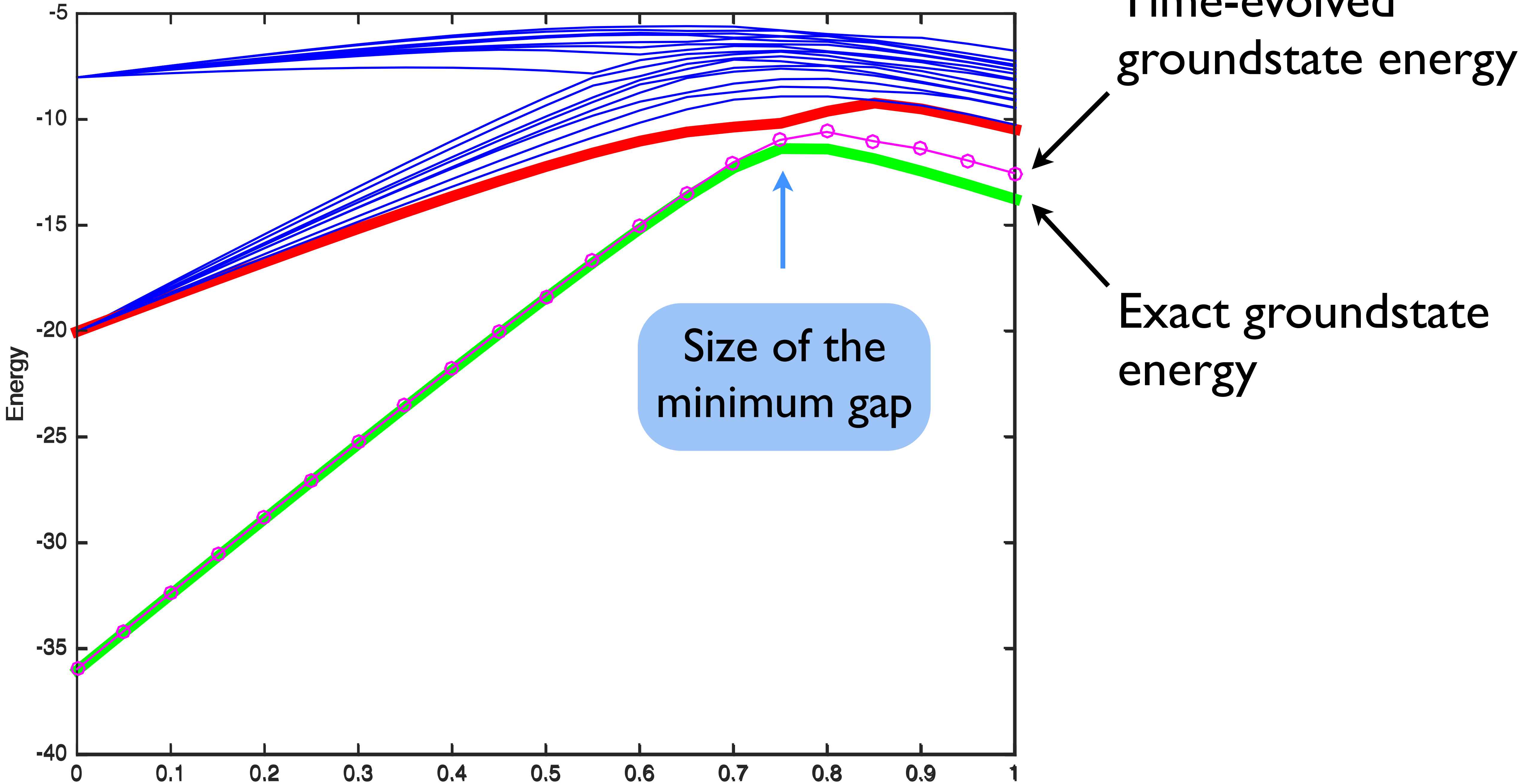
$H_i = \sum_{i<j} r_{ij} X_i X_j$ → Mixed

$r_{ij} \in \{-1, 1\}$

→ Non-stoquatic

Simulating Quantum Annealing

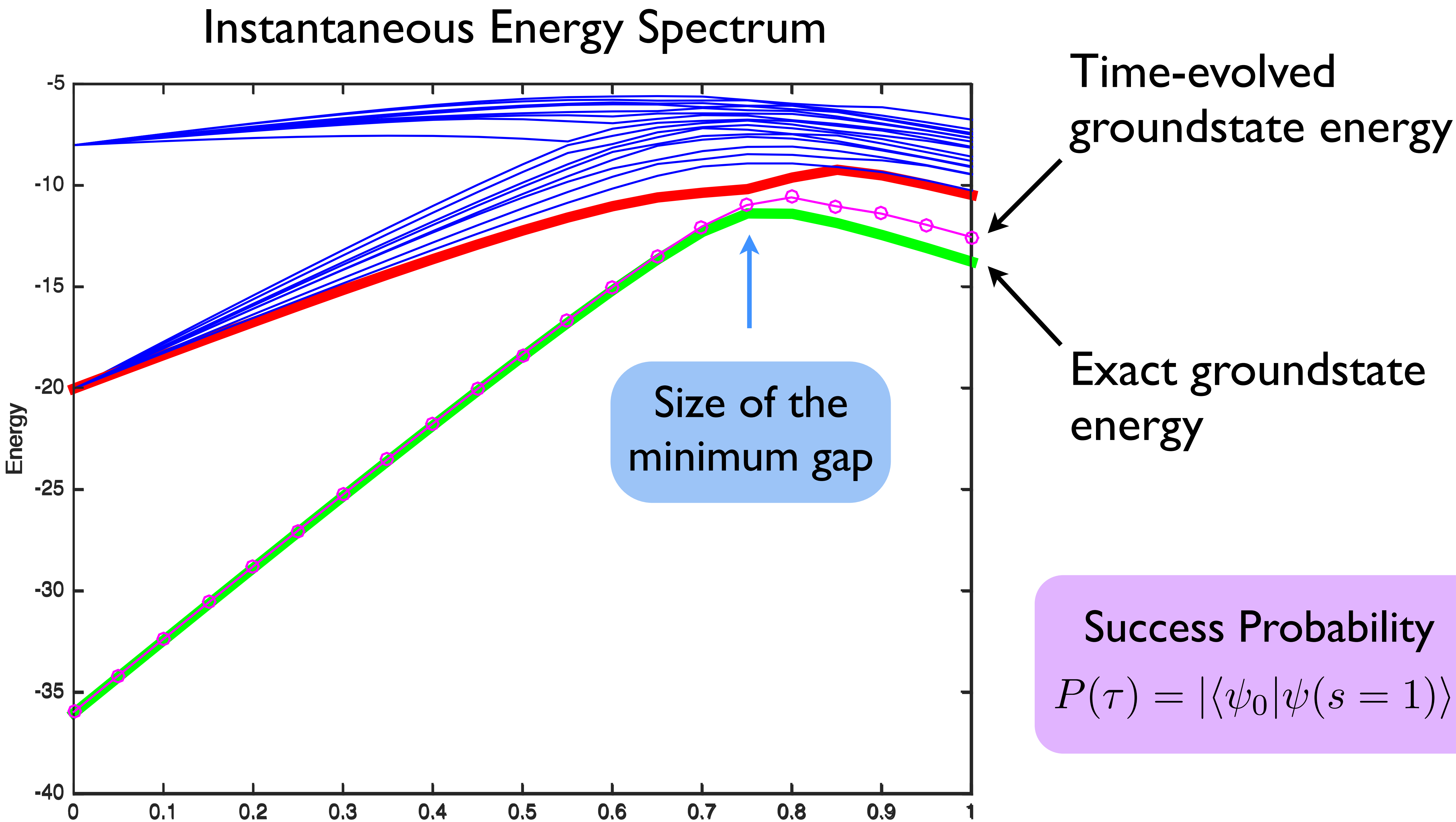
Instantaneous Energy Spectrum



$s = t/\tau$ ← total annealing time

- Exact Diagonalization
- Unitary Schroedinger Dynamics (Simulates Annealing)

Metrics of Comparison



Success Probability

$P(\tau) = |\langle\psi_0|\psi(s=1)\rangle|^2$

$s = t/\tau \longleftarrow$ total annealing time

- Exact Diagonalization
- Unitary Schroedinger Dynamics (Simulates Annealing)

Success Probability Enhancement Metrics

- Success Probability <u>Enhancement Ratio</u>

number of instances with $P^{\alpha} > P^{\beta}, \quad \forall \beta \neq \alpha$

$$R_{en}^{\alpha} = \frac{L^{\alpha}}{L}$$

total number of instances

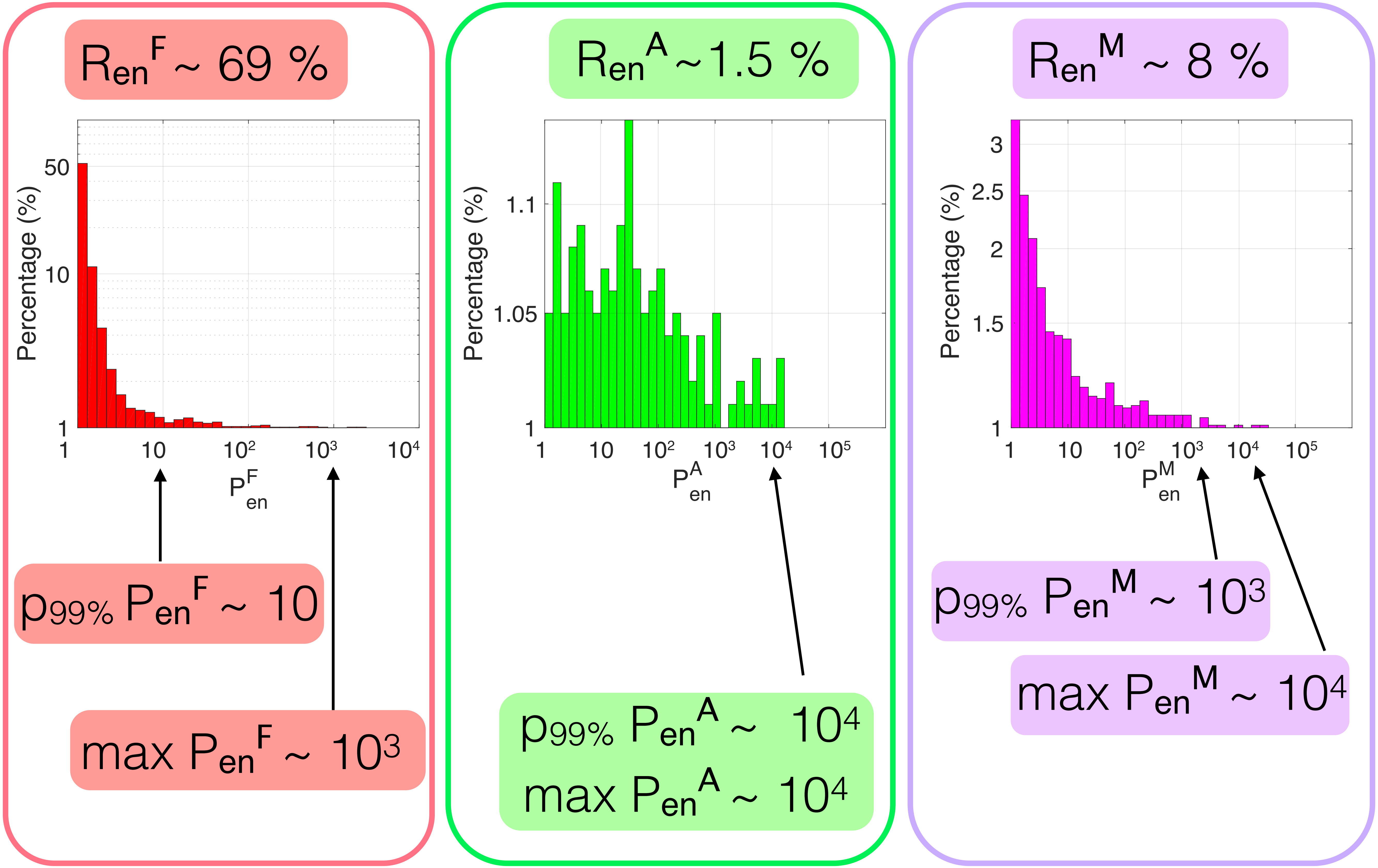
$$\alpha \in \{F, A, M\}$$

- Success Probability <u>Enhancement</u>

$$P_{en}^{\alpha} = \frac{P^{\alpha}}{P^{0}} > 1$$

$$(P^{\alpha} > P^{\beta}, \quad \forall \beta \neq \alpha)$$

Distribution of Success Probability Enhancement



Stoquastic

Non-Stoquastic

Distribution of Success Probability Enhancement

Stoquastic Coupled Hamiltonian:

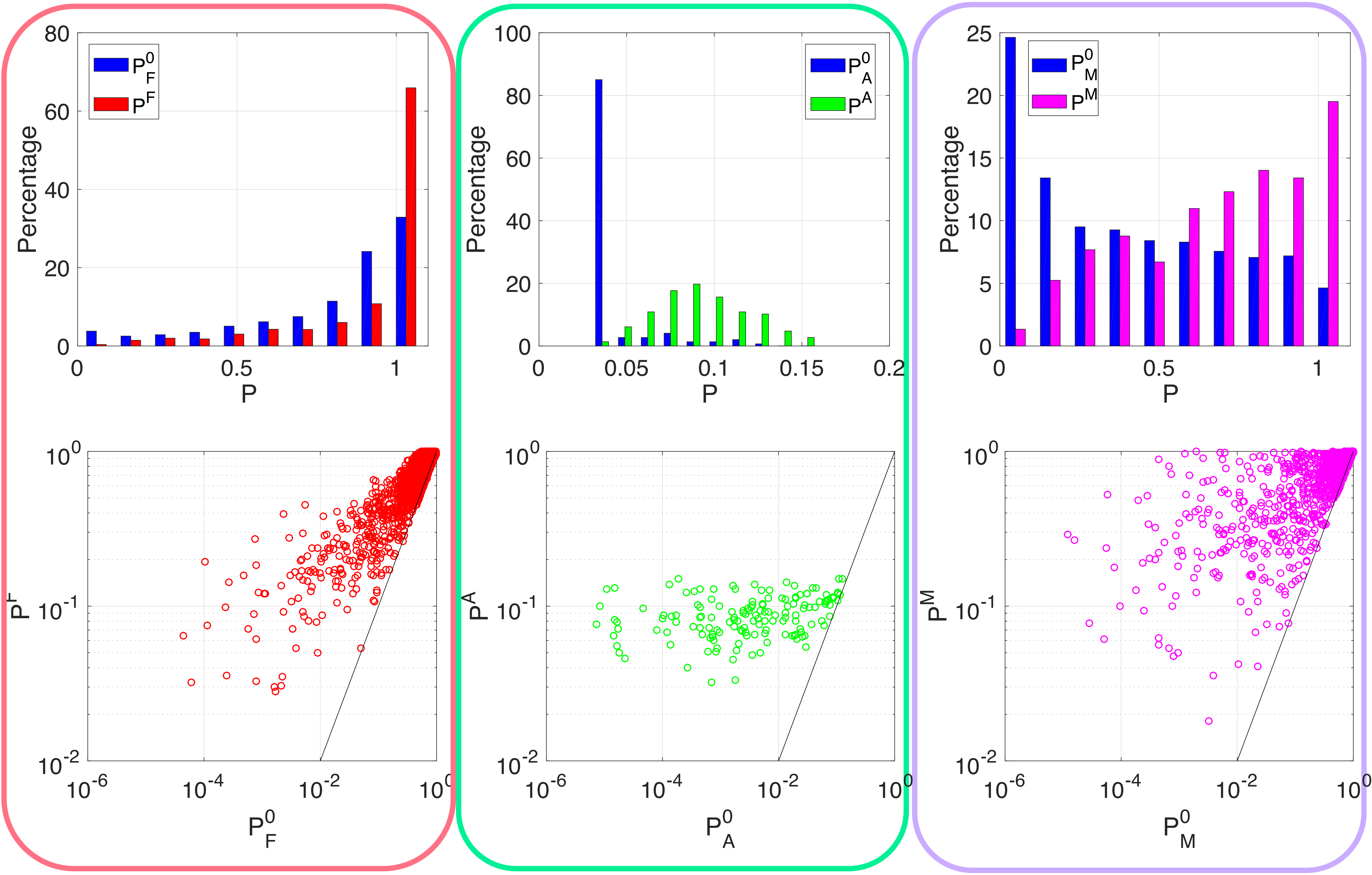
- Improves a large fraction of instances
- The actual improvement is small

Non-Stoquastic Coupled Hamiltonians:

- Improve smaller fractions of instances
- The actual improvement can be huge

Which instances are affected by
each type of Hamiltonian?

Affected Instances: P Distribution



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Distribution of Success Probability Enhancement

Stoquastic Coupled Hamiltonian:

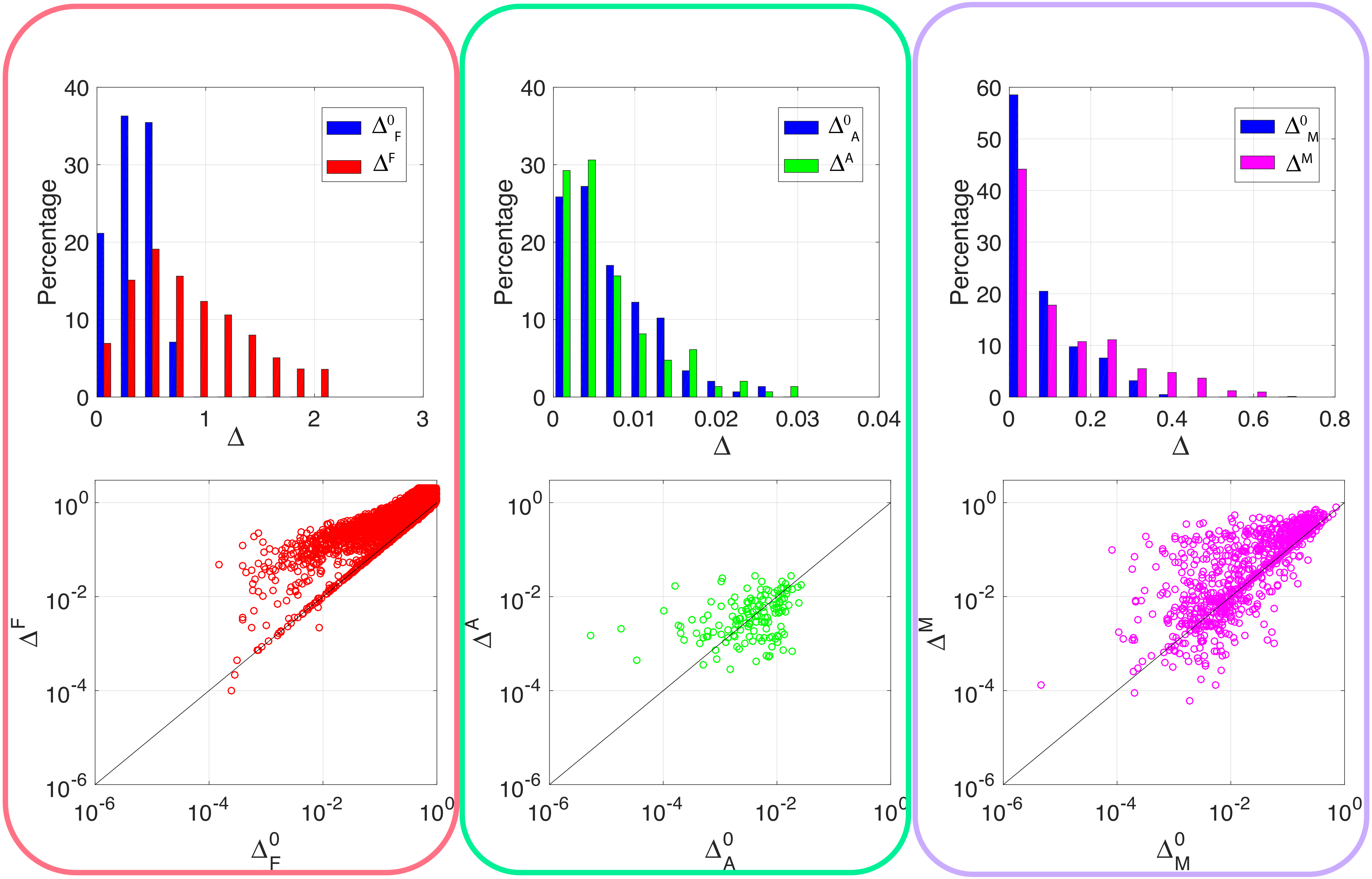
- Improves a large fraction of instances
- The actual improvement is small
- **Tends to improve on easier problems**

Non-Stoquastic Coupled Hamiltonians:

- Improve smaller fractions of instances
- The actual improvement can be huge
- **Mainly improves on harder problems**

What is the relation to the minimum gap?

Affected Instances: Min Gap Distribution



Stoquastic

Non-Stoquastic

Relation to the Size of Minimum Gap

Stoquastic Coupled Hamiltonian:

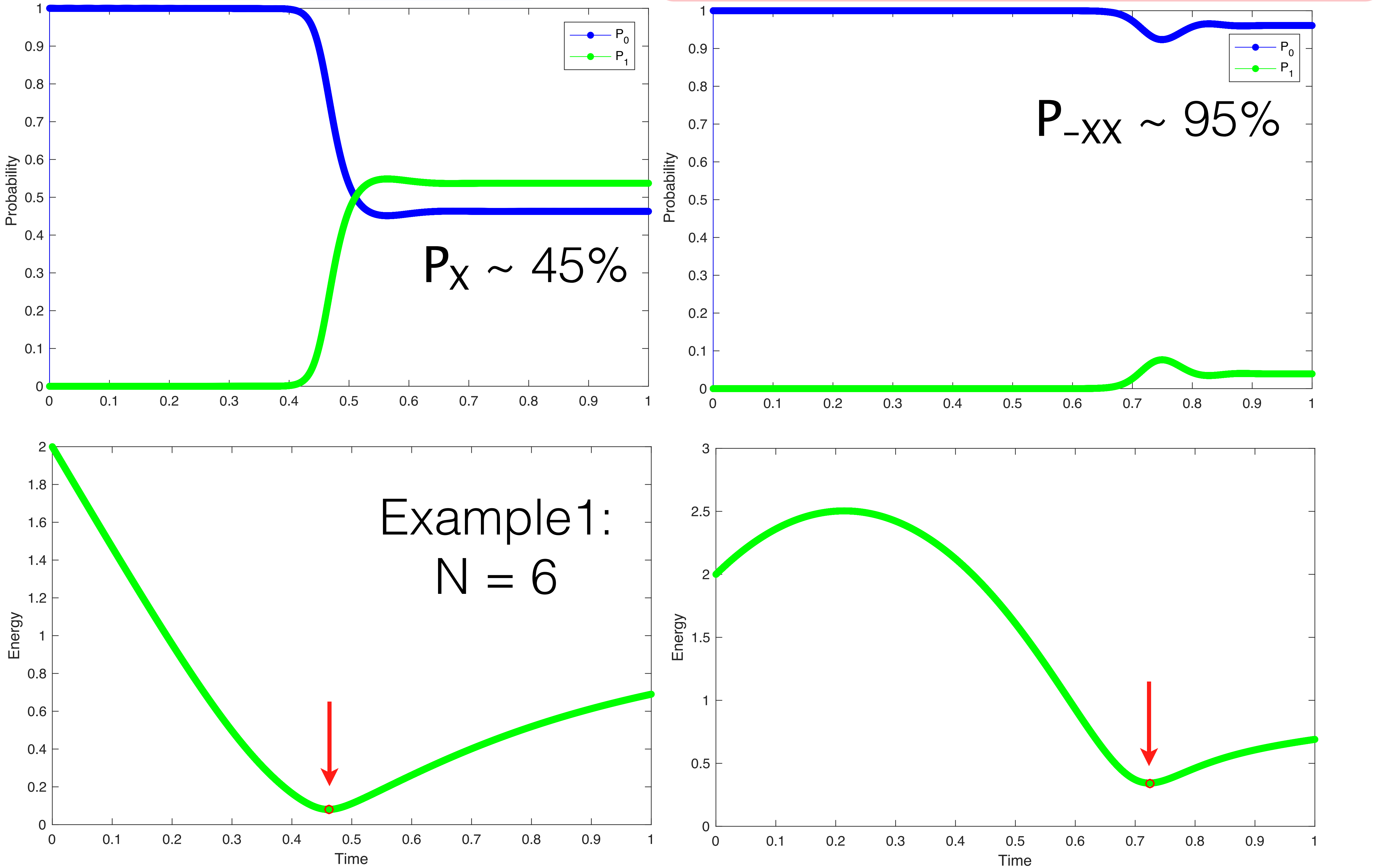
- Affects instances with a large range of gaps
- The size of the gap almost always increases.

The Stoquastic Hamiltonian seems to improve the probability by increasing the gap.

Success Probability & Minimum Gap

$$H_i = 0$$

Stoquastic: $H_i = -\sum_{i<j} X_i X_j$



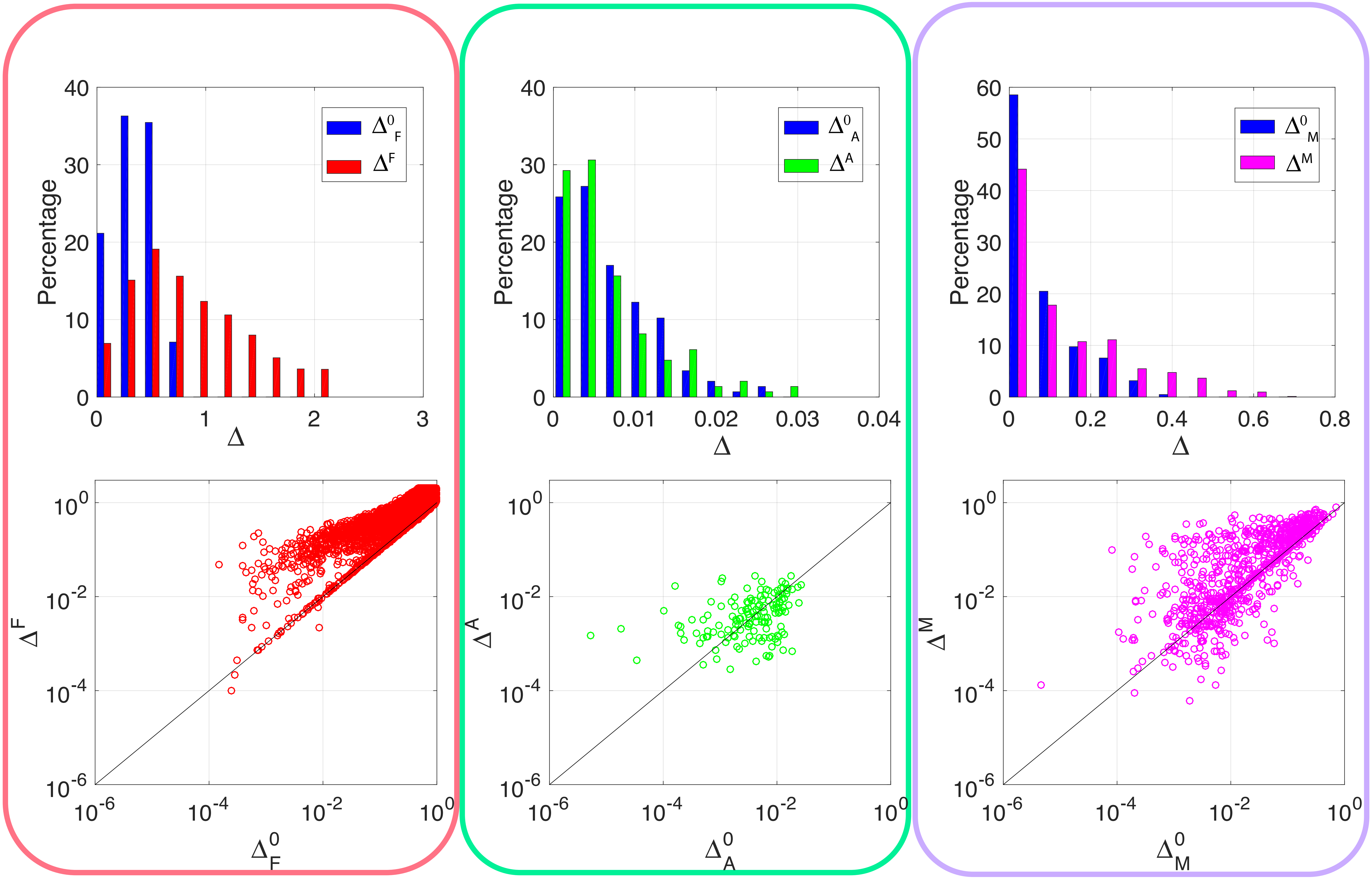
Relation to the Size of Minimum Gap

Stoquastic Coupled Hamiltonian:

- Affects instances with a large range of gaps
- The gap always gets bigger.

Stoquastic Hamiltonians improve the probability by increasing the size of the gap ✓

Affected Instances: Min Gap Distribution



Stoquastic

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Relation to the Size of Minimum Gap

Stoquastic Coupled Hamiltonian:

- Affects instances with a large range of gaps
- The gap always gets bigger.

Stoquastic Hamiltonians improve the probability by increasing the size of the gap ✓

Non-Stoquastic Coupled Hamiltonians:

- Affects problems with smaller gaps
- No clear correlation with the change in the size of minimum gap

What is going on here?

Frustration and Degeneracy

$$H = \sum X_i + \sum X_i X_j + \sum J_{ij} Z_i Z_j + \sum h_i Z_i$$

Anti-ferromagnetic Couplings on a fully-connected graph

$\Downarrow$

Frustration in the X Component of the Spins

$\Downarrow$

Near-degenerate States

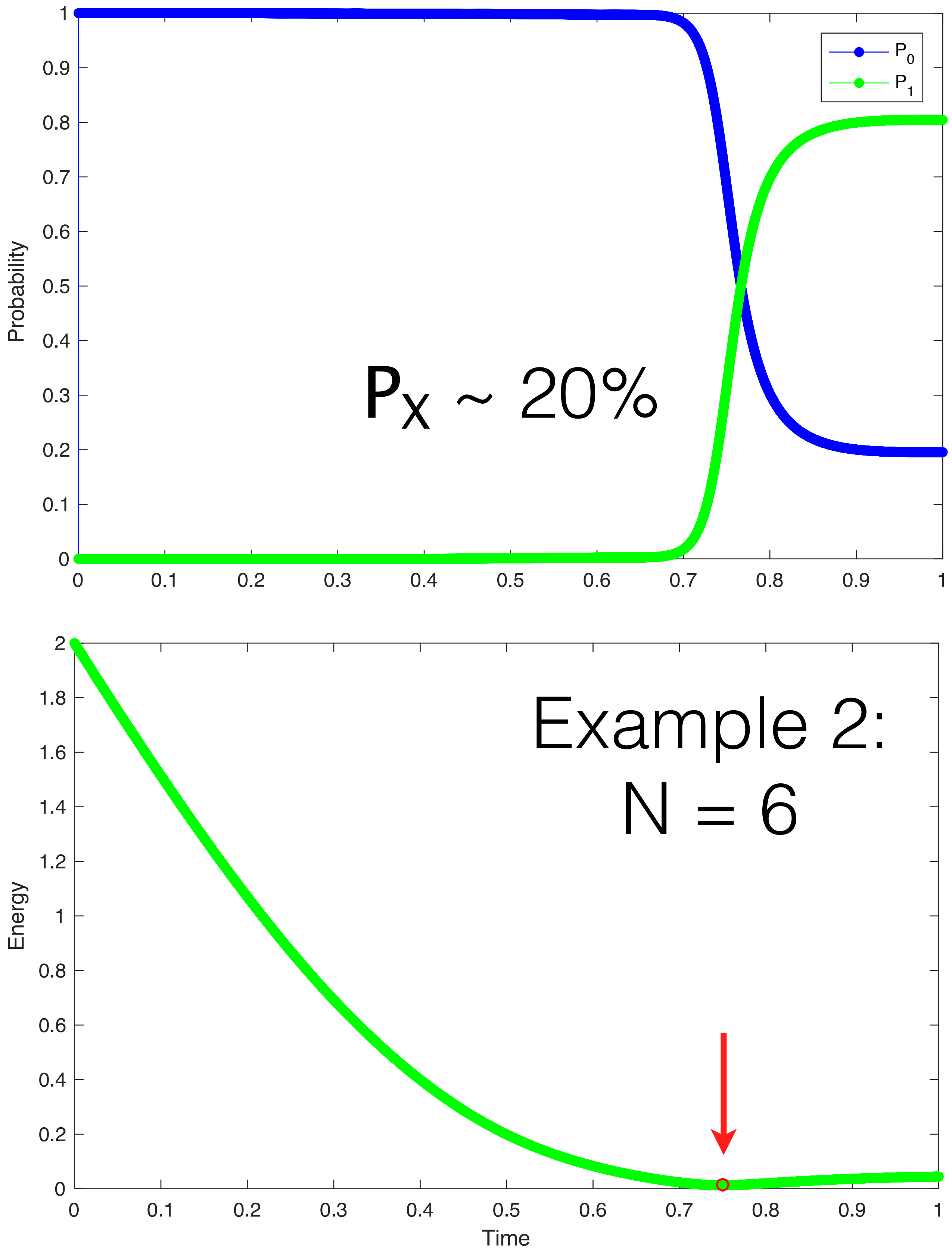
$\Downarrow$

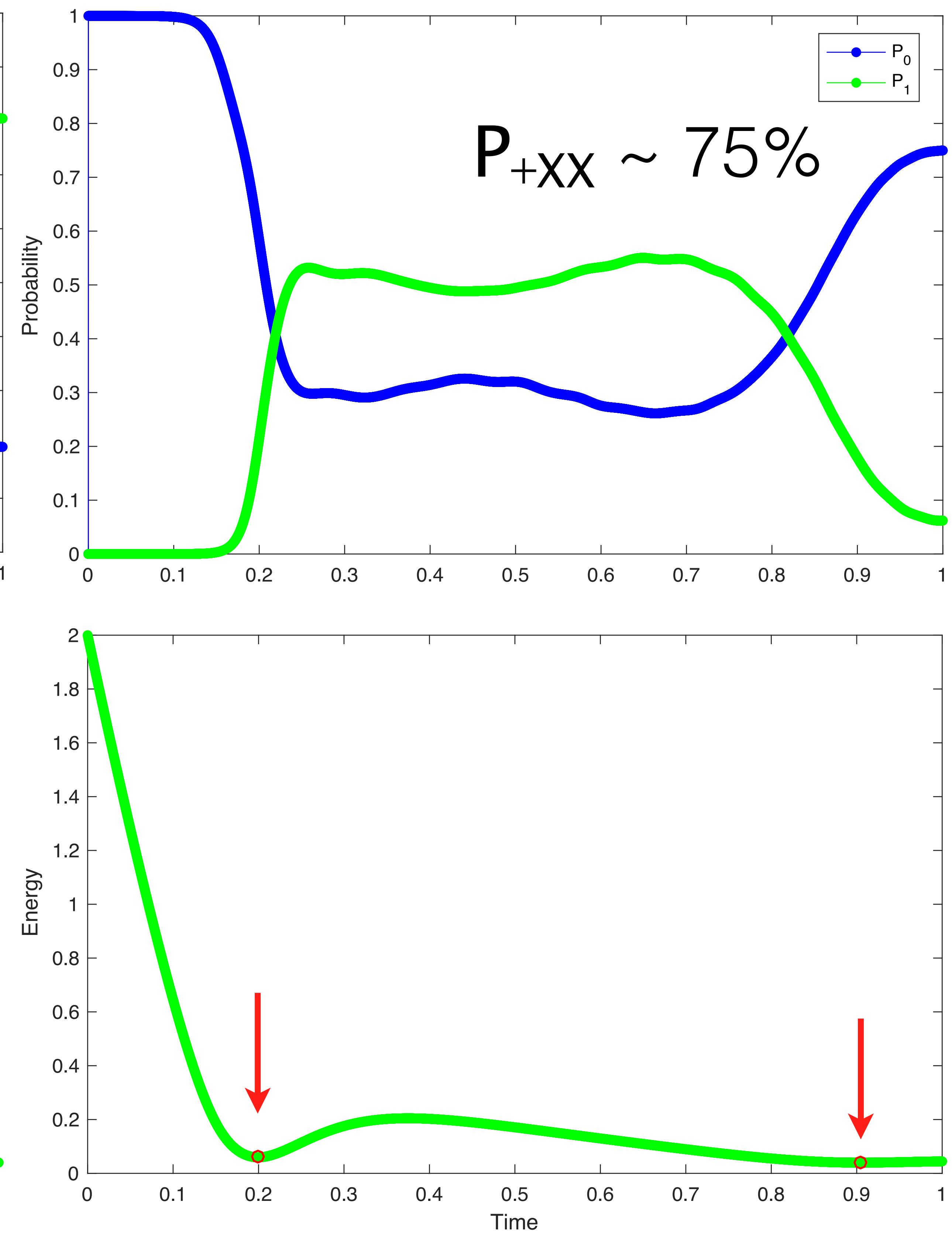
Additional Anti-crossings

Success Probability & Minimum Gap

$H_i = 0$

Non-Stoquastic: $H_i = +\sum_{i<j} X_i X_j$

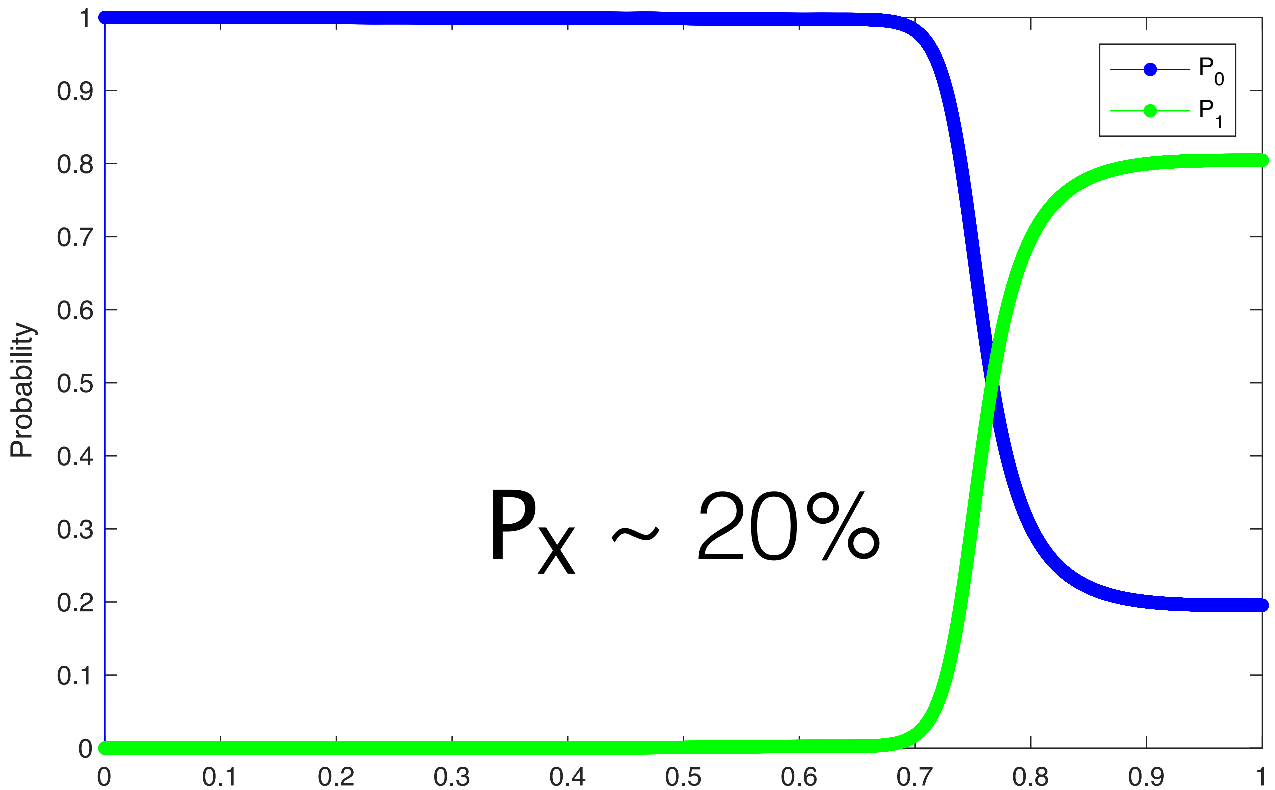


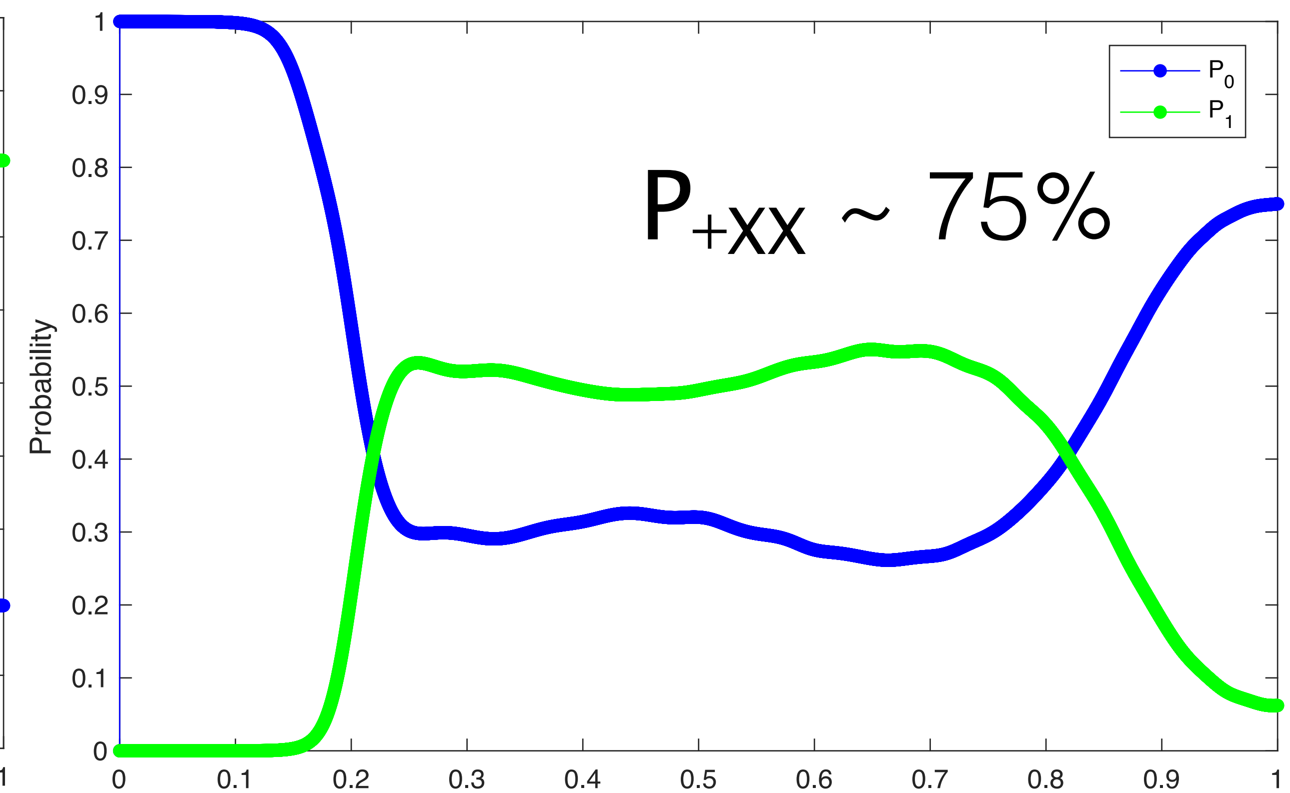


Success Probability & Minimum Gap

$$H_i = 0$$

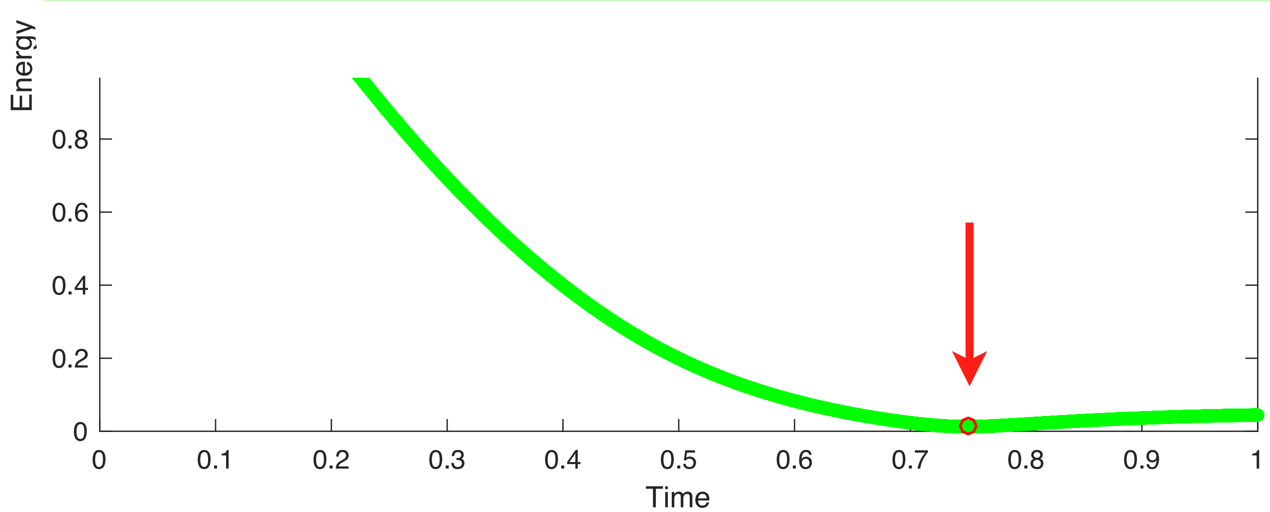
Non-Stoquastic: $H_i = +\sum_{i<j} X_i X_j$

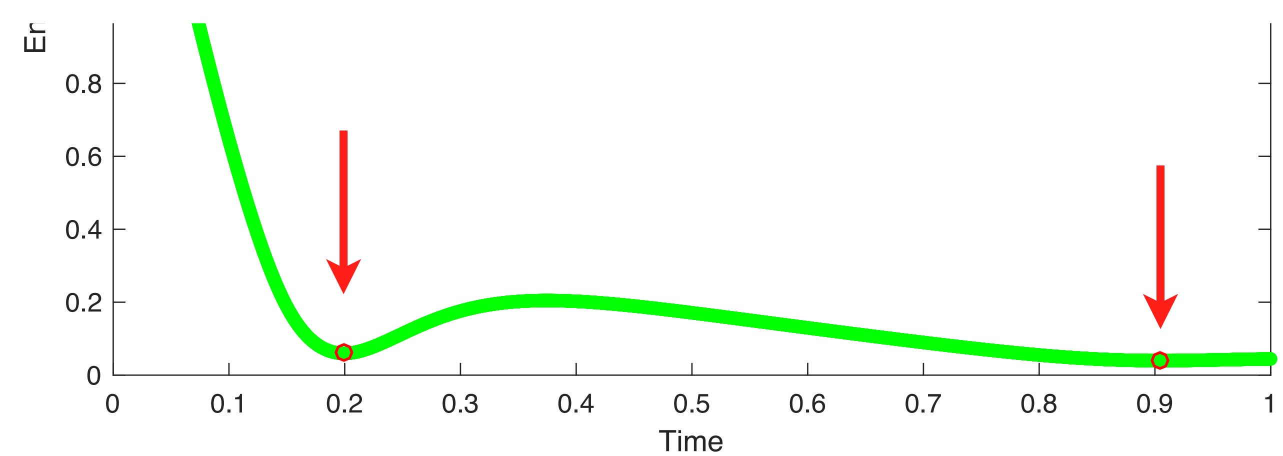




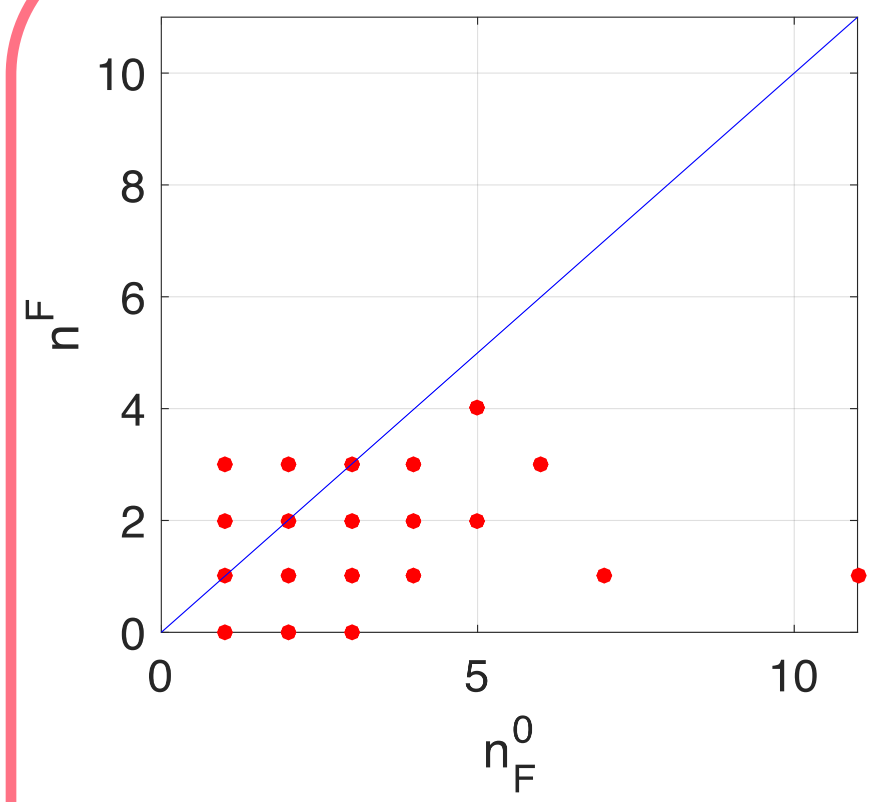
Crosson et al, '14

Similar phenomenon has been reported for the worst cases of MAX 2-SAT.

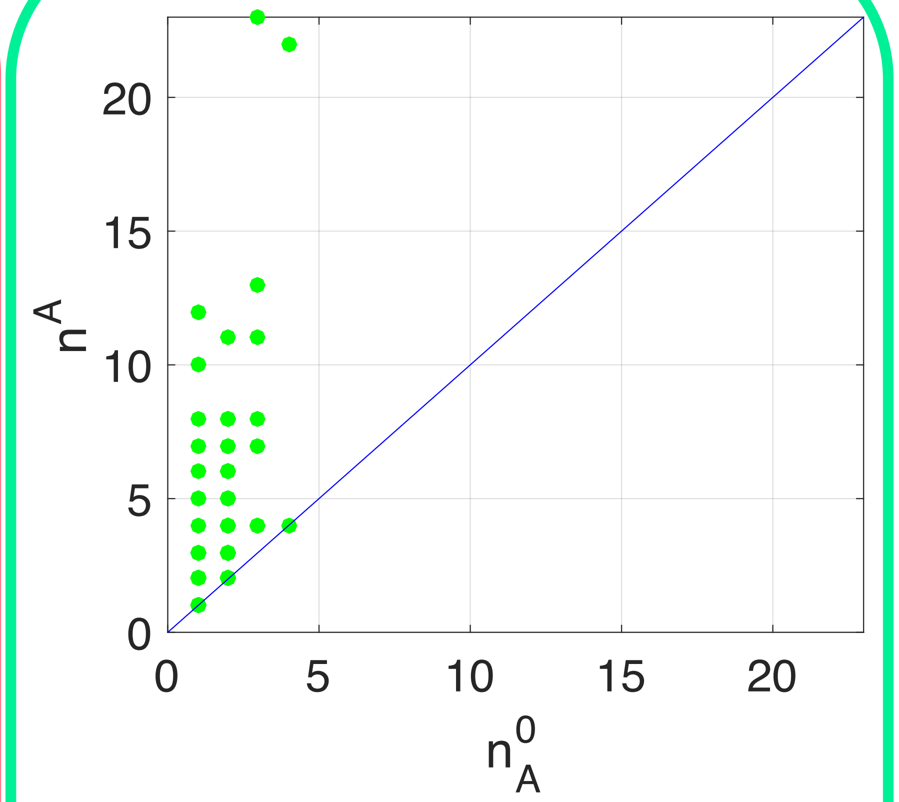




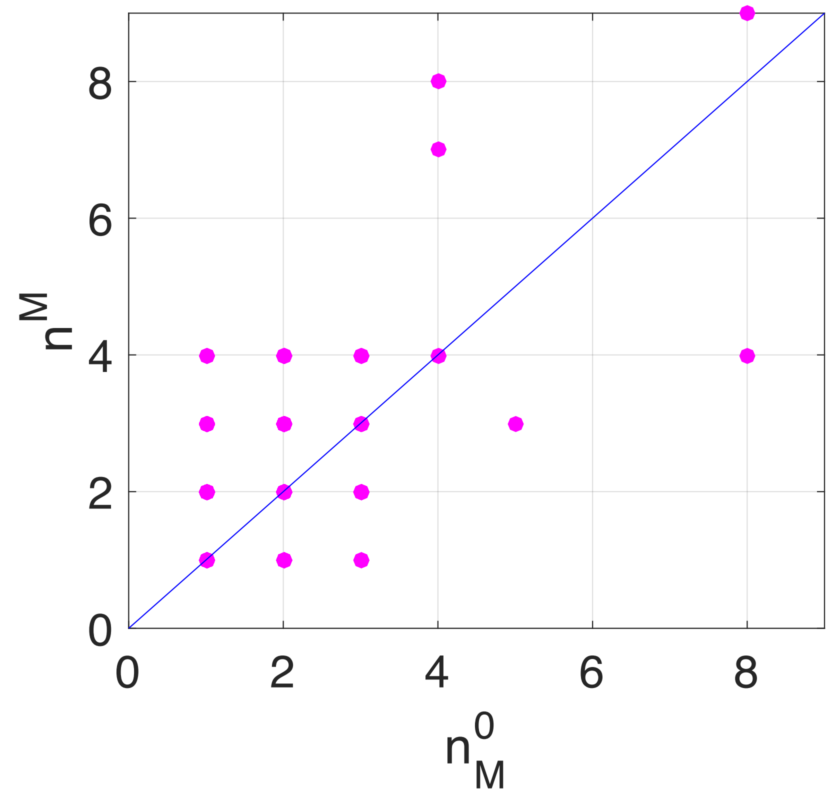
Number of Anti-Crossings



$\langle n_F \rangle < \langle n^0_F \rangle$



$\langle n_A \rangle > \langle n^0_A \rangle$



$\langle n_M \rangle > \langle n^0_M \rangle$

Stoquastic

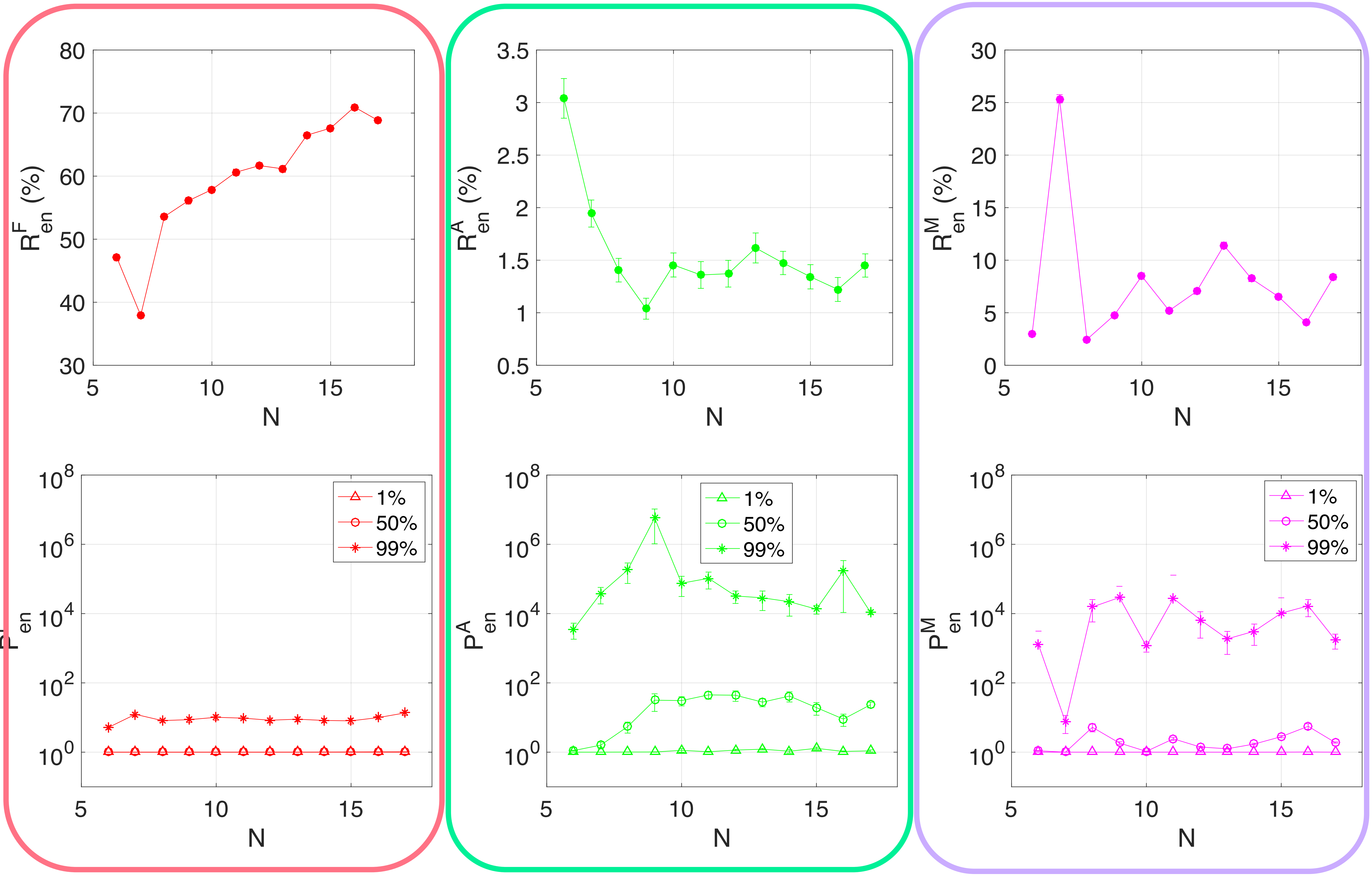
Non-Stoquastic

Relation to the Size of Minimum Gap

Stoquastic Hamiltonian seems to improve the success probability by increasing the size of the minimum gap.

Non-Stoquastic Hamiltonians might be improving the success probability by increasing the number of anti-crossings.

Enhancements & Trends v. System Size



Stoquastic

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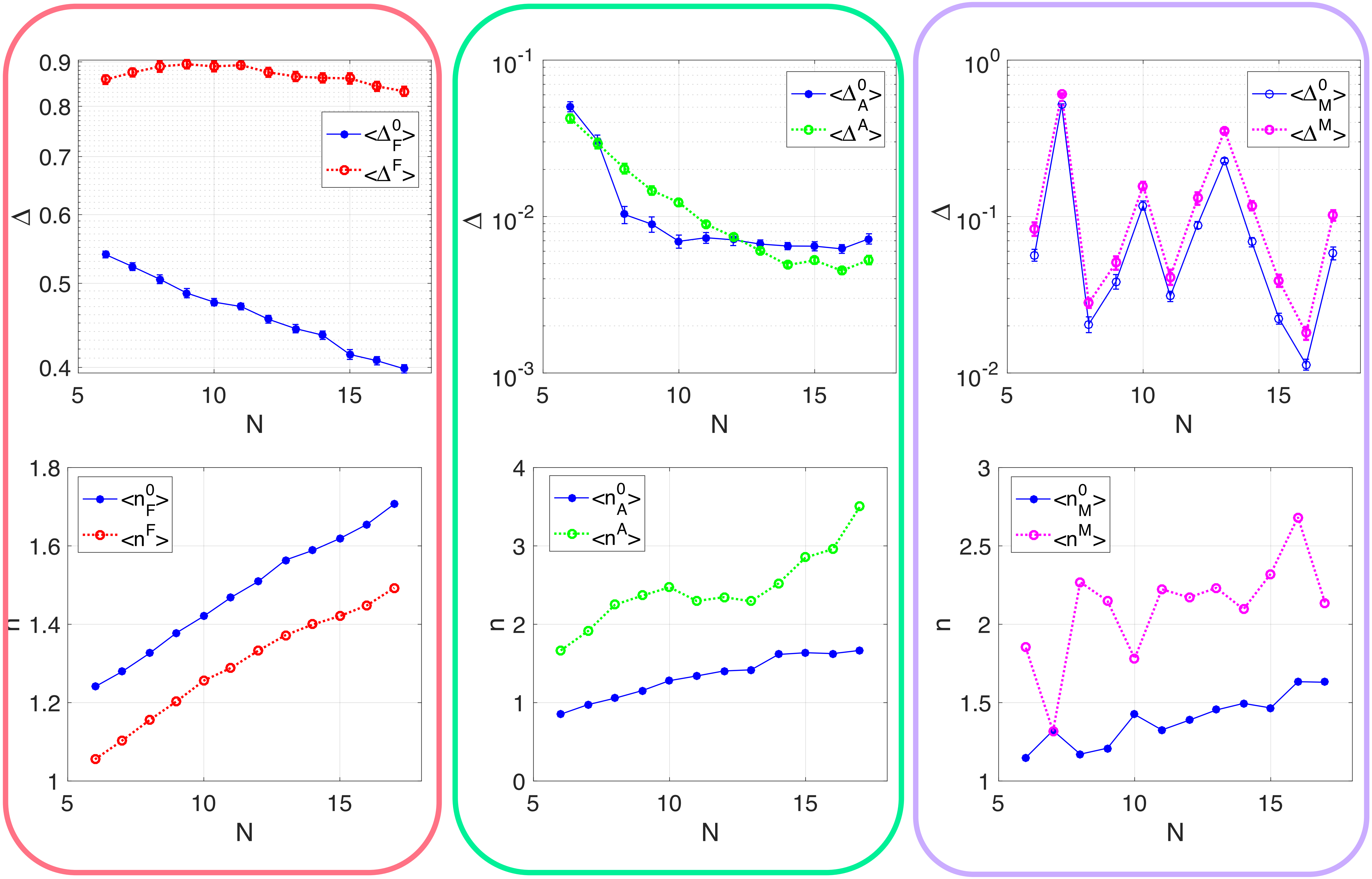
Enhancements & Trends v. System Size



Stoquastic

Non-Stoquastic

Summary

Stoquastic Coupled Hamiltonians:

- Improve large fractions of instances.
- Fractions grow with the system size.
- The actual improvement is small.
- Tend to improve on easier problems with larger gaps.
- <u>Seem to improve the probability by increasing the minimum gap</u>.

Non-Stoquastic Coupled Hamiltonians:

- Improve smaller fractions of instances.
- Fractions remain constant as the system size grows.
- The actual improvement can be huge.
- Mainly improve on harder problems with smaller gaps.
- <u>Might be improving the probability by increasing the number of anti-crossings</u>.

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