Quantum Annealing
and
Quantum Phase Transition

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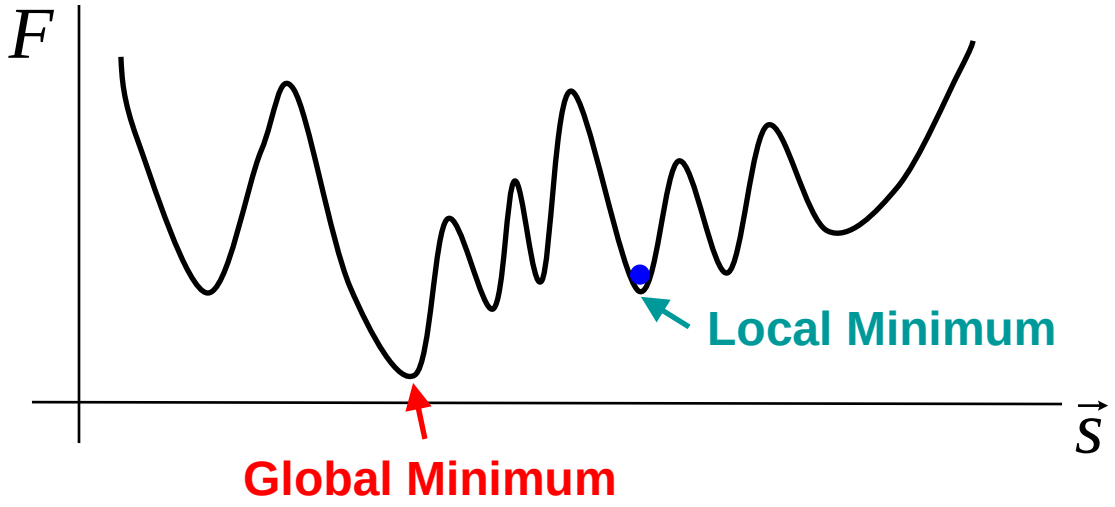
Annealing as a Way of Optimization

Ising Problem:

Find a set of $s_i = \pm 1$ that minimizes

$$F(\vec{s}) = \sum_{i=1}^{N} h_i s_i + \sum_{i,j=1}^{N} J_{ij} s_i s_j, \qquad \vec{s} = [s_1, s_2, \ldots, s_N]$$

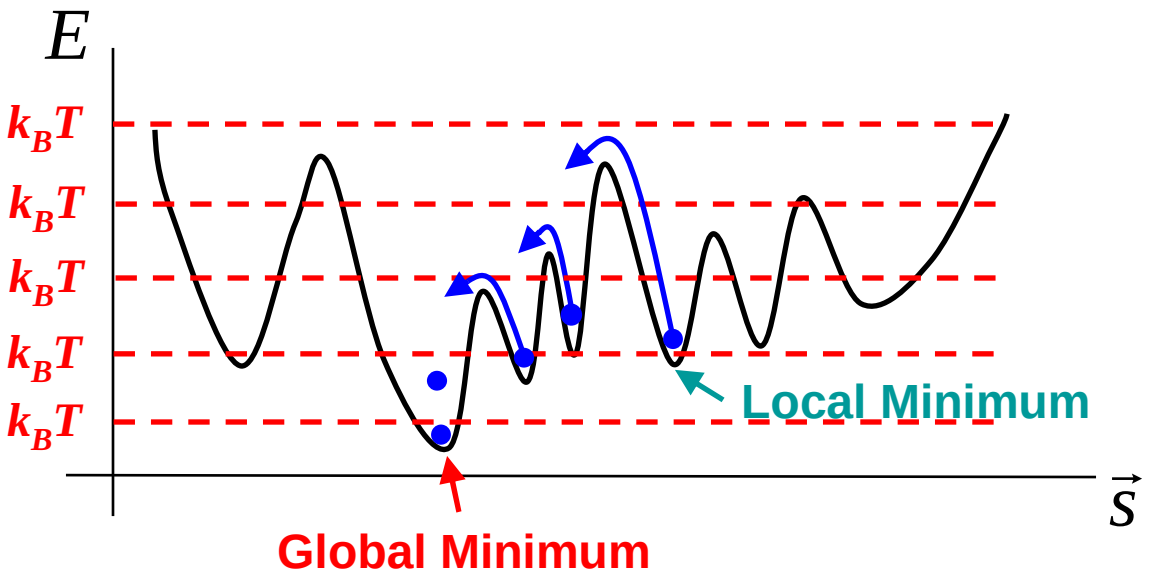


Ising Problem is NP-Hard

Classical (Thermal) Annealing

Consider a physical system with energy:

$$H = E\left(\sum_{i=1}^{N} h_i s_i + \sum_{i,j=1}^{N} J_{ij} s_i s_j\right)$$



Thermal fluctuations take the system out of the local minima

Classical (Thermal) Annealing

Consider a physical system with energy:

$$H = E\left(\sum_{i=1}^{N} h_i s_i + \sum_{i,j=1}^{N} J_{ij} s_i s_j \right)$$

Boltzmann distribution: $P_n = Z^{-1} e^{-E_n / T}$

Partition function: $Z = \mathrm{Tr}\, e^{-H/T} = \sum_n e^{-E_n / T}$

Thermal annealing: change T slowly from T_{max} to 0

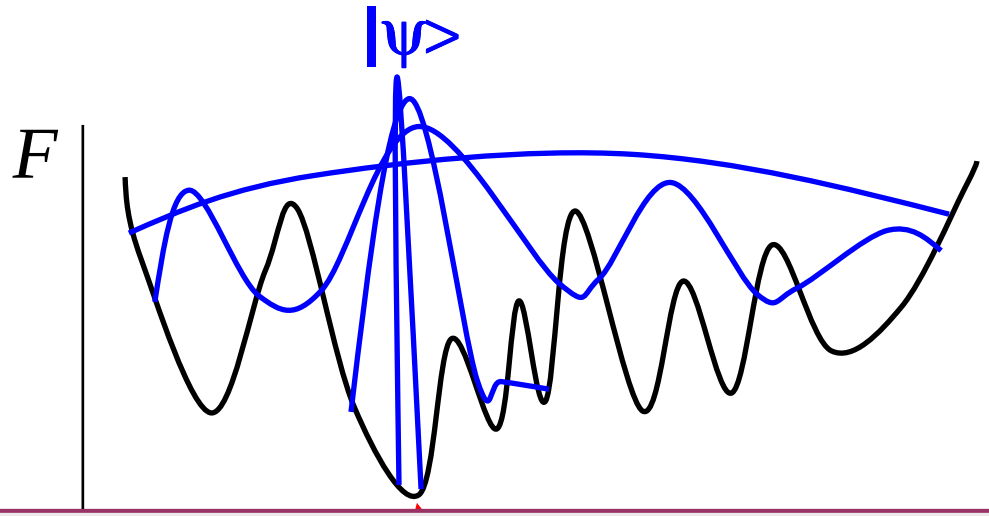
Or: keep T constant and change E from 0 to E_{max}

Quantum Annealing

$$H_P = \sum_{i=1}^{N} h_i \sigma_i^z + \sum_{i,j=1}^{N} J_{ij} \sigma_i^z \sigma_j^z$$

Tunneling amplitude

Hamiltonian: $H = E\left(H_P - \Gamma(t) \sum_{i=1}^{N} \sigma_i^x \right)$ $\Gamma(t) = \dfrac{\Delta(t)}{2E}$



Quantum fluctuations (tunneling) keep the system out of the local minima

Quantum Annealing

$$H_P = \sum_{i=1}^{N} h_i \sigma_i^z + \sum_{i,j=1}^{N} J_{ij} \sigma_i^z \sigma_j^z$$

Hamiltonian: $$H = E\left(H_P - \Gamma(t) \sum_{i=1}^{N} \sigma_i^x \right) \qquad \Gamma(t) = \frac{\Delta(t)}{2E}$$

Quantum annealing: change Γ slowly from Γ_{max} to 0

Phase Transitions

During annealing the system may go through a phase transition

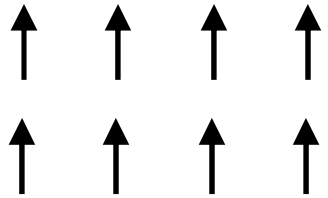
Phase transition: Transformation of a thermodynamic system from one phase to another due to some external change (e.g., temperature, pressure, etc.)

Classical Phase Transition

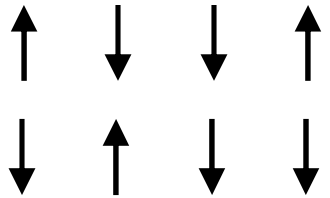
Ferromagnetically coupled spins

$$H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z$$

$T = 0$:

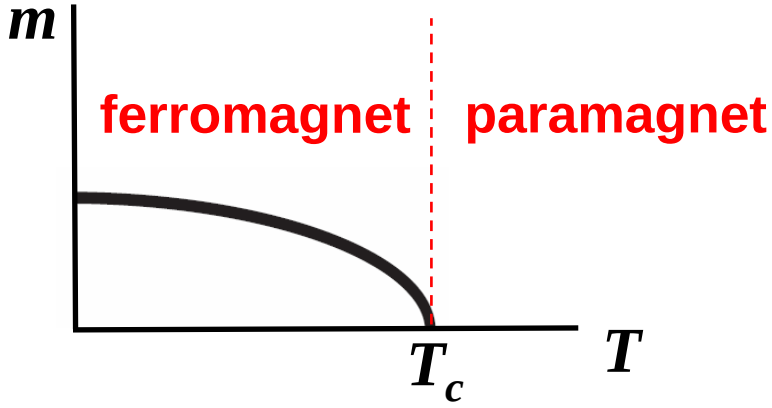


Large T:



Magnetization:

$$m = \left\langle \sum_{i=1}^{N} \sigma_i^z \right\rangle$$



Thermal Equilibrium

P_i **= Probability of finding the system in state** i **with energy** E_i

Boltzmann distribution:

$$P_i = \frac{e^{-E_i / k_B T}}{Z}$$

Partition function:

$$Z = \sum_i e^{-E_i / k_B T}$$

Free Energy

Let us write

$$Z = \sum_i e^{-E_i / k_B T} = e^{-F / k_B T}$$

$$\Rightarrow \quad F = -k_B T \ln Z$$

Free energy

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$$P_i = \frac{e^{-E_i / k_B T}}{Z} \quad \Rightarrow \quad F = -k_B T \ln Z = E_i - k_B T \ln P_i$$

Free Energy

Let us write

$$Z = \sum_i e^{-E_i / k_B T} = e^{-F / k_B T}$$

$$P_i = \frac{e^{-E_i / k_B T}}{Z} \quad \Rightarrow \quad F = -k_B T \ln Z = E_i - k_B T \ln P_i$$

$$\Rightarrow \quad \sum_i P_i F = \sum_i P_i E_i - k_B T \sum_i P_i \ln P_i$$

Free Energy

Let us write

$$Z = \sum_i e^{-E_i / k_B T} = e^{-F / k_B T}$$

$$P_i = \frac{e^{-E_i / k_B T}}{Z} \quad \Rightarrow \quad F = -k_B T \ln Z = E_i - k_B T \ln P_i$$

$$\Rightarrow \quad \sum_i P_i F = \sum_i P_i E_i - k_B T \sum_i P_i \ln P_i$$

$$\sum_i P_i = 1 \quad \Rightarrow \quad \boxed{F = \overline{E} - TS}$$

Average energy:

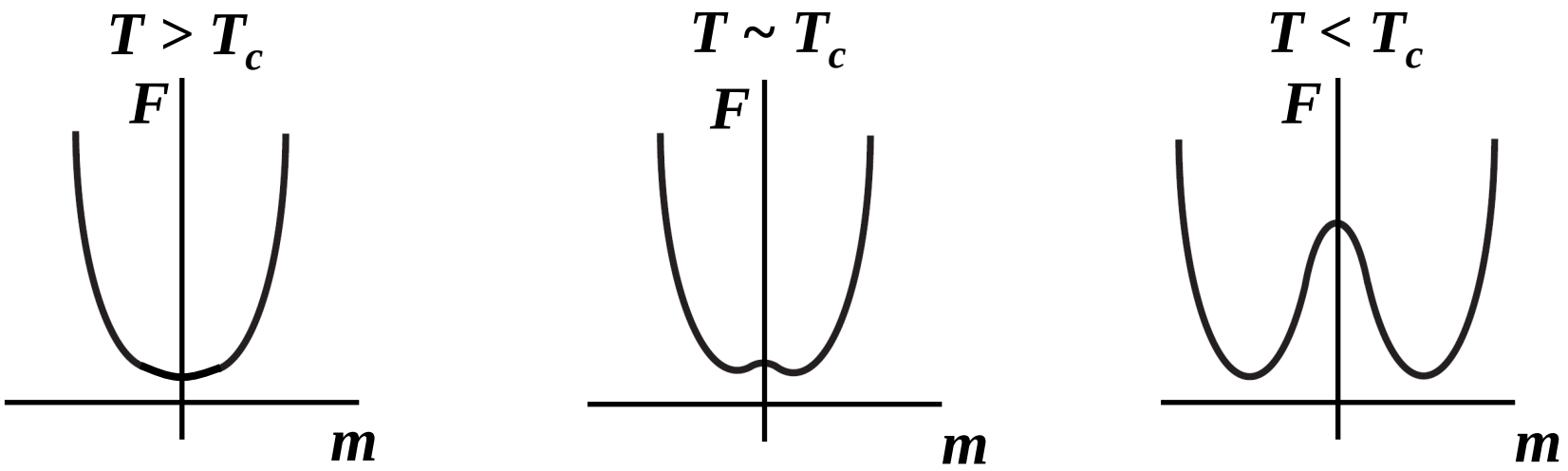
$$\overline{E} = \sum_i P_i E_i$$

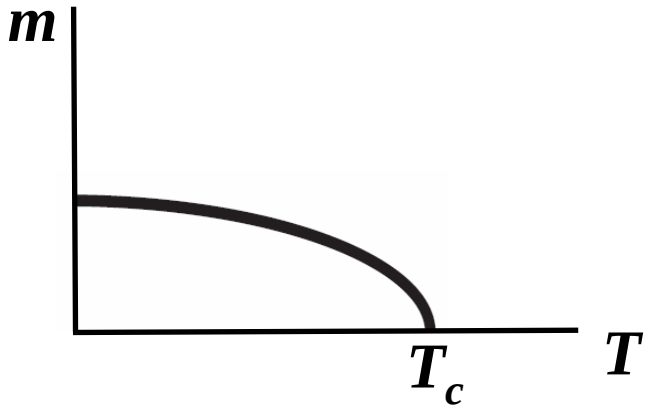
Equilibrium (Boltzmann) distribution is the minimum of the free energy

Second Order Phase Transition

Order parameter (magnetization)

$$m = \left\langle \sum_{i=1}^{N} \sigma_i^z \right\rangle$$

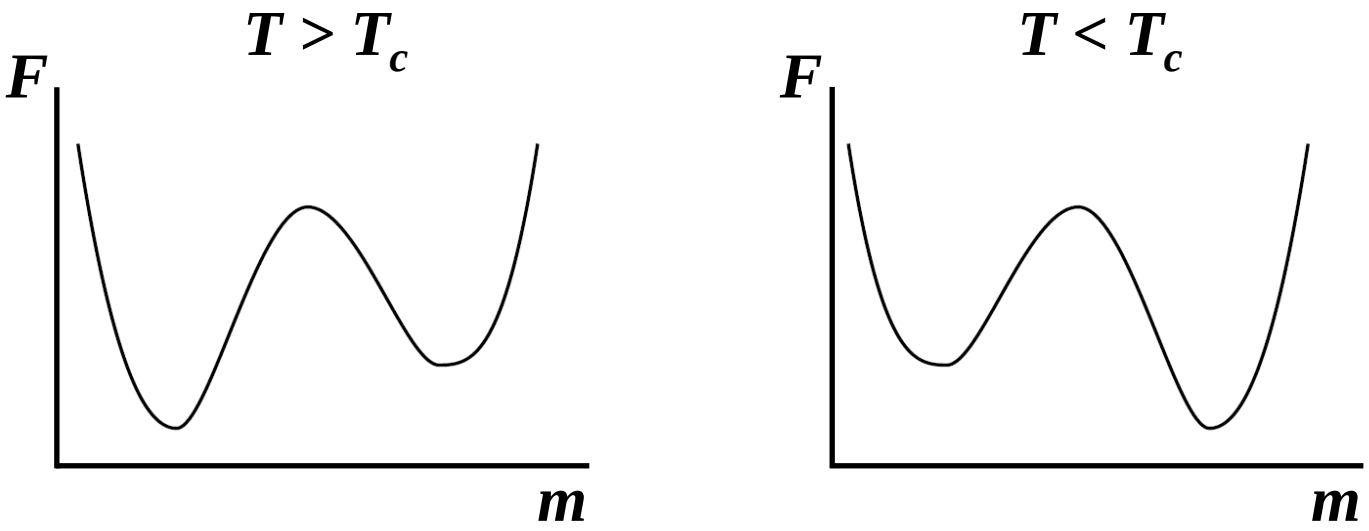


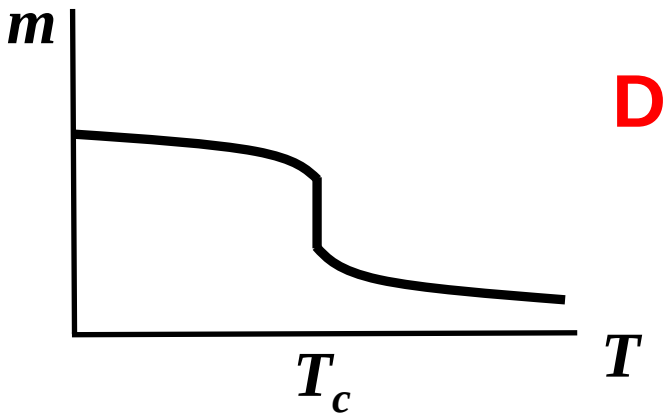


Continuous transition

First Order Phase Transition

Order parameter (magnetization) $m = \left\langle \sum_{i=1}^{N} \sigma_i^z \right\rangle$



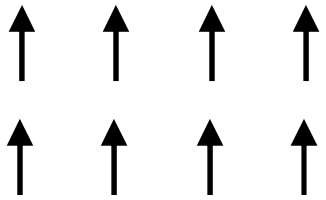


Discontinuous transition

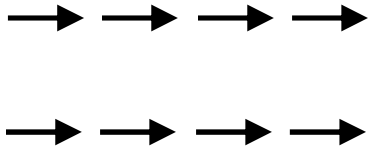
Quantum Phase Transition

Hamiltonian: $H = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - \Gamma \sum_i \sigma_i^x$

$\Gamma = 0$:



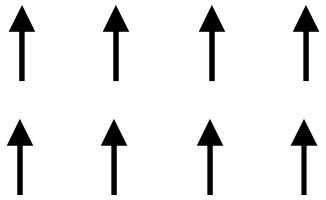
Large Γ:



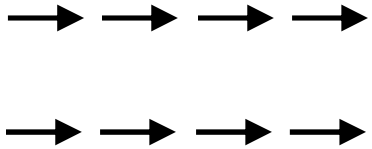
Quantum Phase Transition

Hamiltonian: $H = -J\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x$

$\Gamma = 0$:



Large Γ:



Free energy: $F = \langle\psi|H|\psi\rangle = \overline{E} - \Gamma K$

$\overline{E} = -J\langle\psi|\sum_{\langle i,j\rangle}\sigma_i^z\sigma_j^z|\psi\rangle$

$K = \langle\psi|\sum_i \sigma_i^x|\psi\rangle$

Minimum of the free energy is the ground state

Classical vs. Quantum

	Classical	Quantum
Free energy:	$F = \overline{E} - TS$	$F = \overline{E} - \Gamma K$
Measure of disorder:	$S = -k_B \sum_i P_i \ln P_i$	$K = \langle \psi \vert \sum_i \sigma_i^x \vert \psi \rangle$
Free energy minimum:	**Thermal equilibrium**	**Ground state**
Disorder:	**Thermal mixing**	**Superposition**
Control parameter	T	Γ

AQC and Quantum Phase Transition

AQC Hamiltonian:

$$H = (1-\lambda)H_B + \lambda H_P = \lambda\left(H_P - \Gamma \sum_{i=1}^{N} \sigma_i^x \right)$$

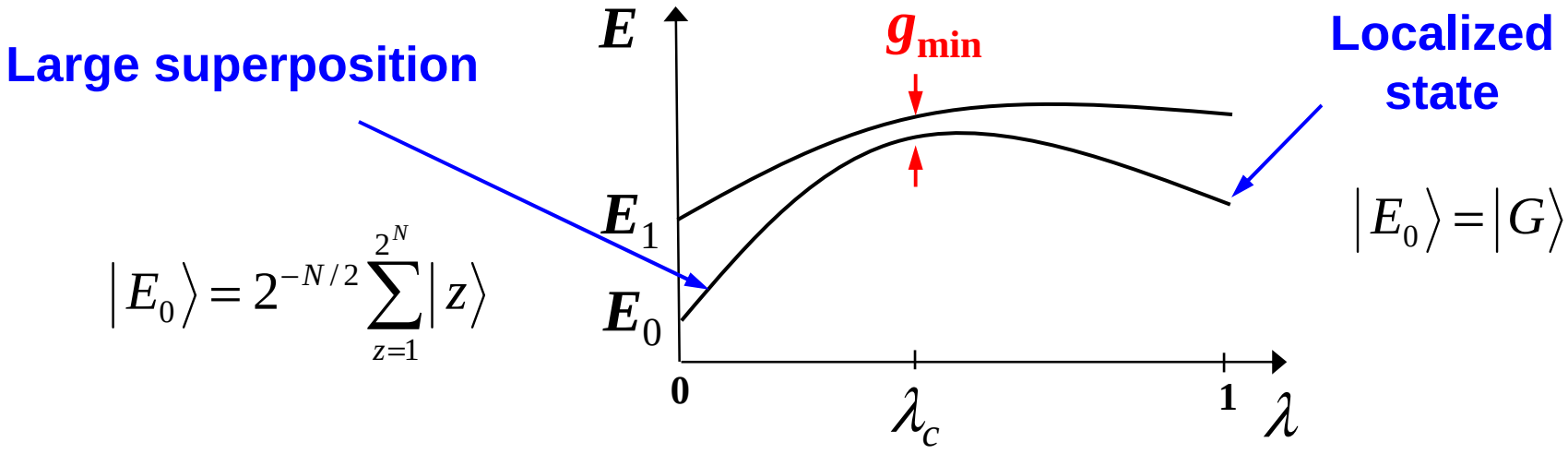
$$\Gamma = \frac{\Delta(1-\lambda)}{\lambda}$$

$\lambda = 0$ **Complete disorder (superposition)**

$\lambda = 1$ **Complete order (unique ground state)**

$\lambda = \lambda_c$ **Transition from disorder to order (quantum critical point)**

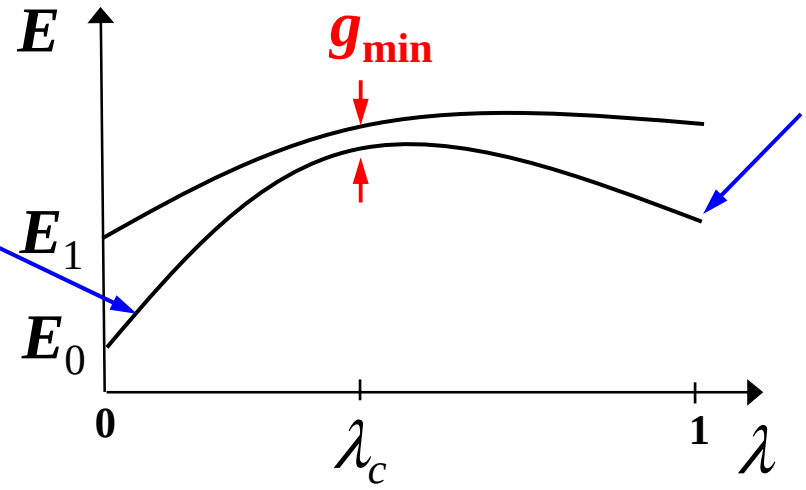
2nd Order Quantum Phase Transition



2nd Order Quantum Phase Transition

Large superposition

$$|E_0\rangle = 2^{-N/2}\sum_{z=1}^{2^N}|z\rangle$$

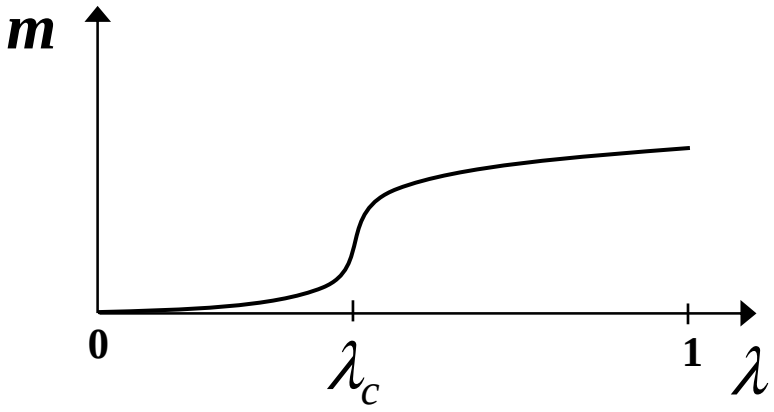


Localized state

$$|E_0\rangle = |G\rangle$$

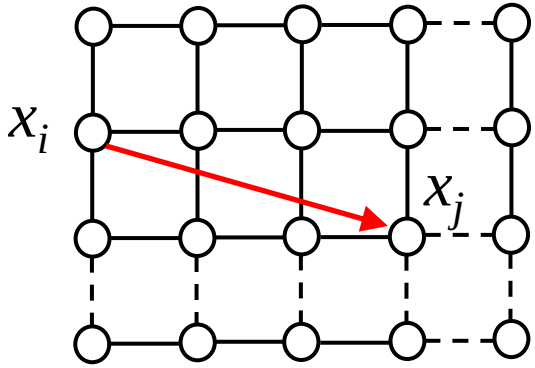
Order Parameter

$$m = \left\langle \sum_{i=1}^{N} \sigma_i^z \right\rangle$$



Spectral Gap

S. Sachdev, "Quantum Phase Transitions", Cambridge University Press (1999)



Correlation function:

$$\left\langle \sigma_i^z \sigma_j^z \right\rangle - \left\langle \sigma_i^z \right\rangle \left\langle \sigma_j^z \right\rangle \sim e^{-|x_i - x_j|/\xi}$$

Correlation length

At the critical point all correlation lengths diverge

Universal behavior:

$$\xi \sim \frac{1}{|\lambda - \lambda_c|^{\nu}}$$

$$g_{\min} \sim \xi^{-z}$$

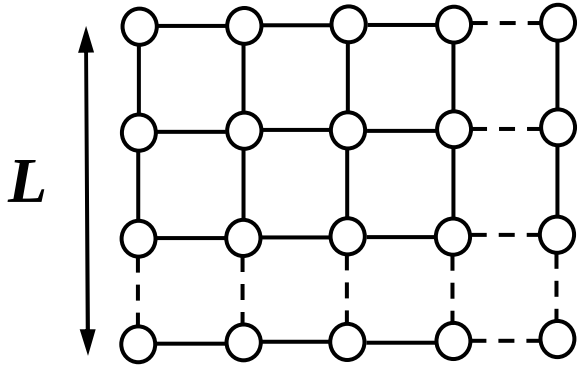
Critical exponents

Spectral Gap

For an infinitely large system

$$L \to \infty$$

$$\xi \to \infty \qquad g_{\min} \to 0$$



For a finite size system

$$\xi \sim L \sim N^{1/d} \quad \Rightarrow \quad g_{\min} \sim \xi^{-z} \sim L^{-z} \sim N^{-z/d}$$

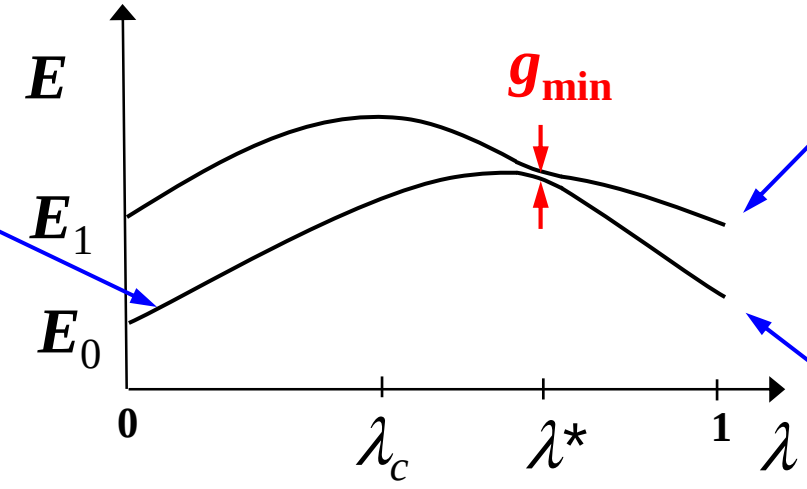
For a 2D lattice ($d = 2$): $g_{\min} \sim N^{-z/2}$

Dynamic critical exponent: $1 \le z \le 2$

1st Order Quantum Phase Transition

Large superposition

$$|E_0\rangle = 2^{-N/2}\sum_{z=1}^{2^N}|z\rangle$$



Local minimum

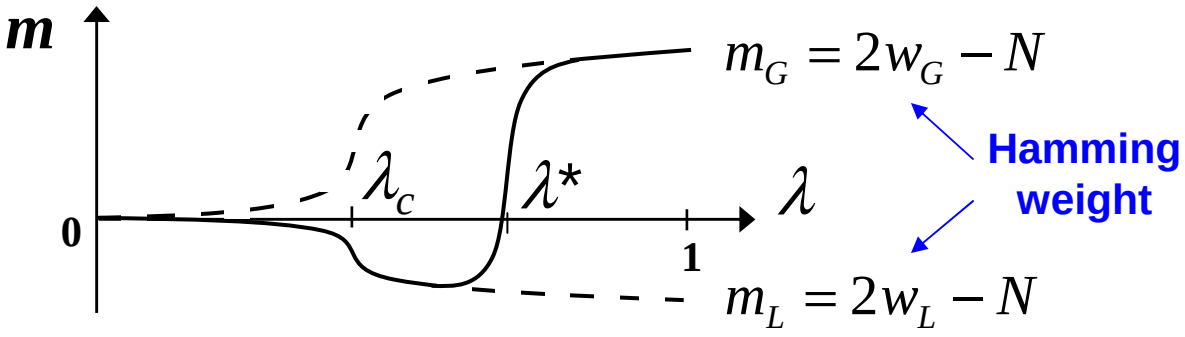
$|E_k\rangle = |L\rangle$

$|E_0\rangle = |G\rangle$

Global minimum

Order Parameter

$$m = \left\langle \sum_{i=1}^{N} \sigma_i^z \right\rangle$$



Perturbation Expansion

M. H. S. Amin and V. Choi, PRA 80, 062326 (2009)

$$H = H_0 + H'$$

Unperturbed Hamiltonian: $H_0 = \lambda H_P$

Perturbation Hamiltonian: $H' = (1-\lambda) H_B$

$$H_P = -\mathcal{E}\left(\sum_j h_j \sigma_j^z + \sum_{j,k} J_{jk}\sigma_j^z \sigma_k^z\right)$$

$$H_B = -\Delta \sum_j \sigma_j^x$$

⇒

Small parameter:

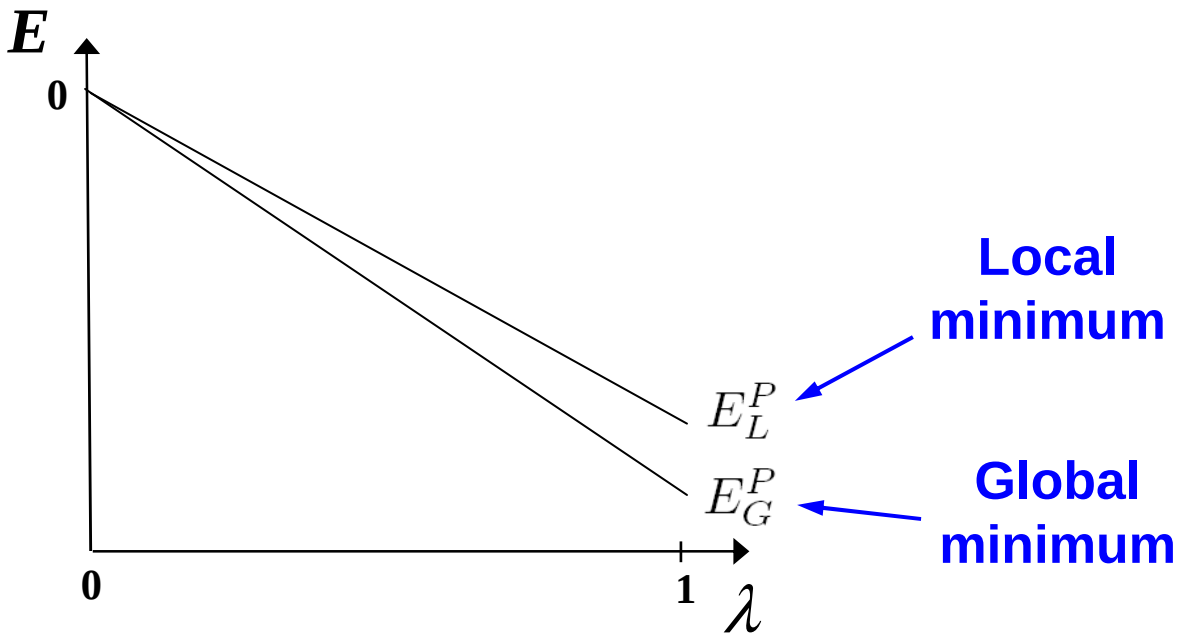
$$\zeta = \frac{(1-\lambda)\Delta}{\lambda \mathcal{E}}$$

H_B can only cause single bit flips

0th Order Perturbation

$$E_\alpha = E_\alpha^{(0)} + E_\alpha^{(1)} + E_\alpha^{(2)} + \ldots$$

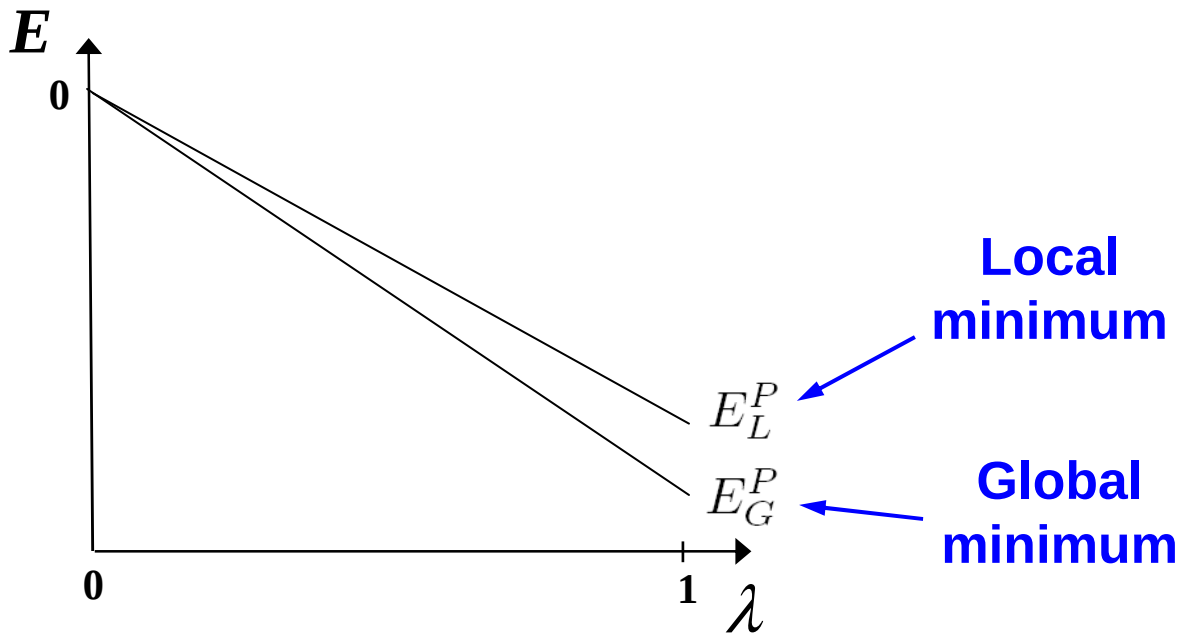
$$H_0 = \lambda H_P \quad \Rightarrow \quad E_\alpha^{(0)} = \lambda E_\alpha^P$$



1st Order Perturbation

$$E_\alpha = E_\alpha^{(0)} + E_\alpha^{(1)} + E_\alpha^{(2)} + \ldots$$

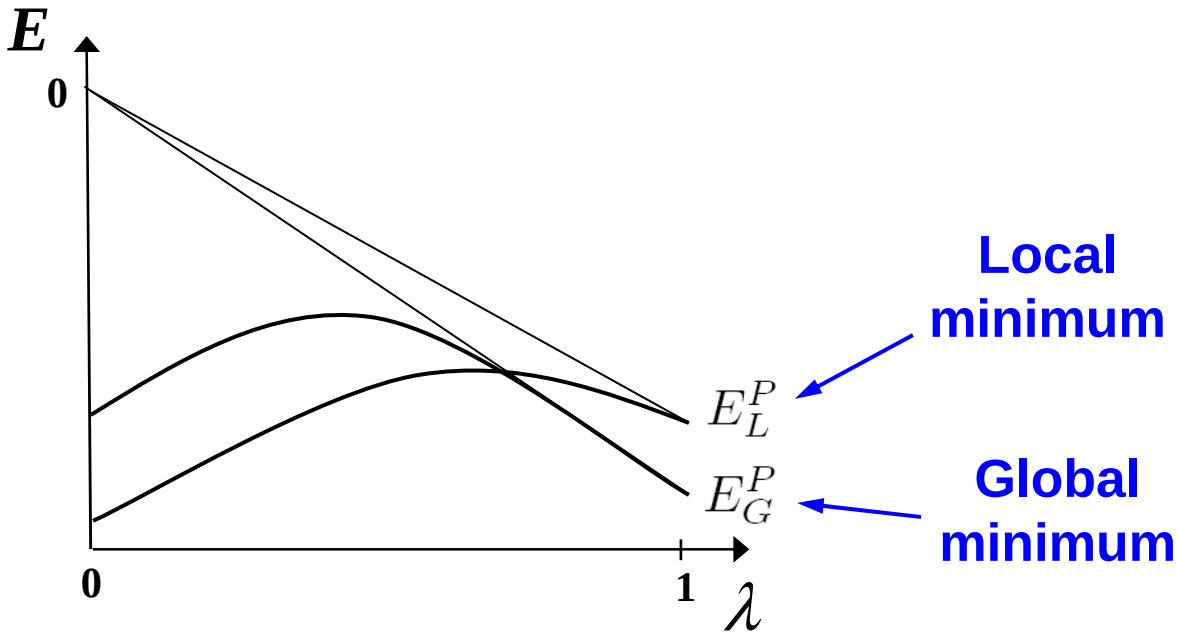
$$E_\alpha^{(1)} = (1-\lambda)\langle \alpha^{(0)} | H_B | \alpha^{(0)} \rangle = 0$$



2nd Order Perturbation

$$E_\alpha = E_\alpha^{(0)} + E_\alpha^{(1)} + E_\alpha^{(2)} + \ldots$$

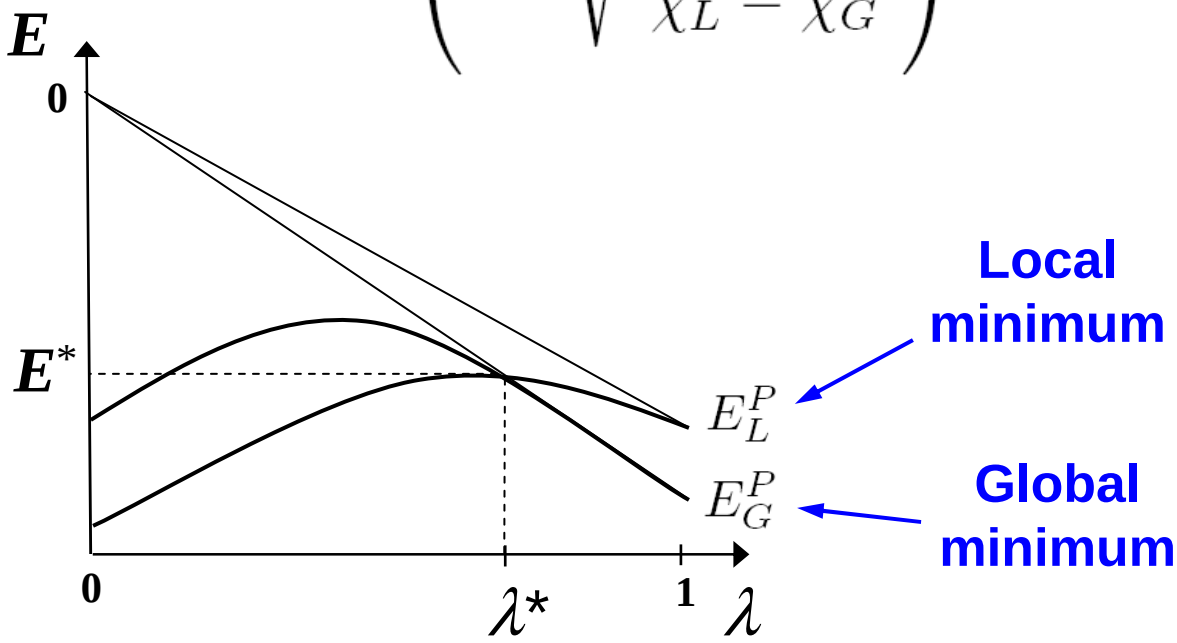
$$E_\alpha^{(2)} = (1-\lambda)^2 \sum_{n \notin \mathcal{S}_\alpha} \frac{|\langle \alpha^{(0)} | H_B | n^{(0)} \rangle|^2}{E_\alpha^{(0)} - E_n^{(0)}} = -\frac{(1-\lambda)^2}{\lambda} \chi_\alpha$$



2nd Order Perturbation

$$E_G = E_L = E^* \quad \Rightarrow \quad \lambda E_L^P - \frac{(1-\lambda)^2}{\lambda}\chi_L = \lambda E_G^P - \frac{(1-\lambda)^2}{\lambda}\chi_G$$

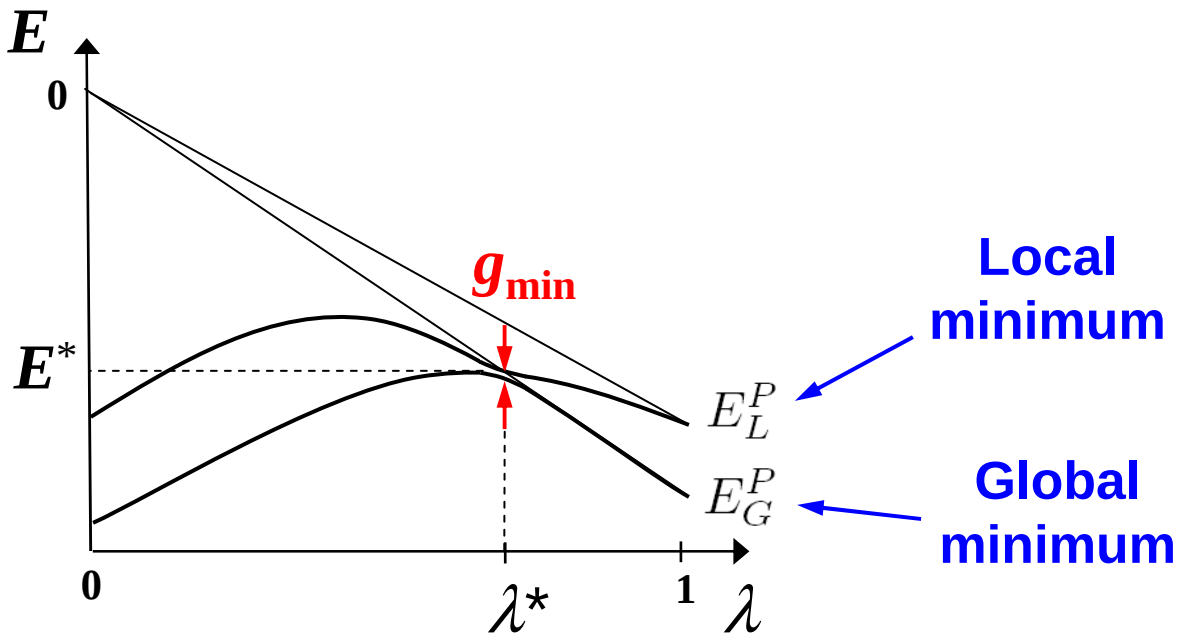
$$\lambda^* = \left(1 + \sqrt{\frac{E_L^P - E_G^P}{\chi_L - \chi_G}}\right)^{-1}$$



Minimum Gap

$$g_{\min} = 2|\langle L|H|G\rangle| = 2|\langle L^{(0)}|\widetilde{H}|G^{(0)}\rangle|$$

Perturbed states **Perturbed Hamiltonian**



Minimum Gap

$$H' = (1-\lambda)\Delta \sum_j \sigma_j^x$$

Minimum bit flips = *f*

$$\widetilde{H}_{LG} = \sum_{l_i \notin \mathcal{S}} \frac{\langle L^{(0)}|H'|l_1^{(0)}\rangle\langle l_1^{(0)}|H'|l_2^{(0)}\rangle ... \langle l_{m-1}^{(0)}|H'|G^{(0)}\rangle}{(E_G^{(0)}-E_{l_1}^{(0)})(E_G^{(0)}-E_{l_2}^{(0)})...(E_G^{(0)}-E_{l_{m-1}}^{(0)})},$$

$$\widetilde{H}_{GL} = \sum_{l_i \notin \mathcal{S}} \frac{\langle G^{(0)}|H'|l_1^{(0)}\rangle\langle l_1^{(0)}|H'|l_2^{(0)}\rangle ... \langle l_{m-1}^{(0)}|H'|L^{(0)}\rangle}{(E_L^{(0)}-E_{l_1}^{(0)})(E_L^{(0)}-E_{l_2}^{(0)})...(E_L^{(0)}-E_{l_{m-1}}^{(0)})}$$

$$g_{\min} = 2\sqrt{\widetilde{H}_{LG}\widetilde{H}_{GL}}$$

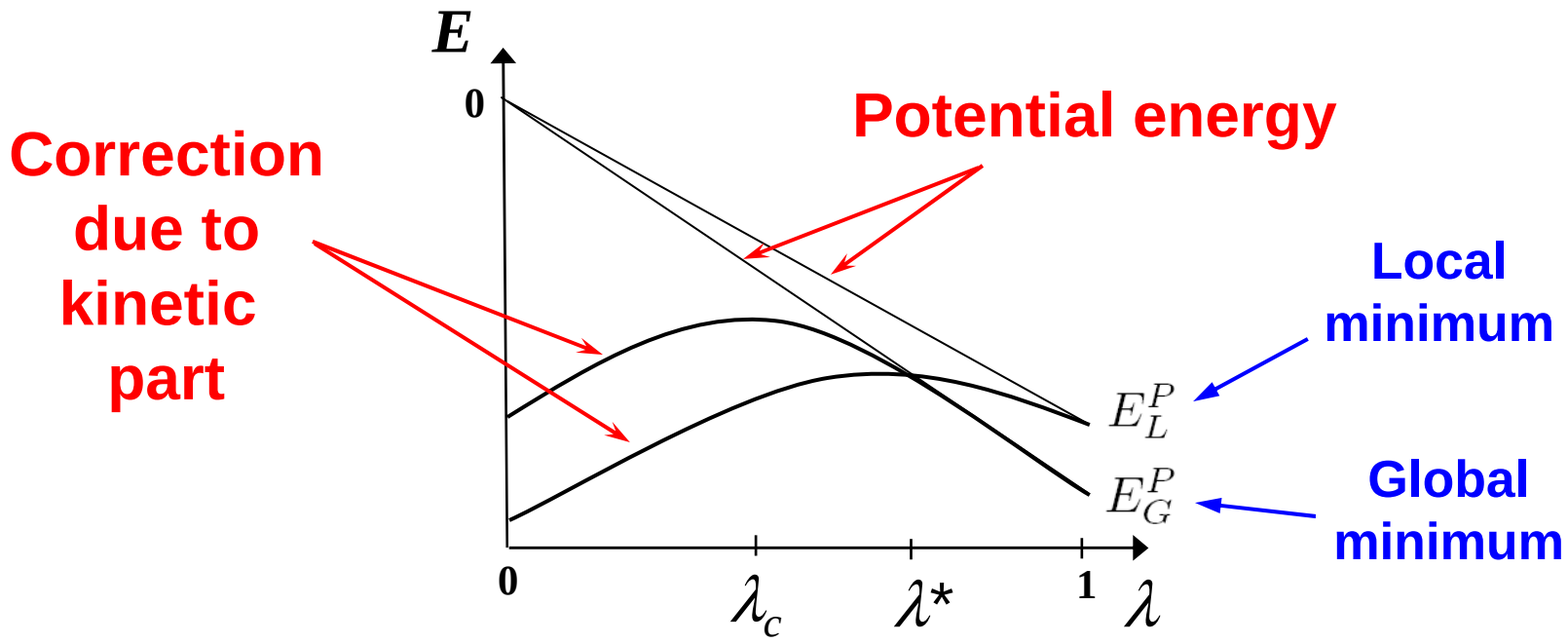
$$g_{\min} \sim \left[\frac{(1-\lambda^*)\Delta}{\lambda^*\mathcal{E}}\right]^{f} \leftarrow \boldsymbol{\kappa}$$

Hamming distance between global and local minima

What type of local minimum can create first order quantum phase transition?

$$H = (1- \lambda)\, H_B + \lambda\, H_P$$

Kinetic part **Potential part**

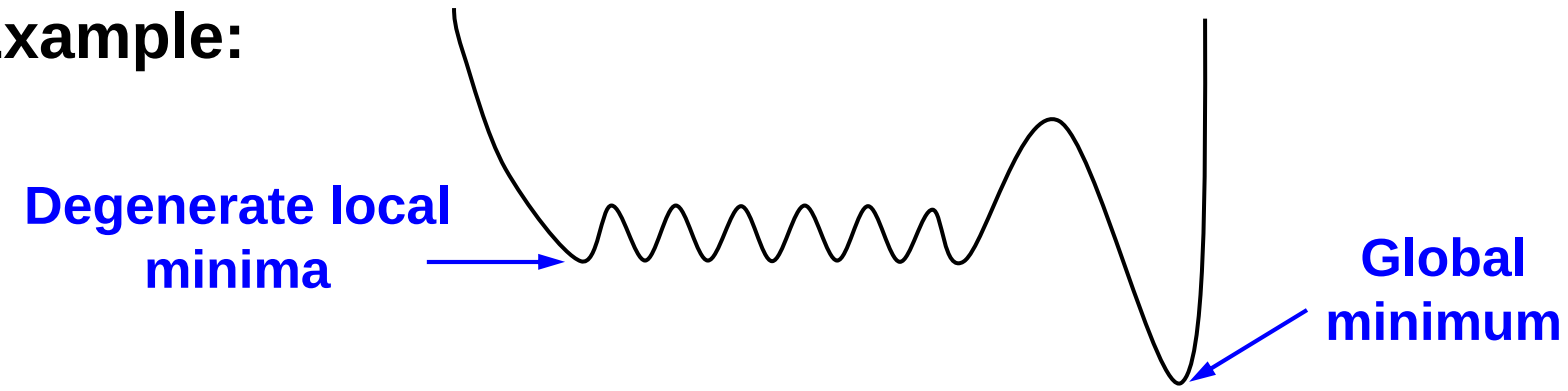


What type of local minimum can create first order quantum phase transition?

Answer: **A local minimum that can benefit more from the kinetic part than the global minimum**

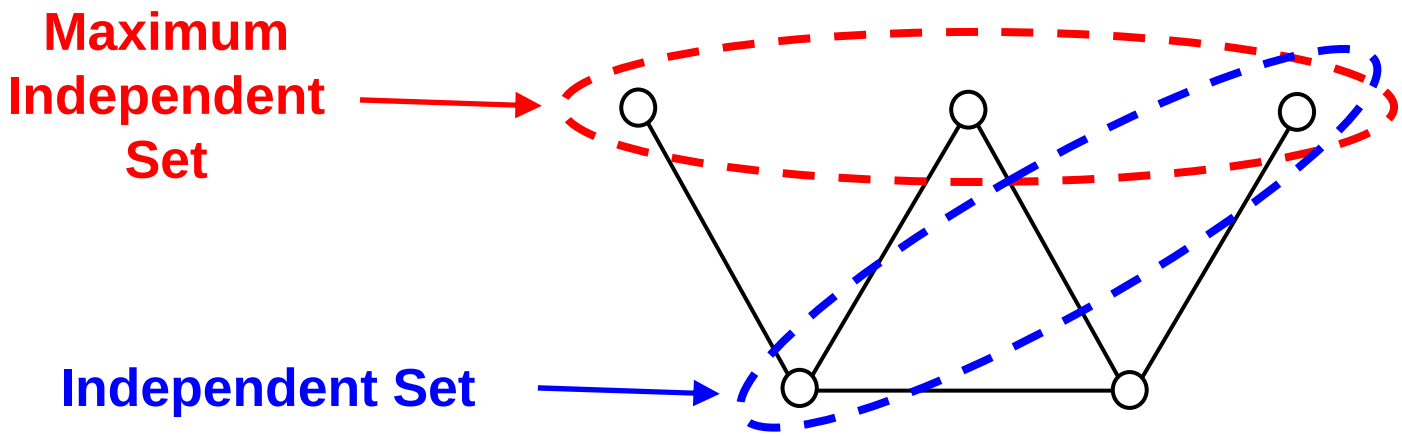
The system should move more freely within the local than the global minimum (more possibilities with less energy cost)

Example:



Maximum Independent Set (MIS) Problem

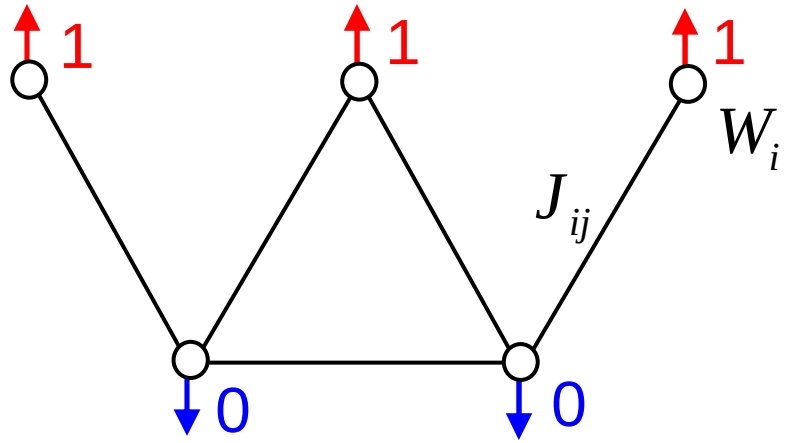
An independent set in a graph is a set of vertices that are not connected directly to each other



MIS is NP-hard

(Weighted) MIS Hamiltonian

$$H_P = -4\left\{\sum_i W_i x_i - \sum_{i,j} J_{ij} x_i x_j\right\} \qquad x_i \in \{0,1\}, \qquad J_{ij} > W_i, W_j$$



(Weighted) MIS Hamiltonian

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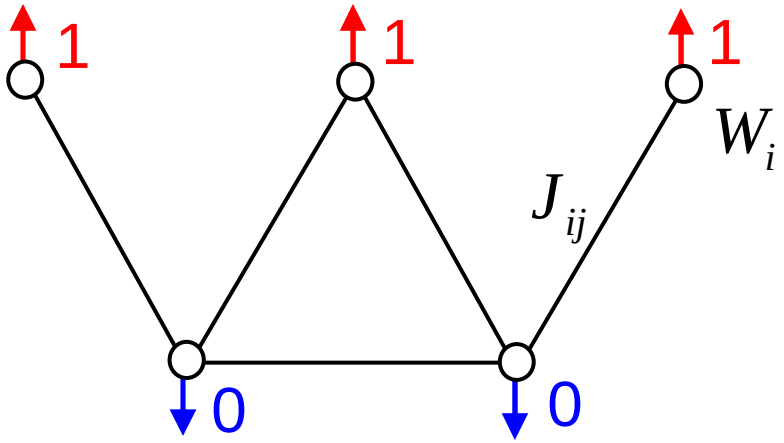
$$x_i = \frac{1+\sigma_i^z}{2}$$

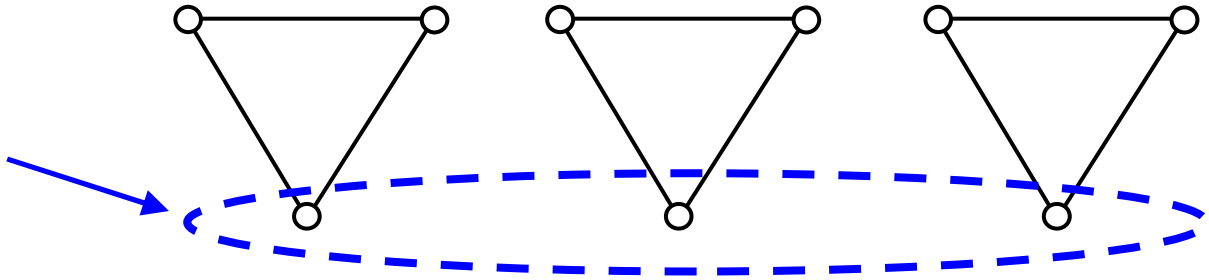
$$H_P = -\sum_i h_i \sigma_i^z + \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z$$

$$h_i = 2W_i - \sum_j J_{ij}$$



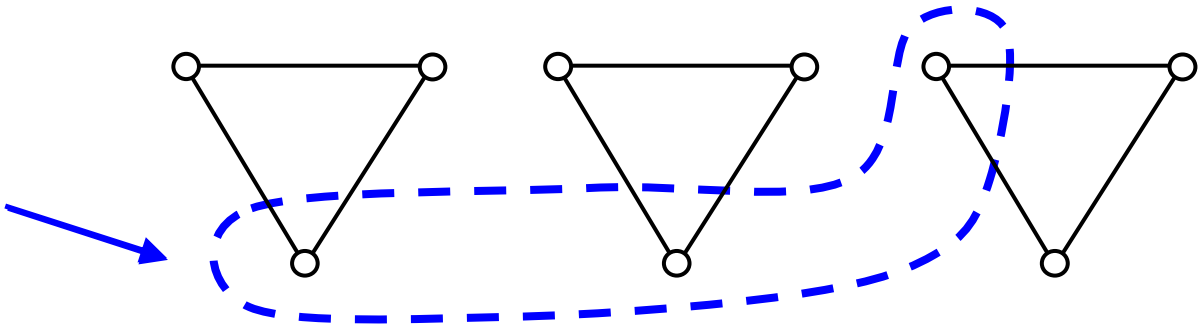
MIS Example

Maximum Independent Set (global minimum)

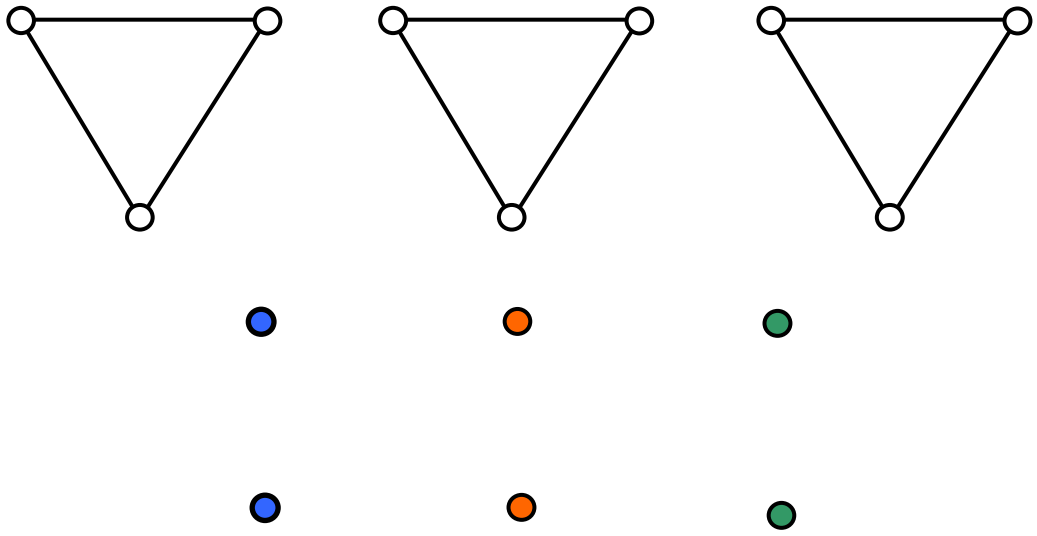


MIS Example

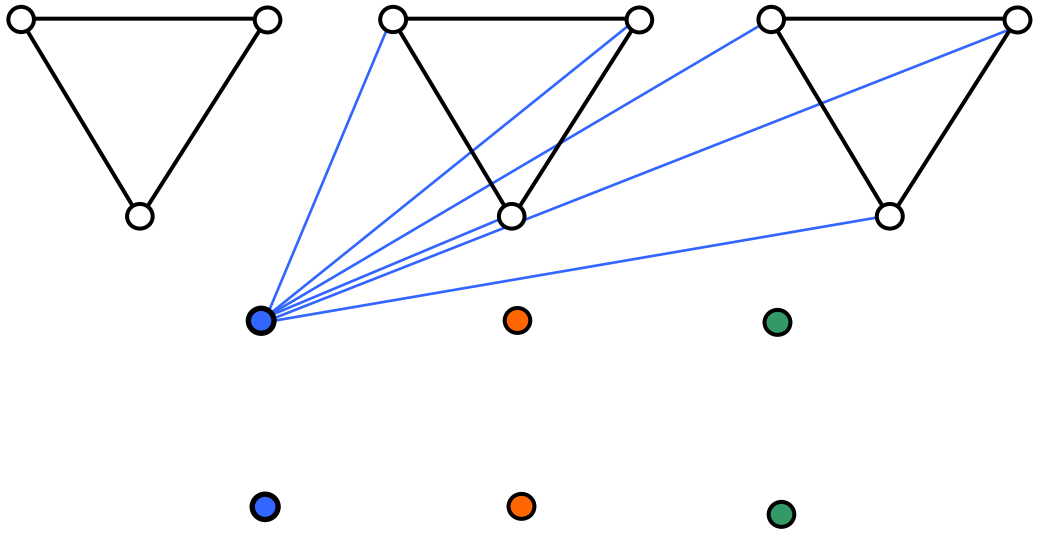
27 Maximum Independent Sets (global minima)



MIS Example

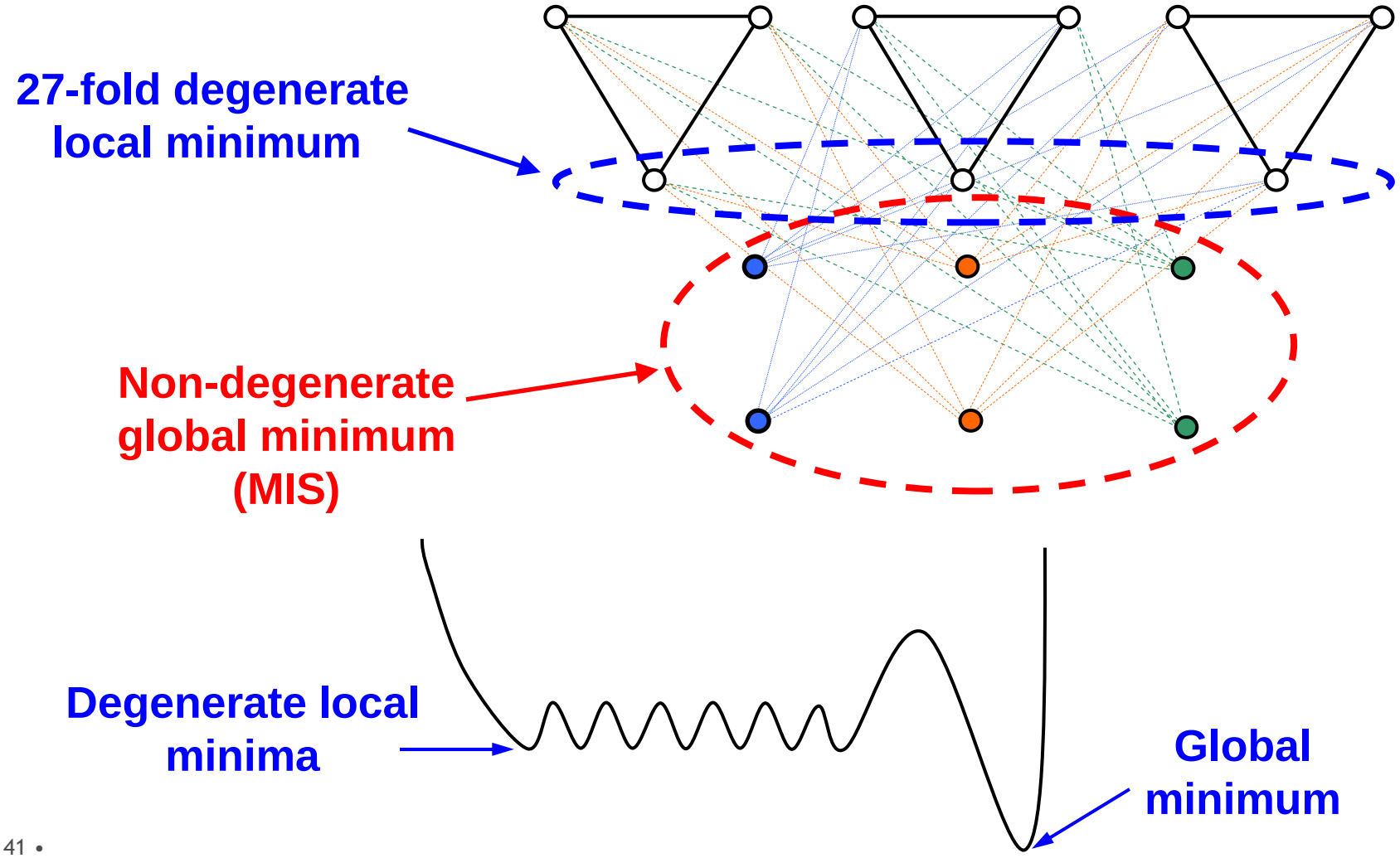


MIS Example

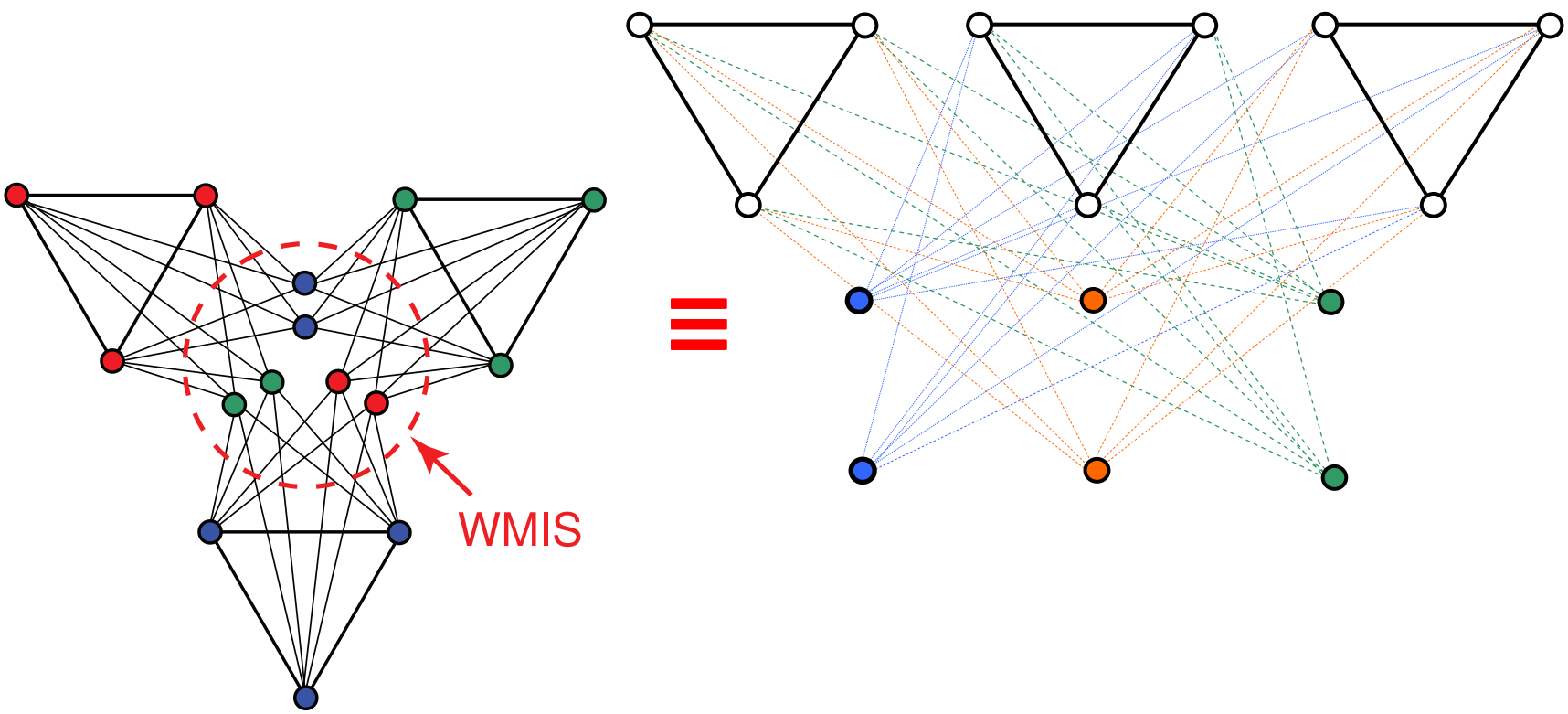


MIS Example

M. H. S. Amin and V. Choi, PRA 80, 062326 (2009)



MIS Example

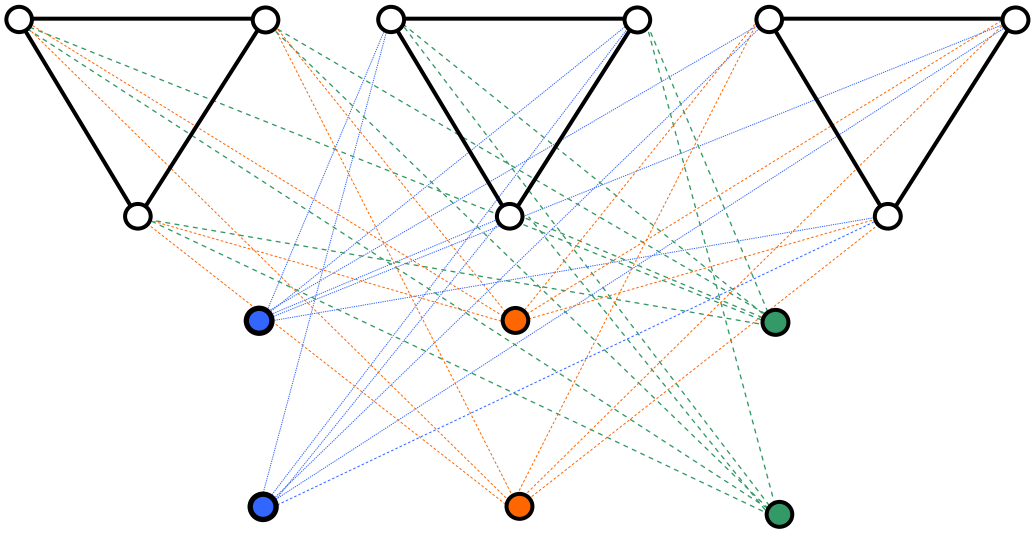


Weighted MIS

$J = 2$ $\Delta = 1$

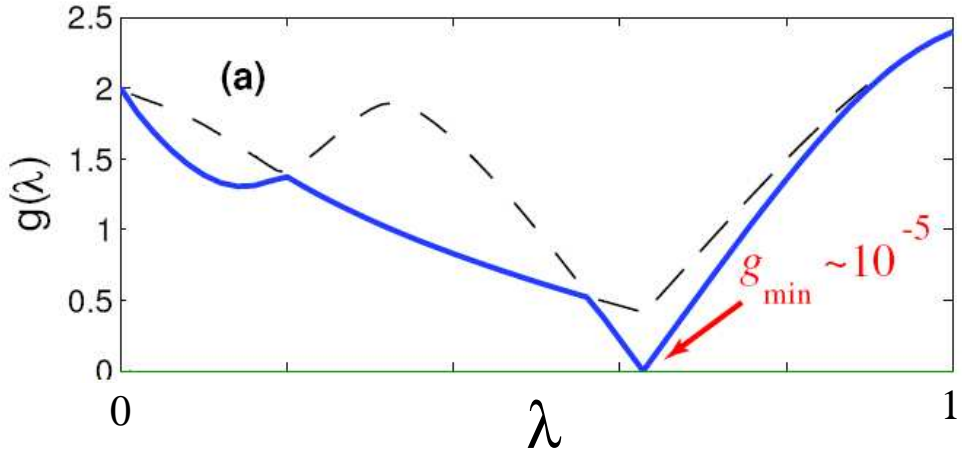
$W_i = W$ ⇨

$W_i = 1$ ⇨



Spectral Gap

$W = 1.8$



Two Interesting Quantities

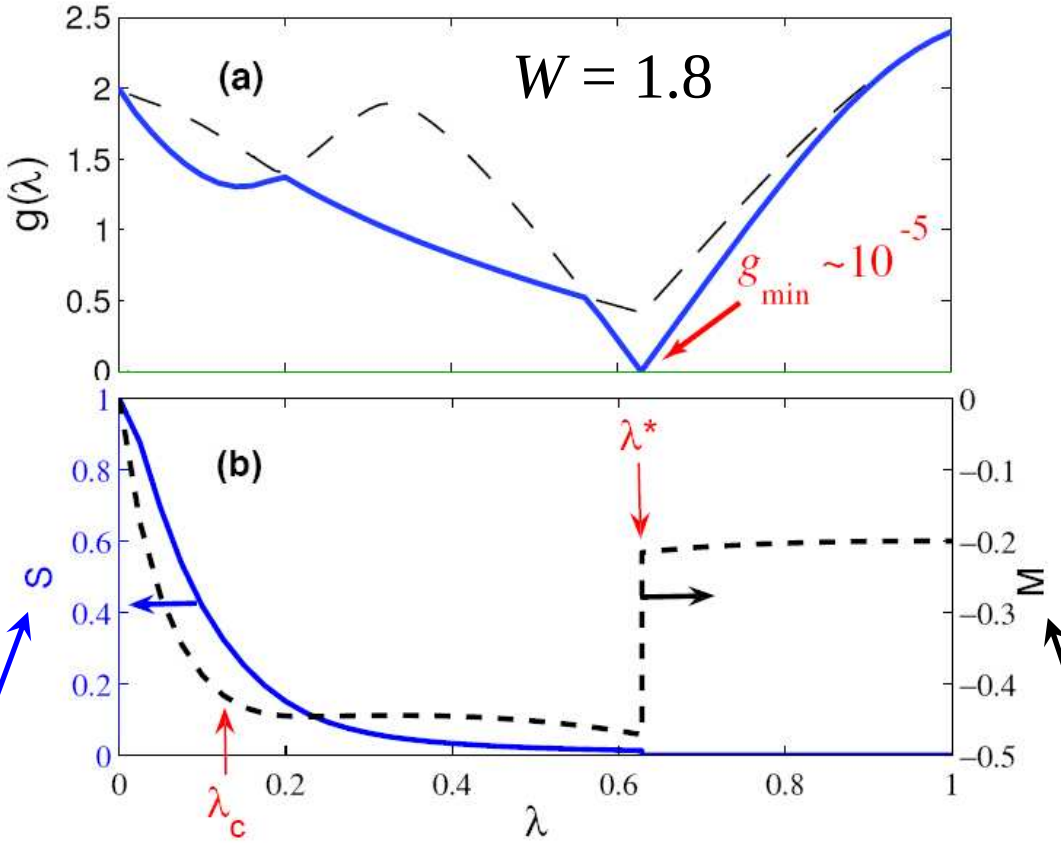
Magnetization (as an order parameter): $M = \frac{1}{N} \sum_{i=1}^{N} \langle \psi_0 | \sigma_i^z | \psi_0 \rangle$

Spread of the wave-function: $S = \frac{1}{2^N} [\sum_{n=1}^{2^N} | \langle \psi_0 | n \rangle | \ ]^2$

$$|\psi_0\rangle = \frac{1}{\sqrt{m}} \sum_{i=1}^{m} |i\rangle \quad \Longrightarrow \quad S = \frac{m}{2^N}$$

S = fraction of states participating in the superposition

Order Parameter & Wave Function Spread



$$S=\frac{1}{2^N}[\sum_{n=1}^{2^N}|\langle\psi_0|n\rangle|\ ]^2$$

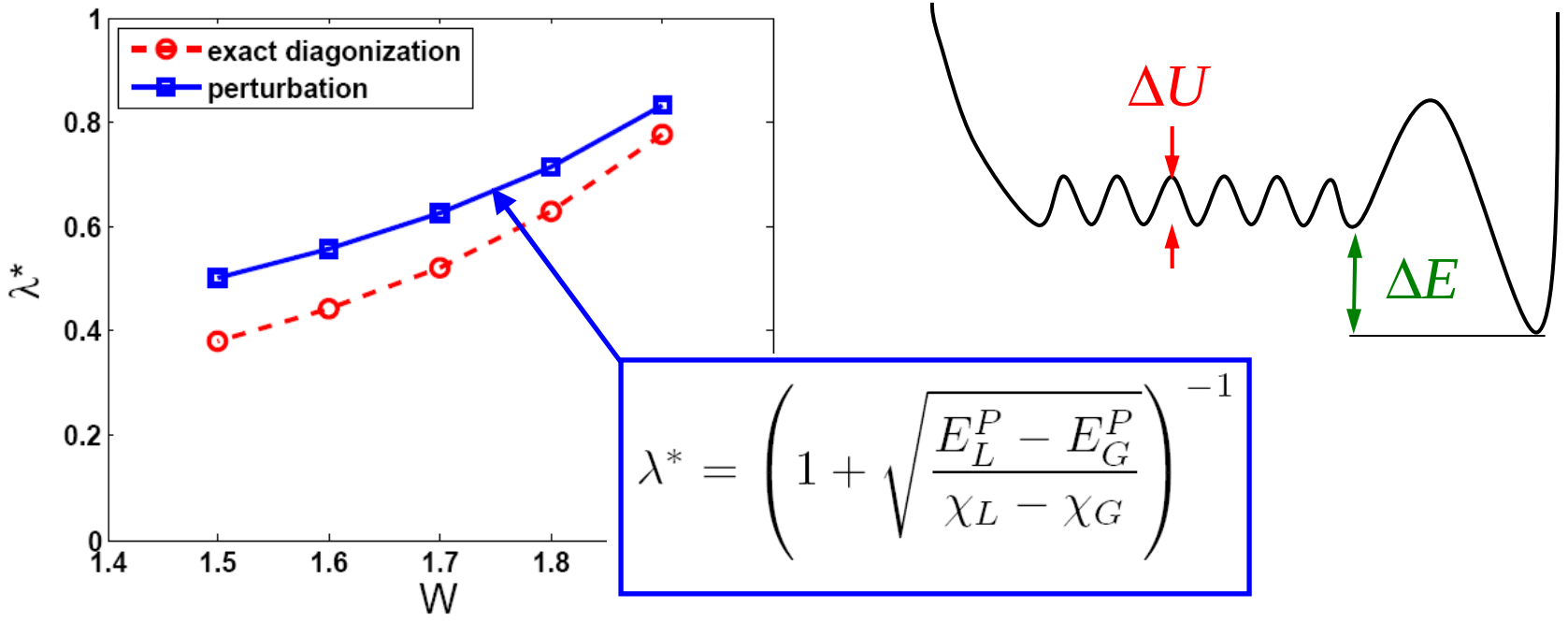
$$M=\frac{1}{N}\sum_{i=1}^{N}\langle\psi_0|\sigma_i^z|\psi_0\rangle$$

Minimum Gap

Barrier height $\Delta U = 4(2-W) \rightarrow 0$

$\Delta E = 12(2-W) \rightarrow 0$

as $W \rightarrow 2$



Minimum Gap

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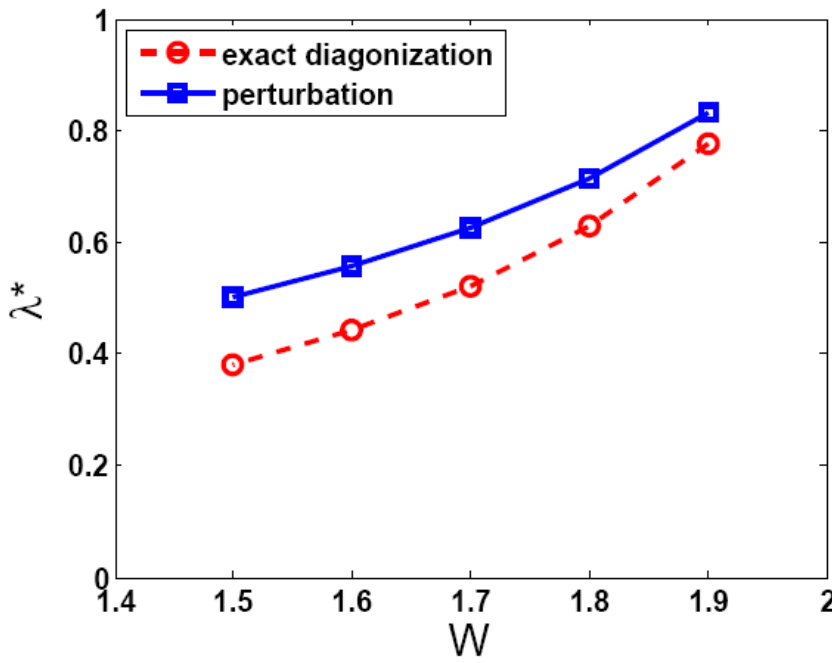

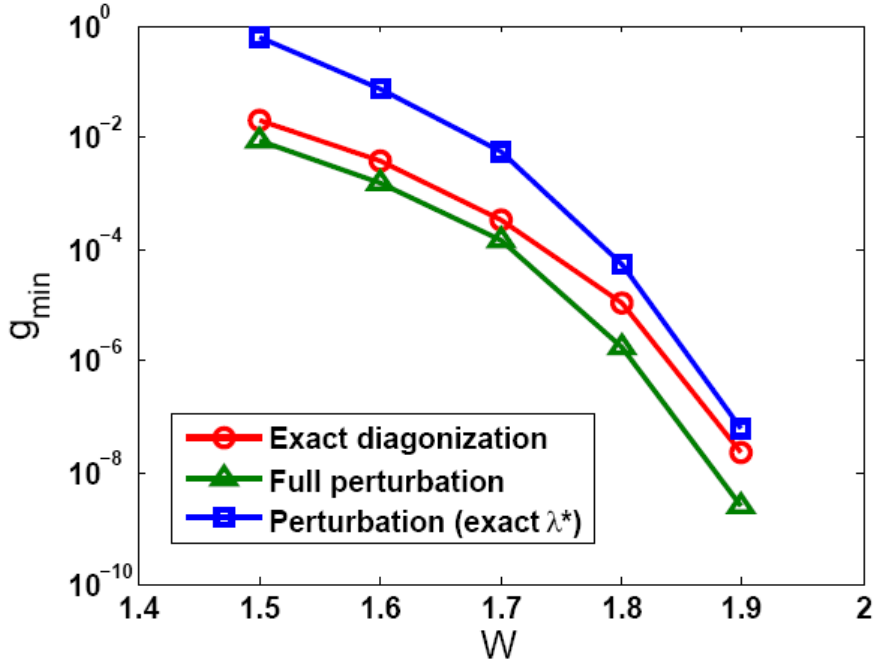

The gap is exponentially sensitive to W

Controversy

M. H. S. Amin and V. Choi, PRA 80, 062326 (2009)

B. Altshuler, H. Krovi, and J. Roland, arXiv:0908.2782,
PNAS 107, 12446 (2010) **(See Altshuler's presentation on July 23)**

E. Farhi, J. Goldstone, D. Gosset, S. Gutmann, H. B. Meyer and P. Shor, arXiv:0909.4766

A.P. Young, S. Knysh, V.N. Smelyanskiy, PRL 104, 020502 (2010)

T. Jorg, F. Krzakala, G. Semerjian, and F. Zamponi, PRL 104, 207206 (2010)

S. Knysh, V.N. Smelyanskiy, arXiv:1005.3011

V. Choi, arXiv:1004.2226 **(See Choi's presentation on July 23)**

N. Dickson, M.H.S. Amin, **(See Dickson's poster on July 24)**

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