Low-lying excitations of quantum spin-glasses

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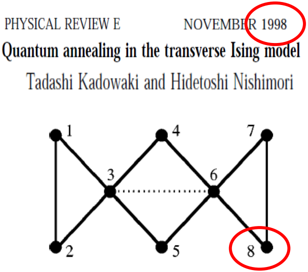
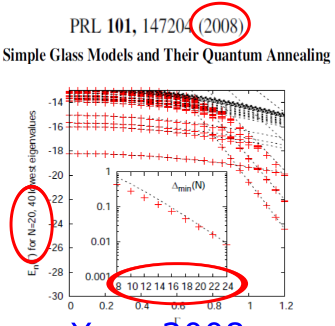
A ‘Personal’ Motivation





Year: 1998
Size: 8 spins

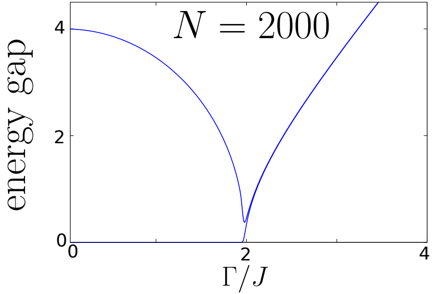
Year: 2008
Size: 24 spins

Difficulty:
Dimension of Hilbert space increases exponentially with system size

Ordered spin systems are easier

Ferromagnet: $H_J = -\frac{J}{N}\left(\sum_{i=1}^{N}\sigma_i^z\right)^2 - \Gamma\sum_{i=1}^{N}\sigma_i^x$

Conserved quantity: $\boxed{[H_J, S^2] = 0}$



For spin-glasses: $\boxed{[H_{J_{ij}}, S^2] \neq 0}$

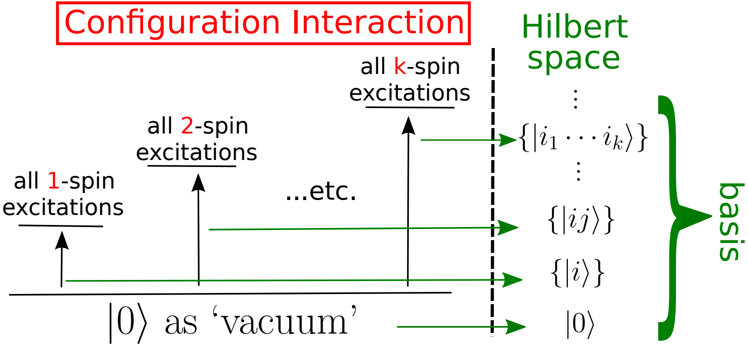
Hartree-Fock and Configuration Interaction Theory

Hartree-Fock approximation

$$|s_1\rangle \otimes \cdots \otimes |s_N\rangle \overset{\text{def.}}{=} |0\rangle$$

Wavefunctions of individual spins factorize.

Configuration Interaction



SK model and its Hartree-Fock Approximation

Sherrington-Kirkpatrick (SK) model:

$$H = -\sum_{i>j} J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x. \quad (1)$$

$\mathrm{Prob}(J_{ij}) = \mathrm{Gaussian}.$

Hartree-Fock wavefunction:

$$|0\rangle = \prod_{i=1}^{N} \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix}. \quad (2)$$

We minimize

$$E^{\mathrm{HF}} = \langle 0|H|0\rangle, \quad (3)$$

with respect to $\{\alpha_i, \beta_i\}$, subjected to $\alpha_i^2 + \beta_i^2 = 1$.

HF Energy, HF Equations, and stability matrix

HF energy:

$$E^{\mathrm{HF}} = -\sum_{i>j} J_{ij}(\alpha_i^2 - \beta_i^2)(\alpha_j^2 - \beta_j^2) - 2\Gamma \sum_i \alpha_i \beta_i. \tag{4}$$

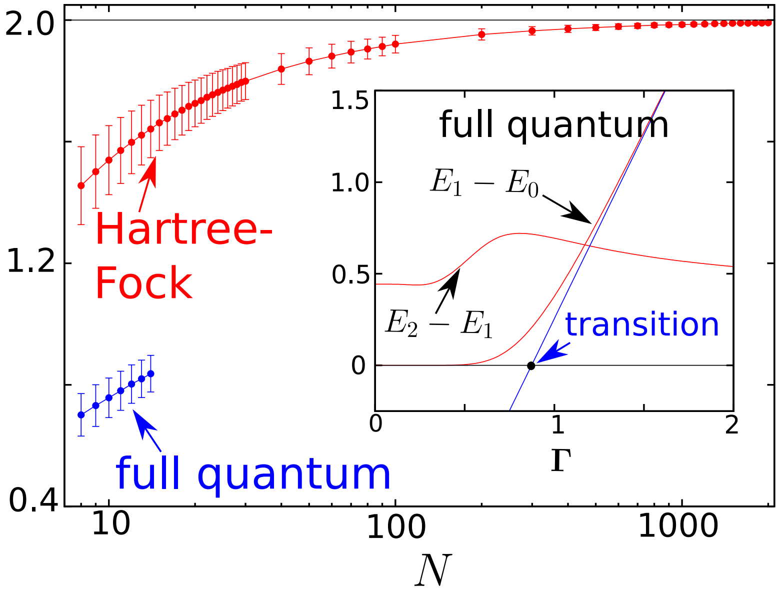
Stationary conditions, $\frac{\partial E^{\mathrm{HF}}}{\partial \alpha_i} = 0$ (HF equations):

$$\frac{2\Gamma(2\alpha_i^2 - 1)}{\sqrt{1-\alpha_i^2}} - 4\alpha_i \sum_{a\neq i} J_{ia}(2\alpha_a^2 - 1) = 0. \tag{5}$$

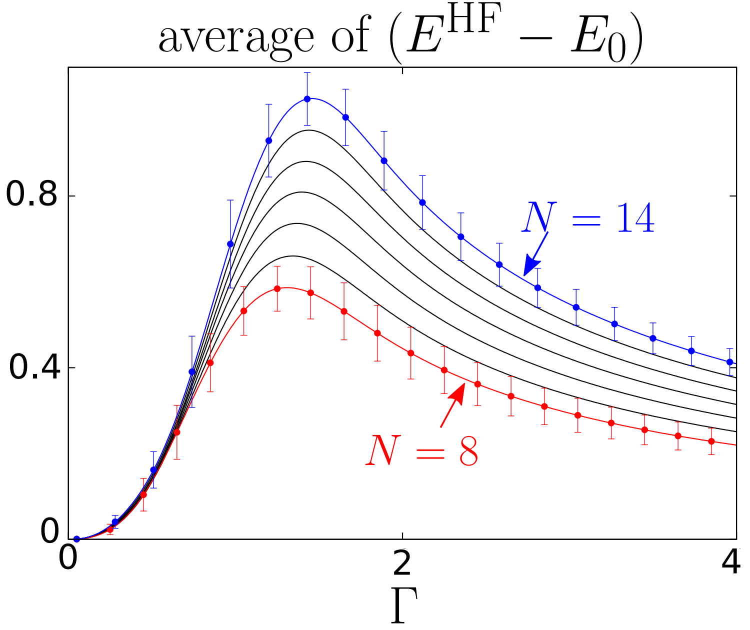
Paramagnetic solution: $\alpha_{\mathrm{para}} = (1/\sqrt{2}, \cdots, 1/\sqrt{2})$.
Its stability:

$$\left.\frac{\partial^2 E^{\mathrm{HF}}}{\partial \alpha_i \partial \alpha_j}\right|_{\alpha_{\mathrm{para}}} = 8(\Gamma\delta_{ij} - J_{ij}). \tag{6}$$

Transition into ordered phase: A HF description



Comparing E^{HF} with exact E_0



Generating Excitations

Since H does not involve y-direction,

$$\sigma^y \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \text{flips the spinor } \begin{pmatrix} \alpha \\ \beta \end{pmatrix}. \tag{7}$$

To excite ith spin of $|0\rangle$,

$$|i\rangle = \sigma_i^y |0\rangle. \tag{8}$$

To excite ith and jth spins of $|0\rangle$,

$$|ij\rangle = \sigma_i^y \sigma_j^y |0\rangle. \tag{9}$$

etc.

We generate a subspace spanned by $\{|0\rangle, |i\rangle, |ij\rangle\}$.

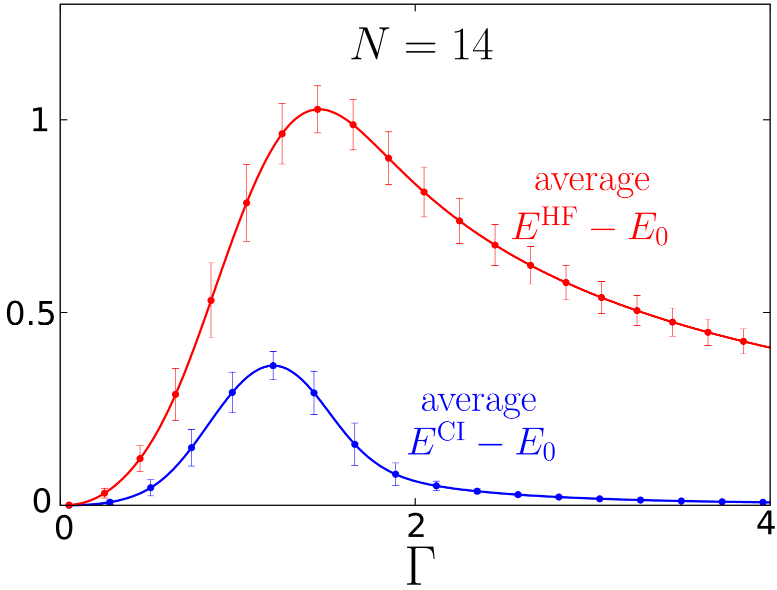
Configuration Interaction Matrix

truncated CI matrix

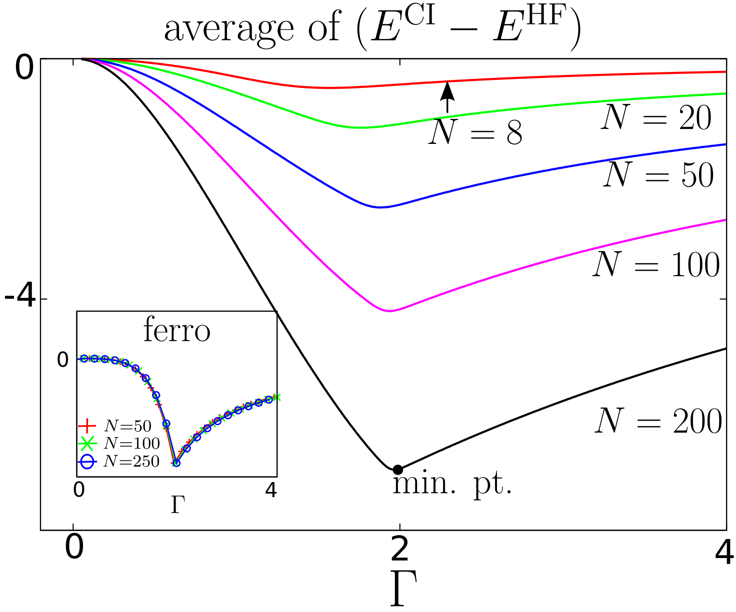
$$
\begin{array}{cc}
 & \begin{array}{ccccc} |0\rangle & |i\rangle & |ij\rangle & |ijk\rangle & \cdots \end{array} \\
\begin{array}{c} |0\rangle \\ |i\rangle \\ |ij\rangle \\ |ijk\rangle \\ \vdots \end{array} &
\begin{pmatrix}
E^{\mathrm{HF}} & \langle 0|H|i\rangle & \langle 0|H|ij\rangle & \cdots \\
\langle i|H|0\rangle & \langle i|H|i\rangle & \langle i|H|ij\rangle & \cdots \\
\langle ij|H|0\rangle & \langle ij|H|i\rangle & \langle ij|H|ij\rangle & \cdots \\
\vdots & \vdots & \vdots & \\
 & & &
\end{pmatrix}
\end{array}
$$

dim. of matrix: $O(N^2)$

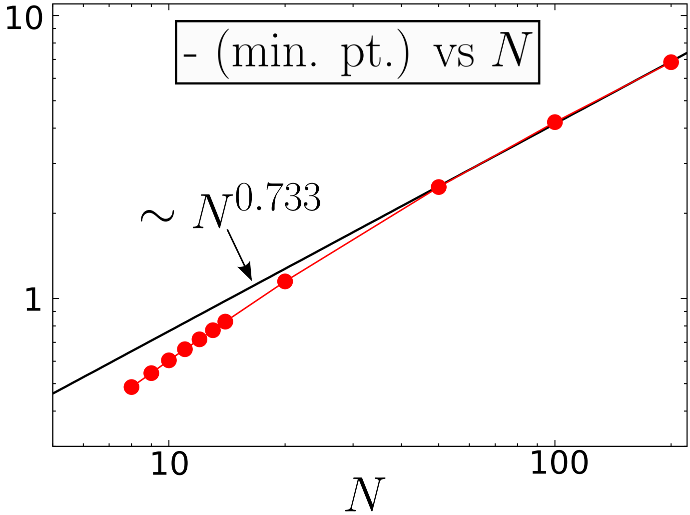
Improvement of E^{CI} over E^{HF}



Correction to extensive part of E_0



Scaling of sub-extensive correction to E^{HF}

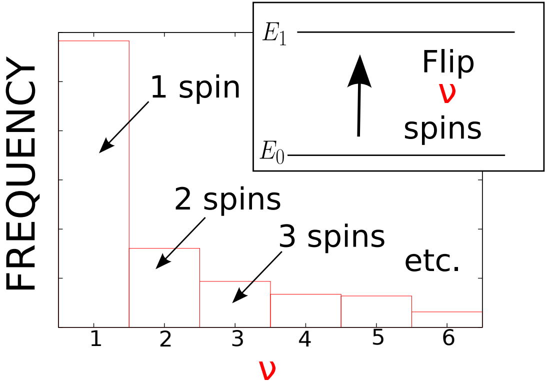


$$E_0 = NC_1 + N^{0.733} C_2 + \cdots$$

Energy gap

The first excited-state is quite complex...

Classical SK energy: $-\sum_{i>j} J_{ij}\sigma_i\sigma_j$



We simplify by assuming $\nu = 1$ for all J_{ij}.

A Formula for the Energy Gap

Energy gap:

$$\Delta = E_1 - E_0 \tag{10}$$

Consider an 'excitation' operator A:

$$|E_1\rangle = A|E_0\rangle. \tag{11}$$

We define a generating function:

$$G(\gamma) = \langle E_0|e^{-i\gamma A} H e^{i\gamma A}|E_0\rangle. \tag{12}$$

Expanding $e^{\pm i\gamma A}$,

$$\gamma^0 C_0 + \gamma^1 C_1 - \frac{\gamma^2}{2}\langle E_0|HA^2 + A^2 H - 2AHA|E_0\rangle + O(\gamma^3) \tag{13}$$

Expanding $G(\gamma)$, and equating:

$$\Delta(|E_0\rangle, A) = \frac{1}{2}\frac{1}{\langle E_0|A^2|E_0\rangle}\left.\frac{\partial^2 G}{\partial\gamma^2}\right|_{\gamma=0}. \tag{14}$$

Only $|E_0\rangle$ is needed! Use approximate HF/CI wavefunctions.
But how do we compute $\partial^2 G/\partial\gamma^2$?

Example: Let $|E_0\rangle = |0\rangle$. Let $A = A_1$.

Let

$$A = A_1 = \sum_{i=1}^{N} y_i \sigma_i^y, \tag{15}$$

y_i: parameters.
We want $G_1^{\mathrm{HF}}(\gamma) = \langle 0|e^{-i\gamma A_1} H e^{i\gamma A_1}|0\rangle$.

$$|\bar{0}\rangle = e^{i\gamma A_1}|0\rangle = \prod_i e^{i\gamma y_i \sigma_i^y} \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} = \prod_i \begin{pmatrix} \bar{\alpha}_i(\gamma) \\ \bar{\beta}_i(\gamma) \end{pmatrix}. \tag{16}$$

So

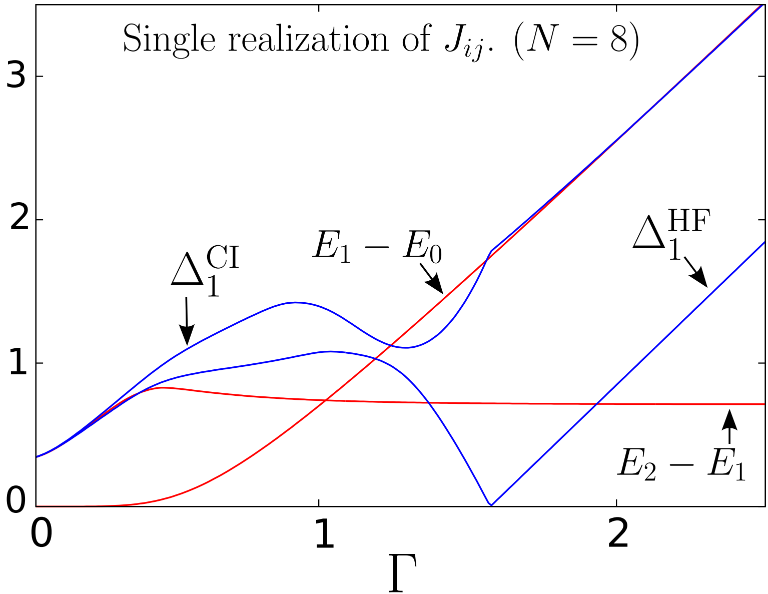
$$G_1^{\mathrm{HF}}(\gamma) = \langle \bar{0}|H|\bar{0}\rangle = E^{\mathrm{HF}}(\bar{\alpha}_i(\gamma), \bar{\beta}_i(\gamma)). \tag{17}$$

Hence

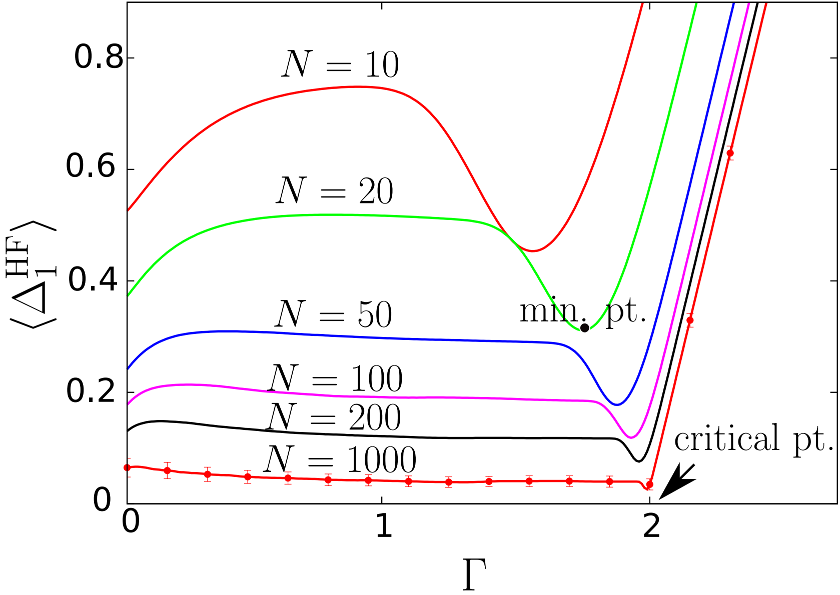
$$\Delta_1^{\mathrm{HF}} = \frac{1}{2}\frac{\partial^2 E^{\mathrm{HF}}(\gamma)}{\partial \gamma^2} = -8\sum_{i\neq j} J_{ij}\alpha_i\alpha_j\beta_i\beta_j y_i y_j + \Gamma \sum_i \frac{y_i^2}{\alpha_i\beta_i}. \tag{18}$$

Minimize Δ_1^{HF} with respect to $\{y_i\}$ to obtain gap.

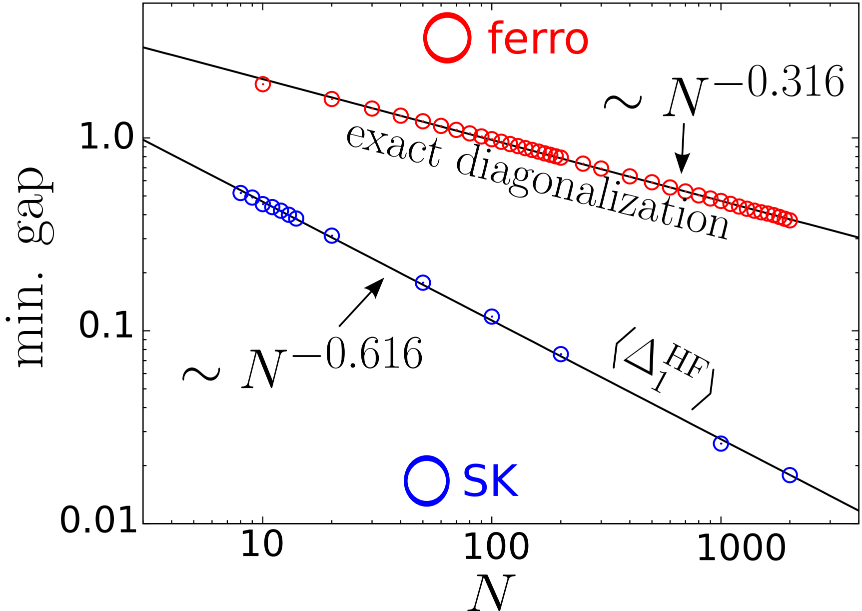
Small N: Comparing with full quantum



Average HF gap

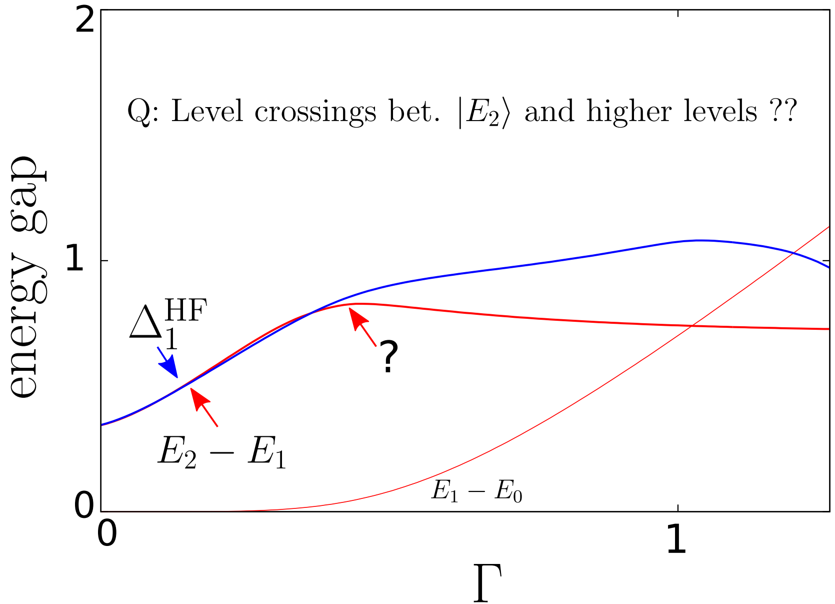


Scaling of gap near critical point

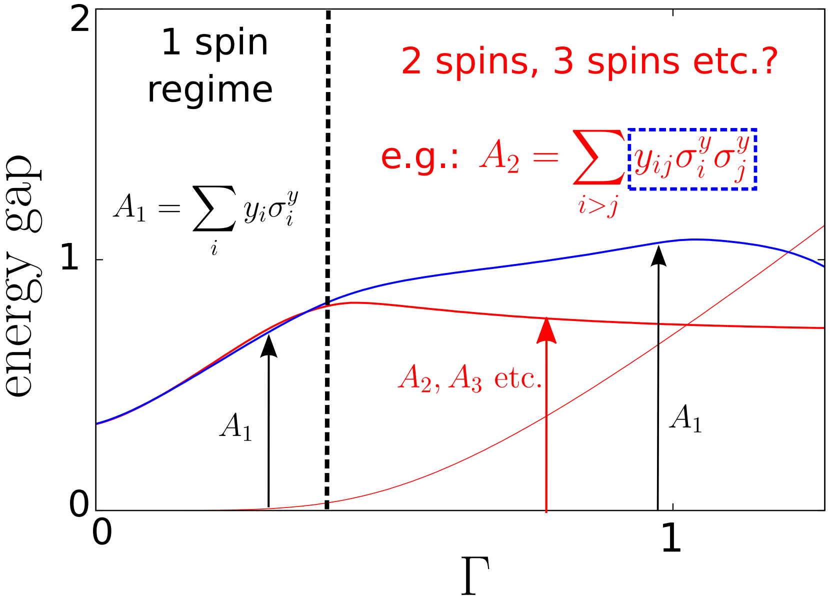


Some speculations...

Complexity of gap in the glass phase...



Different A's for different regimes?

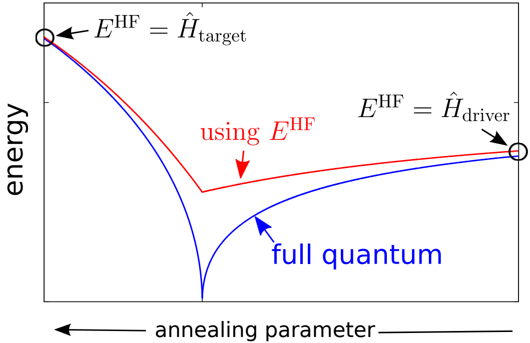


'Hartree-Fock' annealing?

Simulated annealing: $F = -\frac{1}{\beta} \ln \mathrm{Tr}\left[\exp\left(-\beta H_{\mathrm{target}}\right)\right]$ → thermal fluctuations

Quantum annealing: $\hat{H} = \hat{H}_{\mathrm{target}} + \hat{H}_{\mathrm{driver}}$ → quantum fluctuations

'Hartree-Fock' annealing: $E^{\mathrm{HF}} = \langle 0|\hat{H}|0\rangle$



Possible merits of HF annealing

1. No operators are involved. Recall that for SK model

$$E^{\mathrm{HF}} = -\sum_{i>j} J_{ij}(\alpha_i^2 - \beta_i^2)(\alpha_j^2 - \beta_j^2) - 2\Gamma \sum_i \alpha_i \beta_i$$

   α_i, β_i are just numbers. Simpler than annealing $\hat{H}$ itself.

2. Dependence on annealing parameter (Γ) is simple. Simpler than simulated annealing.

3. Hardware implementation of E^{HF} using a classical machine?