Nature of the Spin Glass Phase in finite dimensional (Ising) Spin Glasses

J. J. Ruiz-Lorenzo

Dep. Física & ICCAEx (Univ. de Extremadura) & BIFI (Zaragoza)
http://www.eweb.unex.es/eweb/fisteor/juan/juan_talks.html

Ising Lectures-2019
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Outline of the Talk

- Tuesday
  - What are spin glasses?
  - Different Theories and Models:
    - Droplet
    - Chaotic Pairs
    - RSB
  - Spin glass in presence of a magnetic field.
    - Phase transition in $d = 4$.
    - But in $d = 3$?

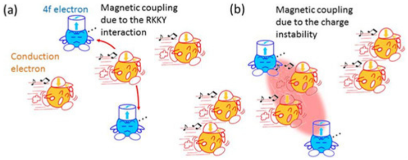
Outline of the Talk

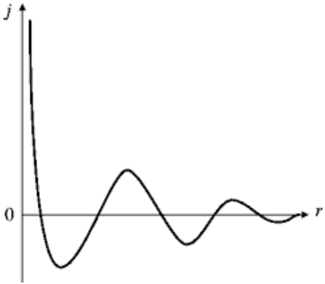
- Wednesday
  - Fluctuation-Dissipation relations out of equilibrium.
    - Theoretical basis.
    - Static-Dynamics Relation: Computation of $P(q)$.
    - Measurement of $P(q)$.
  - Phases and Thermodynamic limit in Disordered systems: The Metastate.
    - Numerical construction of the Aizenman-Wehr Metastate
    - Observables and Numerical Simulations.
    - Results.
  - Conclusions and Open Problems.

What are Spin glasses

- Materials with disorder and fustration.
- Quenched disorder.
- Canonical Spin Glass: Metallic host (Cu) with magnetic impurities (Mn).
- RKKY interaction between magnetic moments: $J(r) \sim \frac{\cos(2k_F r)}{r^3}$.
- Role of anisotropy: Ag:Mn at 2.5% (Heisenberg like), $CdCr_{1.7}IN_{0.3}S_4$ (also Heisenberg like) and $Fe_{0.5}Mn_{0.5}TiO_3$ (Ising like).

RKKY interaction



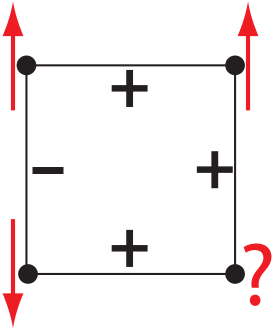


Simplification: We take the J_{ij} as random variables! For instance, Gaussian or from a bimodal probability distribution.

Frustration

Energy:

$$E = -\sum_{<ij>} J_{ij} S_i S_j$$



Quenched and Annealed Disorder

- We compute the partition function for a given realization of the couplings:

$$\mathcal{Z}_J = \sum_{[S_i]} \exp(-\beta \mathcal{H}_J) = \sum_{[S_i]} \exp(\beta \sum_{ij} J_{ij} S_i S_j)$$

- Next, we compute its free energy:

$$F_J = -\frac{1}{\beta} \log \mathcal{Z}_J$$

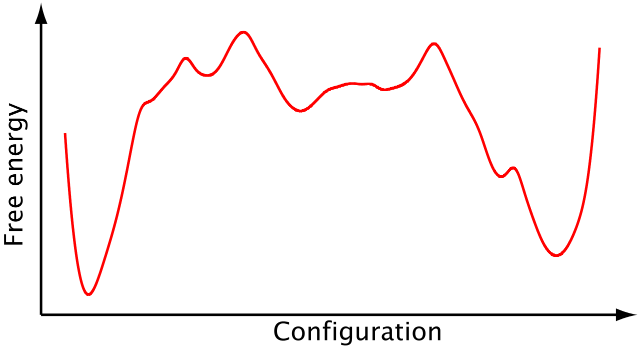
- Finally, we average the different free energies

$$F = \overline{F_J} = \int d[J] p[J] F_J$$

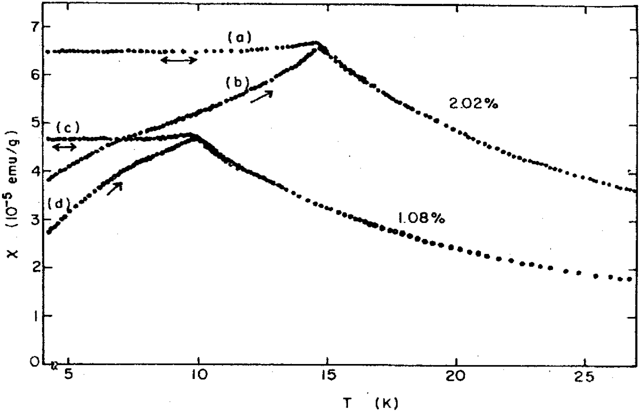
- Annealed average:

$$F = -\frac{1}{\beta} \log \int d[J] p[J] \sum_{[S_i]} \exp(-\beta \mathcal{H}_{\mathcal{J}})$$

Free energy landscape (Disorder+Frustration)



Some experiment (ZF and F-cooled susceptibility)



Some Definitions

- The typical Spin Glass Hamiltonian:

$$\mathcal{H} = -\sum_{i,j} J_{ij}\sigma_i\sigma_j$$

$J_{ij} = \pm 1$ with equal probability.

- The order parameter is:

$$q_{\mathrm{EA}} = \overline{\langle \sigma_i \rangle^2}$$

Using two real replicas:

$$\mathcal{H} = -\sum_{i,j} J_{ij}\left(\sigma_i\sigma_j + \tau_i\tau_j\right)$$

Let $q_i = \sigma_i\tau_i$ be the normal overlap, then: $q_{\mathrm{EA}} = \overline{\langle \sigma_i\tau_i \rangle}$.

Different Theories and Models

The Droplet Model

- Based on the Migdal-Kadanoff implementation (approximate) of the Renormalization Group (exact in $D = 1$).
- *Disguished Ferromagnet*: Only two pure states with order parameter $\pm q_{\rm EA}$ (related by spin flip).
- Compact Excitations of fractal dimension d_f. The energy of a excitation of linear size L grows as L^θ.
- Any amount of magnetic field destroys the spin glass phase (even for Heisenberg spin glasses).
- Trivial probability distributions of the overlaps.

Replica Symmetry Breaking

$$\log Z_J = \lim_{n\to 0} \frac{Z_J^n - 1}{n} \,.$$

$$Z_n = \overline{Z_J^n} = \sum_{\{s^a\}} \int \mathrm{d}[J] \exp\left(\beta \sum_{a=1}^{n} \sum_{i<j} J_{ij} s_i^a s_j^a - \frac{1}{2} N \sum_{i<j} J_{ij}^2\right) .$$

$$Z_n = \sum_{\{s^a\}} \exp\left[\frac{1}{4}\beta^2 N n + \frac{1}{2}\beta^2 N \sum_{a<b}^{n} \left(\frac{1}{N}\sum_i s_i^a s_i^b\right)^2\right] .$$

Linearising the sum over the sites by introducing the so-called replica matrix Q_{ab},

$$Z_n = \int \mathrm{d}[Q_{ab}] \sum_{\{s^a\}} \exp\left[\frac{1}{4}\beta^2 N n - \frac{1}{2}\beta^2 N \sum_{a<b}^{n} Q_{ab}^2 + \beta^2 \sum_{a<b}^{n} \sum_i Q_{ab} s_i^a s_i^b\right] .$$

Replica Symmetry Breaking

$$Z_n = \int \mathrm{d}[Q_{ab}] e^{-\mathcal{H}_n\{Q_{ab}\}},$$

where the effective Hamiltonian is

$$\mathcal{H}_n\{Q_{ab}\} = -\frac{Nn}{4}\beta^2 + \frac{N}{2}\beta^2 \sum_{a<b} Q_{ab}^2 N \log\left[\sum_{\{s^a\}} \exp\left(\beta^2 \sum_{a<b} Q_{ab} s^a s^b\right)\right] .$$

The Mean Field solution is given by

$$\delta\mathcal{H}_n / \delta Q_{ab} = 0$$

which can be written as

$$Q_{ab} = \frac{1}{N}\sum_i \langle s_i^a s_i^b \rangle_{\mathcal{H}_n} \ , \ a \neq b, \tag{1}$$

Replica Symmetry Breaking

0-step: $Q_{ab} = (1 - \delta_{ab}) q$

$$\hat{Q}_{0-\mathrm{step}} = \begin{pmatrix} 0 & & q_0 \\ & \ddots & \\ q_0 & & 0 \end{pmatrix}$$

$$q = \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{\sqrt{2\pi}} \exp(-z^2/2) \tanh^2(\beta z \sqrt{q}).$$

Problem: Negative Entropy!!

Replica Symmetry Breaking ($D < \infty$)

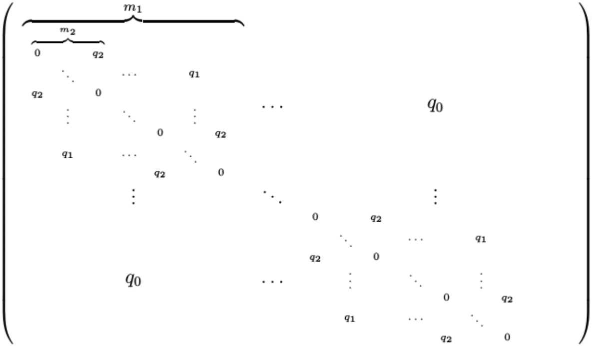
$$H_n = \int d^D x \left[(\partial_\mu Q_{ab})^2 + \tau \mathrm{Tr} Q^2 + g_3 \mathrm{Tr} Q^3 + g_4 \mathrm{Tr} Q^4 + \lambda \sum Q_{ab}^4 \right]$$

- $\lambda \neq 0$. The symmetry group is S_n.
- When $\lambda = 0$. $S_n \to O(n)$.
- $(\lambda = 0)$, $Q_{ab} = (1 - \delta_{ab})q$. $O(n)$ Spontaneously broken: Goldstone Bosons.
- But when $\lambda \neq 0$, $O(n)$ explicitly broken. Goldstone bosons adquire mass (negative!). Unstable solution.

Replica Symmetry Breaking

$$\hat{Q}_{0-\text{step}} = \begin{pmatrix} 0 & & q_0 \\ & \ddots & \\ q_0 & & 0 \end{pmatrix}$$

$$\hat{Q}_{1-\text{step}} = \begin{pmatrix} \overbrace{\begin{matrix} 0 & & q_1 \\ & \ddots & \\ q_1 & & 0 \end{matrix}}^{m_1} & q_0 & \cdots & q_0 \\ q_0 & \begin{matrix} 0 & & q_1 \\ & \ddots & \\ q_1 & & 0 \end{matrix} & \cdots & q_0 \\ \vdots & \vdots & \ddots & \vdots \\ q_0 & q_0 & \cdots & \begin{matrix} 0 & & q_1 \\ & \ddots & \\ q_1 & & 0 \end{matrix} \end{pmatrix}$$



$n > m_1 > m_2 > \ldots > 1.$

Replica Symmetry Breaking

The matrix elements can be described by the probability distribution

$$P(q) = \frac{1}{n(n-1)} \sum_{a \neq b} \delta(Q_{ab} - q)$$

$$= \frac{n}{n(n-1)} \left[(n - m_1)\delta(q - q_0) + (m_1 - m_2)\delta(q - q_1) \right. \quad (2)$$

$$\left. + (m_2 - m_3)\delta(q - q_2) + \ldots \right] \quad (3)$$

Finally, we have to take the limit $n \to 0$,

$$P(q) = m_1\delta(q - q_0) + (m_2 - m_1)\delta(q - q_1) + (m_3 - m_2)\delta(q - q_2) + \ldots$$

Notice that now (after $n \to 0$): $0 < m_1 < m_2 < \ldots < 1.$
In the limit of infinite RSB steps we obtain a continuous variation, so $q_k \to q(x)$, with $x \in [0, 1]$.
Hence, the spin-glass order parameter is a function,

$$\frac{\mathrm{d}x}{\mathrm{d}q} = P(q).$$

Ultrametricity

- Metric Space: $d(A, B) \leq d(A, C) + d(B, C)$.
- Ultrametric Space: $d(A; B) \leq \max(d(A, C), d(B, C))$.

M. C. Espejo et al. Biochemical Systematics and Ecology, 22, 894 (1994)

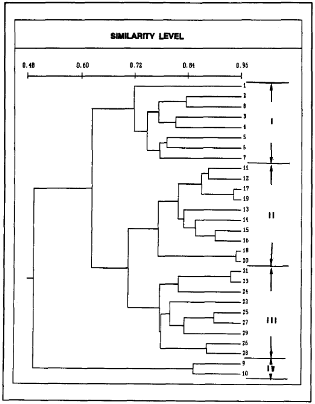
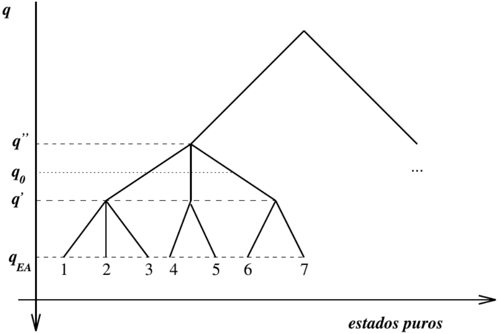


FIG. 2. UPGMA DENDROGRAM OF *PHASEOLUS VULGARIS* ACCESSIONS BASED ON ISOENZYMATIC SYSTEM DATA ANALYZED.

Replica Symmetry Breaking (Ultrametricity)

$$D(A,B) = \frac{1}{2}\left(q_{\mathrm{EA}} - q_{AB}\right).$$



Different Theories

- Field Theory of the Replica Symmetry Breaking (RSB) Theory.
- Hamiltonian

$$H_n = \int d^D x \left[(\partial_\mu Q_{ab})^2 + \tau \mathrm{Tr} Q^2 + g_3 \mathrm{Tr} Q^3 + g_4 \mathrm{Tr} Q^4 + \lambda \sum Q_{ab}^4 \right]$$

  $a, b = 1, ..., n$. At the end, $n \to 0$! (The replica trick)
- Propagator ($T > T_c$):

$$G(p) = \frac{1}{p^2 + m^2}$$

- Propagator ($T = T_c$, λ, g_4 are irrelevant: ϕ^3 theory, and the upper critical dimensions is $D = 6$):

$$G(p) = \frac{1}{p^{2-\eta}}$$

Different Theories.

- Propagators (Parisi Matrix) ($T < T_c$ and λ is relevant):

$$G_q(r) \simeq q^2 + A(q) r^{-\theta(q)}$$

  where
  - $\theta(q_M) = D - 2$. This result may be exact (some kind of Goldstone theorem).
  - $\theta(q) = D - 3$ for $q_M > q > q_m$. This result should be modified below $D = 6$.
  - $\theta(q_m) = D - 4$ for $q_m = 0$.
- In the droplet/scaling Theory:

$$G(r) \simeq q_{EA}^2 + A r^{-\theta}$$

  where θ is the standard droplet exponent.

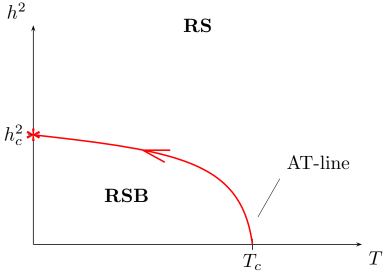
Different Theories: External Magnetic Field

RG from the paramagnetic phase:

- The upper critical dimension in a field is still six (Bray and Moore).
- Due to a dangerous irrelevant variable, some observables change behavior at eight dimensions (Fisher and Sompolinsky).
- Projecting the theory (replicon mode) no fixed points were found (Bray and Roberts).
- However, starting with the most general Hamiltonian of the RS phase and relaxing the $n = 0$ condition a stable fixed point below six dimensions was found (Dominicis, Temesvári, Kondor and Pimentel)
- Temesvári is able to build the dAT slightly below $D = 6$ (but Bray and Moore, Temesvári and Parisi, Moore,...)

Different Theories: External Magnetic Field

Renormalization group predictions (from Temesvári and Parisi):



(a) (b)

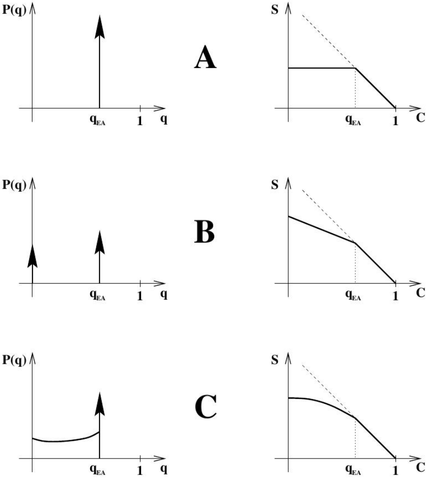
Replica Symmetry Breaking

Summary

- Exact in $D = \infty$.
- Infinite number of phases (pure states) not related by any kind of symmetry.
- These (pure) states are organized in a ultrametric fashion.
- The spin glass phase is stable under (small) magnetic field.
- The excitations of the ground state are space filling.
- Overlap equivalence: All the definitions of the overlap are equivalent.
- Stochastic Stability. The Spin Glass Hamiltonian is "generic" under Random Perturbations.

Note: In a pure state, α, the clustering property holds:
$\langle S_i S_j \rangle_\alpha - \langle S_i \rangle_\alpha \langle S_j \rangle_\alpha \to 0$ as $|i - j| \to \infty$.

Different Theories and Models (Comparison).



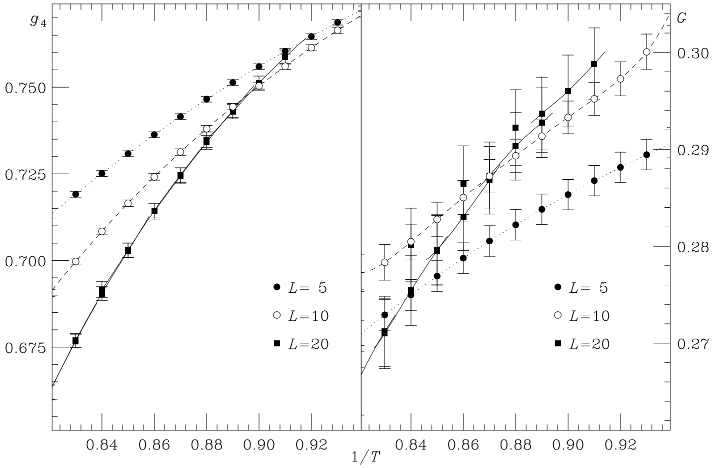
$h = 0$. Binder analysis

$$g_4 = \frac{3}{2} - \frac{1}{2} \frac{\overline{\langle q^4 \rangle}}{\overline{\langle q^2 \rangle}^2} \,.$$

$$g_2 = \frac{\overline{\langle q^2 \rangle^2} - \overline{\langle q^2 \rangle}^2}{\overline{\langle q^2 \rangle}^2} \,.$$

$$G = \frac{g_2}{2 - 2 g_4}$$

$h = 0$. Binder analysis



$h = 0$

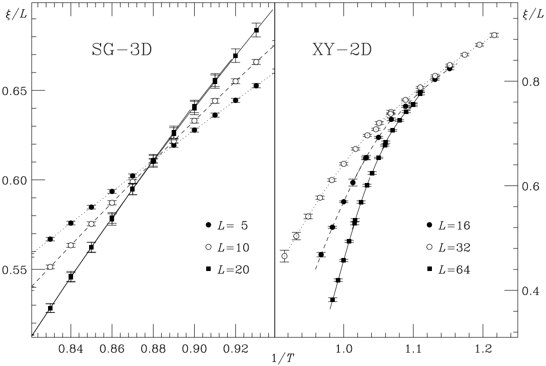
$$G(\boldsymbol{r}) = \frac{1}{L^3} \sum_{\boldsymbol{x}} \overline{\langle S_{\boldsymbol{x}} S_{\boldsymbol{x}+\boldsymbol{r}} \rangle^2}$$

Correlation Length:

$$\xi_2 = \frac{1}{2\sin(\pi/L)} \left(\frac{\hat{G}(0)}{\hat{G}(\boldsymbol{k}_1)} - 1 \right)^{1/2},$$

where $\boldsymbol{k}_1 = (2\pi/L, 0, 0)$ (and two perm.).

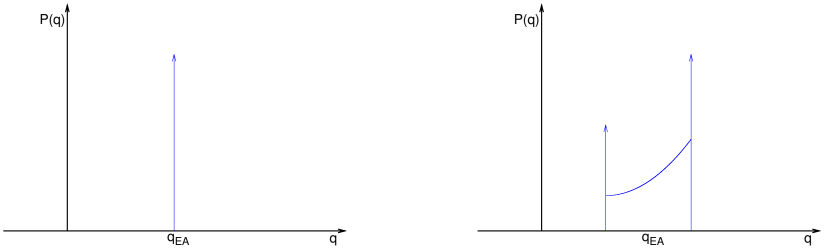
$h = 0$



$T_c = 1.1019(29)$, $\nu = 2.562(42)$, $\eta = -0.3900(36)$, $\omega = 1.12(10)$ Janus. Coll. Phys. Rev. B 88, 224416 (2013)

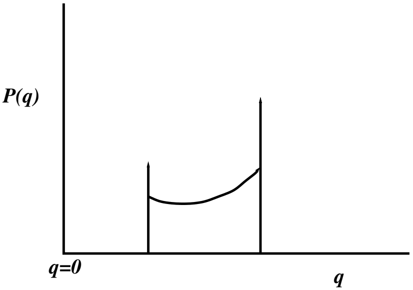
External Magnetic Field

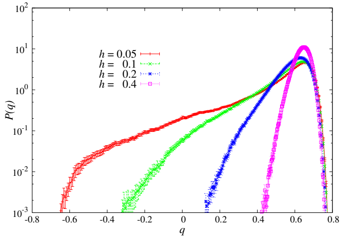
Different behavior of $P(q)$ in a magnetic field (droplet-left, RSB-right):



The negative overlap problem

- $P(q)$ in a magnetic field: SK results and numerical ones.





- The negative overlap region induces large corrections in $\tilde{G}(0)$!!

The correlation length

- Correlation Functions ($D=4$): The replicon Propagator:

$$
\begin{aligned}
G_1(\boldsymbol{r}) &= \frac{1}{L^4}\sum_{\boldsymbol{x}} \overline{\left(\langle S_{\boldsymbol{x}} S_{\boldsymbol{x}+\boldsymbol{r}}\rangle - \langle S_{\boldsymbol{x}}\rangle\langle S_{\boldsymbol{x}+\boldsymbol{r}}\rangle\right)^2}\,, \\
G_2(\boldsymbol{r}) &= \frac{1}{L^4}\sum_{\boldsymbol{x}} \overline{\left(\langle S_{\boldsymbol{x}} S_{\boldsymbol{x}+\boldsymbol{r}}\rangle^2 - \langle S_{\boldsymbol{x}}\rangle^2\langle S_{\boldsymbol{x}+\boldsymbol{r}}\rangle^2\right)}\,.
\end{aligned}
$$

- Correlation Length:

$$
\xi_2 = \frac{1}{2\sin(\pi/L)}\left(\frac{\hat{G}(0)}{\hat{G}(\boldsymbol{k}_1)} - 1\right)^{1/2},
$$

where $\boldsymbol{k}_1 = (2\pi/L, 0, 0, 0)$ (and three perm.)

Numerical Analysis of the Correlation function

- We will avoid the $k = 0$ value by fitting ($k > 0$):

$$\left(\frac{1}{\tilde{G}(k)}\right)^{\text{fit}} = A(L,T) + B(L,T)[\sin(k/2)]^2$$

- We can analyze the L and T dependence of

$$A(L,T) \equiv \lim_{k\to 0} \frac{1}{\tilde{G}(k)}$$

- We fix the L-dependent critical temperature by means:

$$A(L, T_c(L)) = 0$$

A new observable R_{12}

- R_{12}:

$$R_{12} = \frac{\hat{G}(\boldsymbol{k}_1)}{\hat{G}(\boldsymbol{k}_2)},$$

  where $\boldsymbol{k}_1 = (2\pi/L, 0, 0, 0)$, $\boldsymbol{k}_2 = (2\pi/L, 2\pi/L, 0, 0)$ (and permutations)
- We have checked the behavior of this observable in the EA model in $D = 3$ and $D = 4$ ($h = 0$).
- And in the two dimensional (ordered) Ising model. We have been able to compute its value at criticality using Conformal Field Theory:

$$R_{12} = 1.694\ 024...$$

- In a paramagnetic phase, for large L: $R_{12} \to 1$.

Dedicated Computers: Janus.

Some figures

- Built in 2008.
- Ferrara-Rome-Madrid-Extremadura-Zaragoza scientific collaboration.
- Dedicated computer optimized to simulate a wide variety of spin models.
- 16 boards of 16 FPGA's each (Virtex 4).
- Performance. For Ising models: Janus is equivalent to 10000 PC.
- Parallelization inside the boards.
- Previous numerical simulations simulated the 10^{-5} sec region (SSUE).
- Janus allows us to simulate in the 0.1 second time region. Note: Experimental times range from 1 sec to 3000 sec.

Comp. Phys. Comm. 178, 208(2008).

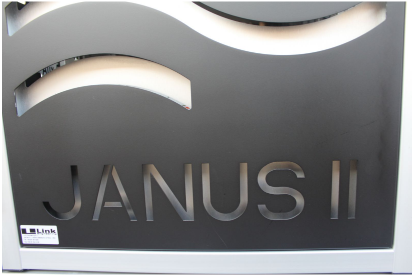
Dedicated Computers: The new Janus II.

Some figures

- Built in 2015.
- ~ 5 times most powerful than Janus.
- Still a dedicated computer optimized to simulate a wide variety of spin models.
- More flexible topology.
- 16 boards of 16 FPGA's each (one IOP and PC integrated on each board) (Virtex 7).
- Janus II will allow us to simulate in the 1 second time region.

Comp. Phys. Comm. 185, 550(2014).

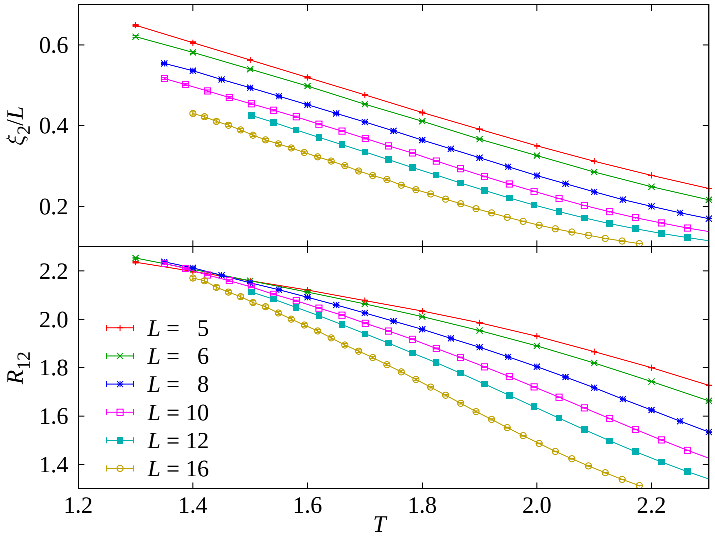
Janus II



$D = 4 \ (h \neq 0)$

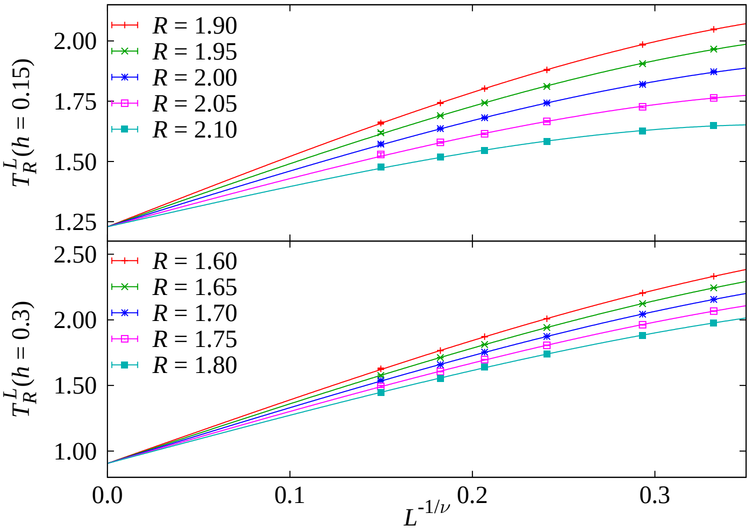
- We have simulated using the JANUS computer.
- $L = 5, 6, 8, 10, 12$ and 16.
- Three (uniform) magnetic Fields: $h = 0.075, 0.150$ and 0.3.
- Parallel Tempering in Temperature (e.g. 32 temperatures in $L = 16$)
- Single sample thermalization protocol.
- We avoid the mode $\boldsymbol{k} = 0$ in the analysis.

$D = 4$ $(h = 0.15)$

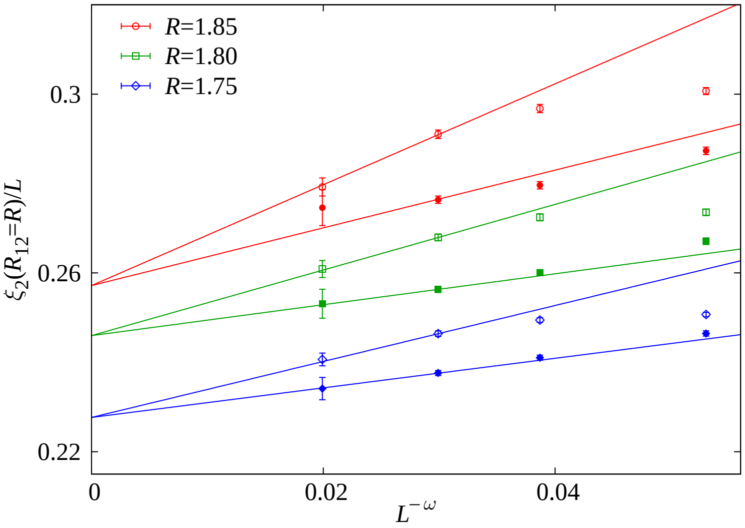


0.6
0.4
0.2
ξ_2/L
2.2
2.0
1.8
1.6
1.4
R_{12}
L = 5
L = 6
L = 8
L = 10
L = 12
L = 16
1.2
1.4
1.6
1.8
2.0
2.2
T

$D = 4$ $(h \neq 0)$: Critical exponents



$D = 4$ $(h \neq 0)$: Corrections to scaling



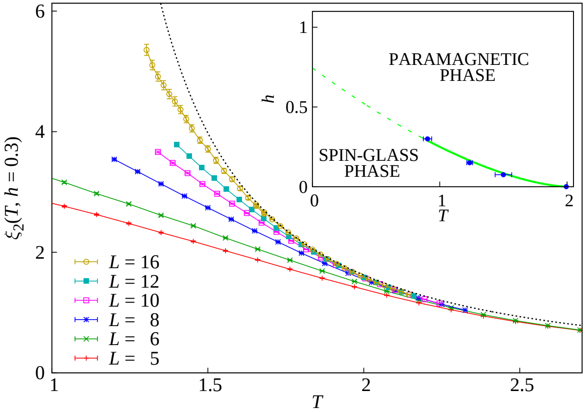
$D = 4$ $(h \neq 0)$: Critical exponents

Parameter	$h = 0.3$	$h = 0.15$	$h = 0.075$
$T_c(h)$	0.906(40)[3]	1.229(30)[2]	1.50(7)
ν	1.46(7)[6]		—
η	−0.30(4)[1]		—
ω	1.43(37)		—

For reference $(h = 0)$:

$T_c^{(0)} = 2.03(3)$, $\nu^{(0)} = 1.025(15)$, $\eta^{(0)} = -0.275(25)$

$D = 4\ (h \neq 0)$: Summary



Fisher-Sompolinsky relation: $h^2(T) \simeq A|T - T_c^{(0)}|^{\beta^{(0)}+\gamma^{(0)}}$

Janus coll. Proc. Nat. Ac. Sci (USA) 109, 6452 (2012)