MEASURING THE FLUCTUATION-DISSIPATION RATIO WITH NO PERTURBING FIELD

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The Fluctuation-Dissipation Ratio (FDR)

- At equilibrium Fluctuation-Dissipation Theorem

$$R(t,s) = \beta\, \partial_s C(t,s)$$

- Off-equilibrium generalization

$$R(t,s) = \beta\, X(t,s)\, \partial_s C(t,s)$$

(Cugliandolo, Kurchan)

The Fluctuation-Dissipation Ratio (FDR) $X(t,s)$ is relevant for

⋆ a complete description of the out of equilibrium dynamics

⋆ the connection with thermodynamics properties

Dynamics to Statics Connection

Off-equilibrium dynamics $\longrightarrow$ threshold states

If the system is stochastically stable (Franz, Mézard, Parisi, Peliti)

$$X(q) = x(q) \equiv \int_0^q P(q')\, dq'$$

Defining (note the added T factor)

$$\chi(t, t_w) \equiv T \int_{t_w}^{t} R(t, s)\, ds$$

$$\Downarrow$$

$$\chi(C) = \int_C^1 X(q)\, dq \quad \Leftrightarrow \quad X(C) = -\partial_C \chi(C)$$

Aim: measure $\chi(C)$ as the limit for $t_w \to \infty$ of $\chi(t, t_w)$ versus $C(t, t_w)$

Objectives of this work

- to check a new method for measuring the FDR with no perturbing field (Chatelain, cond-mat/0303545, to appear in a Special Issue of J. Phys. A)

- to derive a formula easy to use in numerical simulations, avoiding problems related to the measure of the punctual response and $X(t,s)$

- to compare the new method with the old one (finite perturbing field)

- to measure FDR for the 3D Edwards-Anderson model (an old problem!)

FDR with no perturbing field: Analytics

System of N Ising spins and Hamiltonian $\mathcal{H}_0$ (for any given sample)

$$\mathcal{H} = \mathcal{H}_0 - \sum_{i=1}^{N} h_i \sigma_i$$

where $h_i = h\,\varepsilon_i$ with $\overline{\varepsilon_i} = 0$ and $\overline{\varepsilon_i\,\varepsilon_j} = \delta_{i,j}$.

For the observable $A(t) = \sum_i \varepsilon_i \sigma_i(t)$

$$\begin{aligned} NC(t,s) &= \overline{\langle A(t) A(s) \rangle} = \sum_i \langle \sigma_i(t) \sigma_i(s) \rangle \,, \\ NR(t,s) &= \overline{\frac{\partial \langle A(t) \rangle}{\partial h(s)}} = \overline{\sum_i \varepsilon_i \sum_j \frac{\partial \langle \sigma_i(t) \rangle}{\partial h_j(s)} \frac{\partial h_j}{\partial h}} = \\ &= \sum_{i,j} \overline{\varepsilon_i \varepsilon_j} \frac{\partial \langle \sigma_i(t) \rangle}{\partial h_j(s)} = \sum_i \frac{\partial \langle \sigma_i(t) \rangle}{\partial h_i(s)} \,, \end{aligned}$$

Both correlation and response functions factorize over the sites thanks to the choice of $A(t)$.

FDR with no perturbing field: Analytics

Discrete-time dynamics (as in a simulation)

Time t counts the number of single spin flips

Heat-bath probabilities

$$\text{prob}(\sigma_i = \sigma) = \frac{\exp[\beta\sigma(h_i^{\text{W}} + h_i)]}{2\cosh[\beta(h_i^{\text{W}} + h_i)]} \quad ,$$

Weiss field $h_i^{\text{W}} = \sum_{j \neq i} J_{ij}\sigma_j$ for 2-spin interactions

$$\langle \sigma_j(t) \rangle = \text{Tr}_{\vec{\sigma}(t')} \left[\sigma_j(t) \prod_{t'=1}^{t} W_{I(t')} \Big(\vec{\sigma}(t') | \vec{\sigma}(t'-1) \Big) \right]$$

$I(t)$: index of the spin updated at time t

FDR with no perturbing field: Analytics

Transition probability

$$W_i(\vec{\sigma}|\vec{\tau}) = \frac{\exp[\beta\sigma_i(h_i^{\mathsf{W}} + h_i)]}{2\cosh[\beta(h_i^{\mathsf{W}} + h_i)]} \prod_{j \neq i} \delta_{\sigma_j, \tau_j} \ .$$

Note: $h_i^{\mathsf{W}}(\vec{\sigma}) = h_i^{\mathsf{W}}(\vec{\tau})$ (does not depend on σ_i)

$$\left.\frac{\partial W_i(\vec{\sigma}|\vec{\tau})}{\partial h_j}\right|_{h=0} = \delta_{i,j}\, W_i(\vec{\sigma}|\vec{\tau})\, \beta\, \left(\sigma_i - \sigma_i^{\mathsf{W}}\right) \ ,$$

$\sigma_i^{\mathsf{W}} \equiv \tanh(\beta h_i^{\mathsf{W}})$

FDR with no perturbing field: Analytics

Infinitesimal probing field is switch on at time t_w on site k

$$h_k(t) = h\,\theta(t - t_w)$$

Transition probabilities W_k are modified for $t > t_w$

$$\chi_{jk}(t, t_w) = T\,\frac{\partial\langle\sigma_j(t)\rangle}{\partial h}\bigg|_{h=0} =$$

$$= \mathrm{Tr}_{\vec{\sigma}(t')}\left[\sigma_j(t)\prod_{t'=1}^{t} W_{I(t')}\left(\vec{\sigma}(t')|\vec{\sigma}(t'-1)\right)\right.$$

$$\left.\sum_{s=t_w+1}^{t}\delta_{I(s),k}\left(\sigma_k(s) - \sigma_k^{\mathrm{W}}(s)\right)\right] =$$

$$= \langle\sigma_j(t)\,\Delta\sigma_k(t, t_w)\rangle$$

with

$$\Delta\sigma_k(t, t_w) = \sum_{s=t_w+1}^{t}\delta_{I(s),k}\left[\sigma_k(s) - \sigma_k^{\mathrm{W}}(s)\right]$$

FDR with no perturbing field: Analytics

Advantages

Always in the linear response regime (by definition)
One has to measure only correlations !!

$$\begin{aligned} C_i(t,t_w) &= \langle \sigma_i(t)\, \sigma_i(t_w) \rangle \\ \chi_i(t,t_w) &= \langle \sigma_i(t)\, \Delta\sigma_i(t,t_w) \rangle \\ \Delta\sigma_i(t,t_w) &= \sum_{s=t_w+1}^{t} \delta_{i,I(s)} \left[\sigma_i(s) - \sigma_i^{\mathsf{W}}(s) \right] \end{aligned}$$

$C = \sum_i C_i/N \quad \chi = \sum_i \chi_i/N$

In a single run, measures can be taken for any t_w

Drawback

$\Delta\sigma_i(t,t_w)$ is a random variable such that

$$\langle \sigma_i \rangle = \sigma_i^{\mathsf{W}} \Rightarrow \langle \Delta\sigma_i \rangle = 0 \qquad \langle \Delta\sigma_k^2 \rangle \propto \frac{t-t_w}{N}$$

The average over thermal histories $\langle . \rangle$ needs a **huge** number of samples for large times: $\mathcal{N}_S \propto \frac{t-t_w}{N}$
Computational complexity $\propto (t_w/N)^2$

FDR with no perturbing field: Analytics

Physical interpretation

When one tries to update spin i

$$\Delta\sigma_i \leftarrow \Delta\sigma_i + (\sigma_i - \sigma_i^{\mathsf{W}})$$

In the $T = 0$ limit

$$\sigma_i - \sigma_i^{\mathsf{W}} = \begin{cases} 0 & \text{if } h_i^{\mathsf{W}} \neq 0 \text{ (frozen spin)} \\ \sigma_i & \text{if } h_i^{\mathsf{W}} = 0 \text{ (free spin)} \end{cases}$$

Only free spins ($h_i^{\mathsf{W}} = 0$) may respond to an infinitesimal field and give contribution to χ

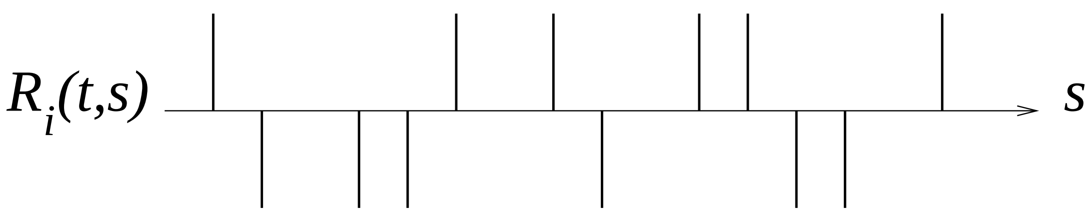
$$\chi_i(t, t_w) = \sum_{s=t_w+1}^{t} \langle \sigma_i(t)\sigma_i(s) \rangle \, \delta_{h_i^{\mathsf{W}},0}$$

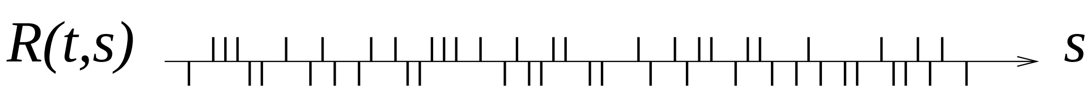
The linear response is a restricted sum of correlation functions

FDR with no perturbing field: Analytics

Problems with the punctual response function

$$R_i(t,s) \simeq \langle \sigma_i(t) \left[\sigma_i(s) - \sigma_i^{\mathsf{W}}(s) \right] \rangle \, \delta_{i,I(s)}$$





$R(t,s) = \frac{1}{N} \sum_i R_i(t,s)$ does not have a straightforward limit for $N \to \infty$

The integrated linear response

$$\chi \propto \int R(t,s) \, ds$$

is a smooth function for $N \to \infty$

NB: the continuous time limit ($t \leftarrow t/N$, $N \to \infty$) is not the usual one !

FDR with no perturbing field: Numerics

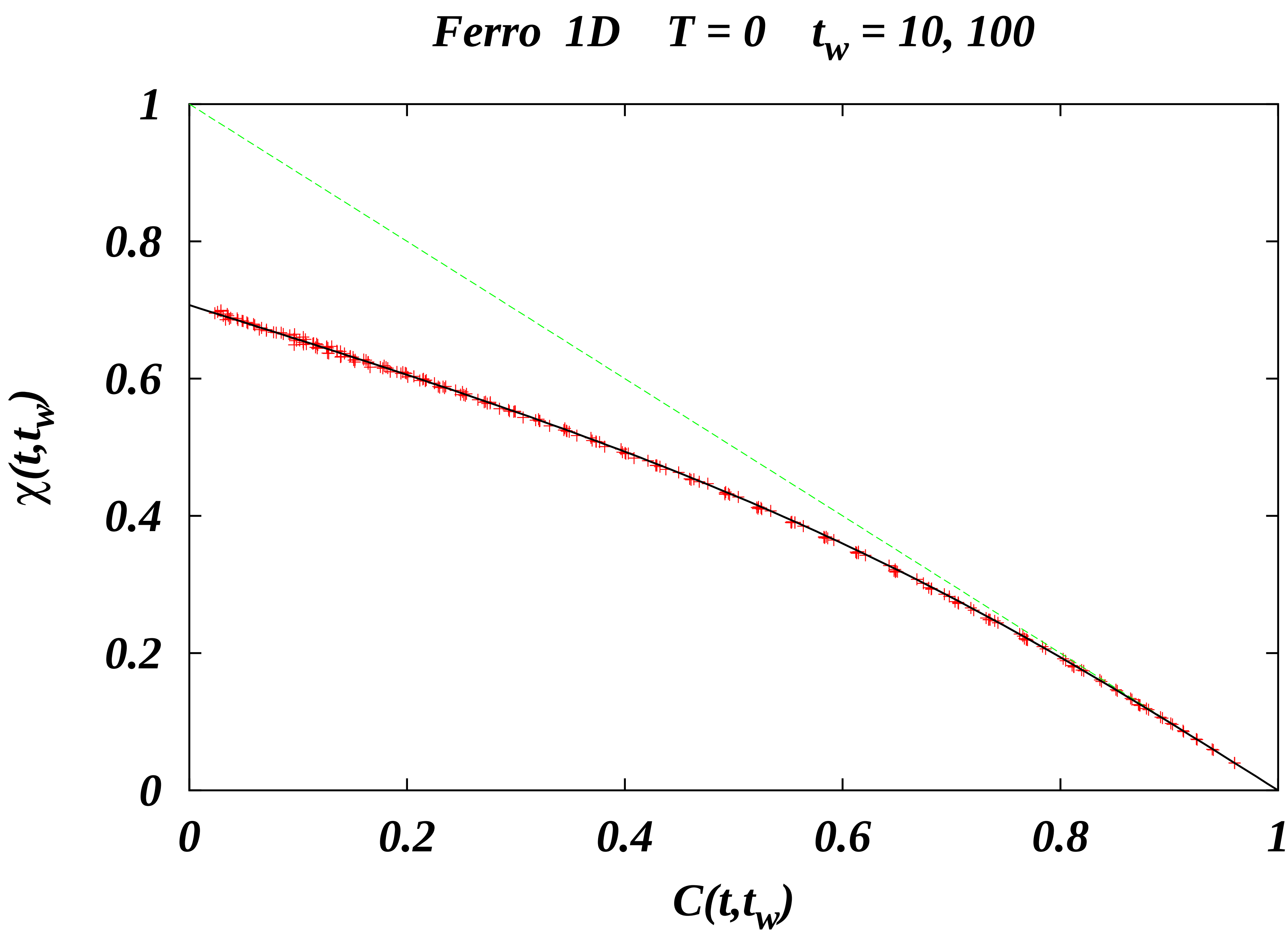
The models

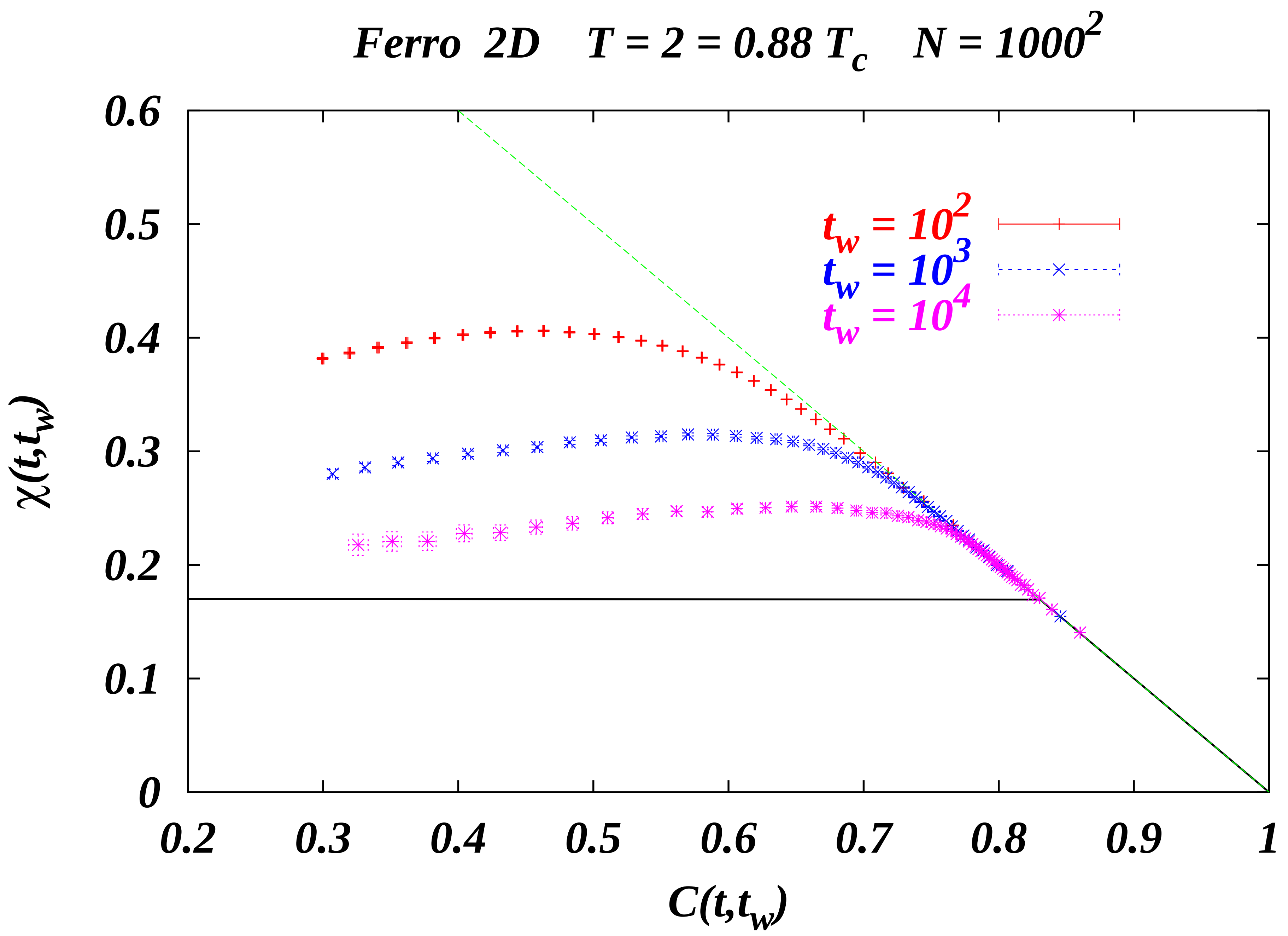
Ferro 1D $\rightarrow$ check vs. analytic solution

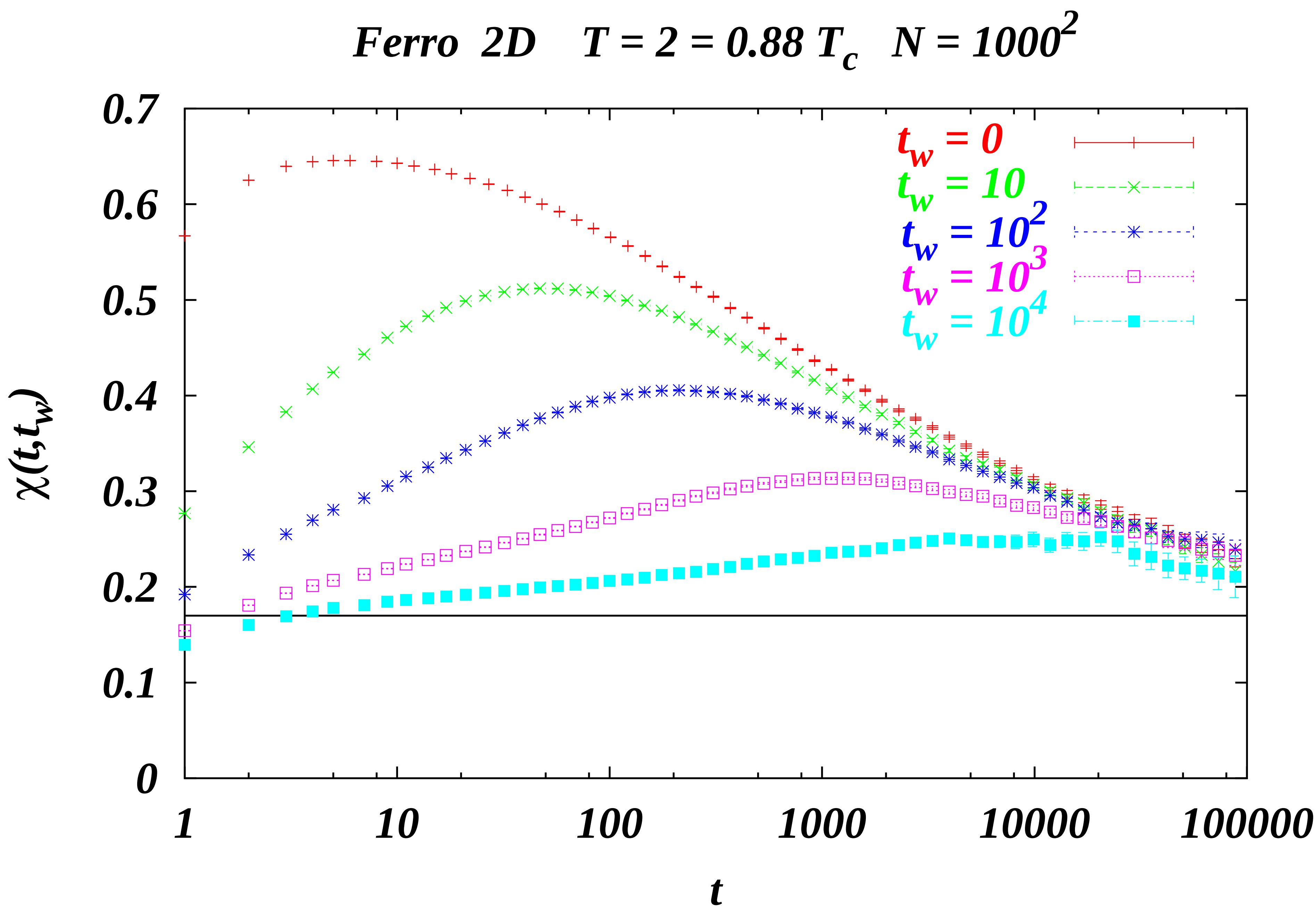
Ferro 2D $\rightarrow$ coarsening dynamics, RS
$X(q) = 0$ for $q < q_{\text{EA}}$

3-spin $\rightarrow$ long-range interactions, fixed conn. 4,
aging dynamics, 1RSB (tiny FRSB effects?)

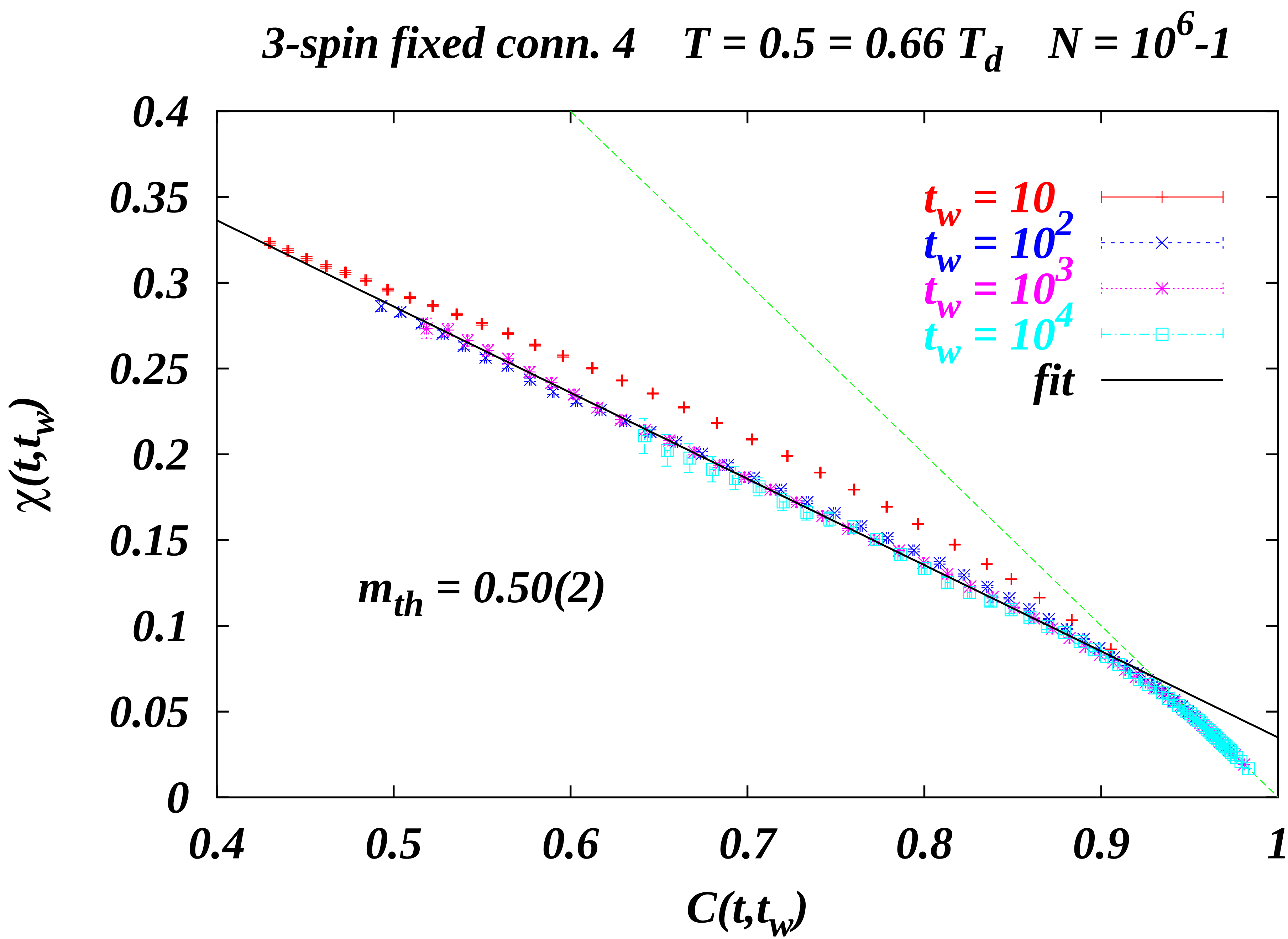
EA 3D $\rightarrow$ the old problem: FRSB vs. RS

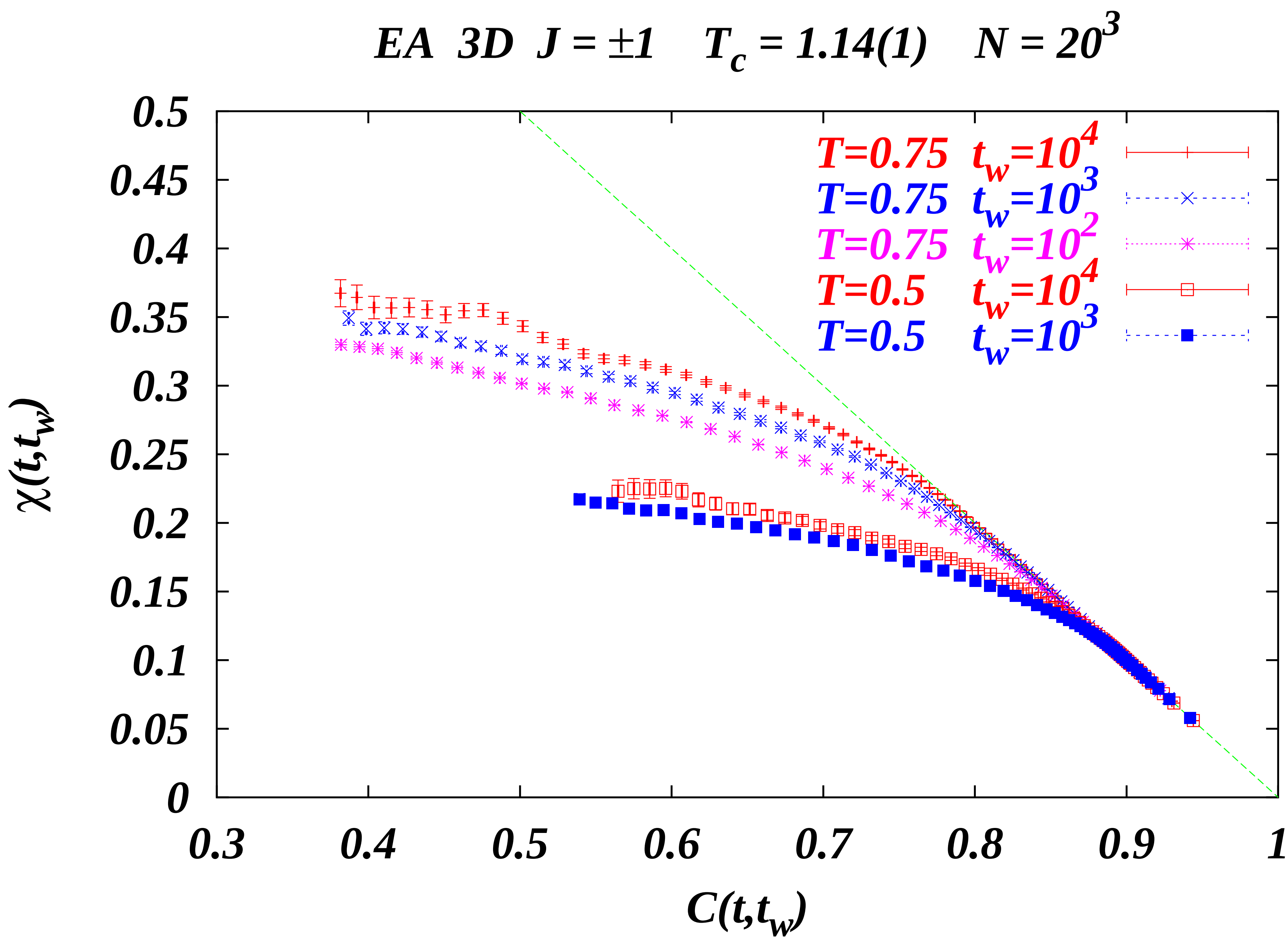

Ferro 1D T = 0 t_w = 10, 100
χ(t,t_w)
C(t,t_w)
0
0.2
0.4
0.6
0.8
1


Ferro 2D T = 2 = 0.88 T_c N = 1000^2
$t_w = 10^2$
$t_w = 10^3$
$t_w = 10^4$
$\chi(t,t_w)$
$C(t,t_w)$
0
0.1
0.2
0.3
0.4
0.5
0.6
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1



Ferro 2D T = 2 = 0.88 T_c N = 1000^2
$t_w = 0$
$t_w = 10$
$t_w = 10^2$
$t_w = 10^3$
$t_w = 10^4$
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
$\chi(t,t_w)$
1
10
100
1000
10000
100000
t


3-spin fixed conn. 4 T = 0.5 = 0.66 T_d N = 10^6-1
t_w = 10
t_w = 10^2
t_w = 10^3
t_w = 10^4
fit
m_{th} = 0.50(2)
$\chi(t,t_w)$
$C(t,t_w)$
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0.4
0.5
0.6
0.7
0.8
0.9
1


EA 3D J = ±1 Tc = 1.14(1) N = 20^3
T=0.75 tw=10^4
T=0.75 tw=10^3
T=0.75 tw=10^2
T=0.5 tw=10^4
T=0.5 tw=10^3
χ(t,tw)
C(t,tw)
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

FDR with no perturbing field: Numerics

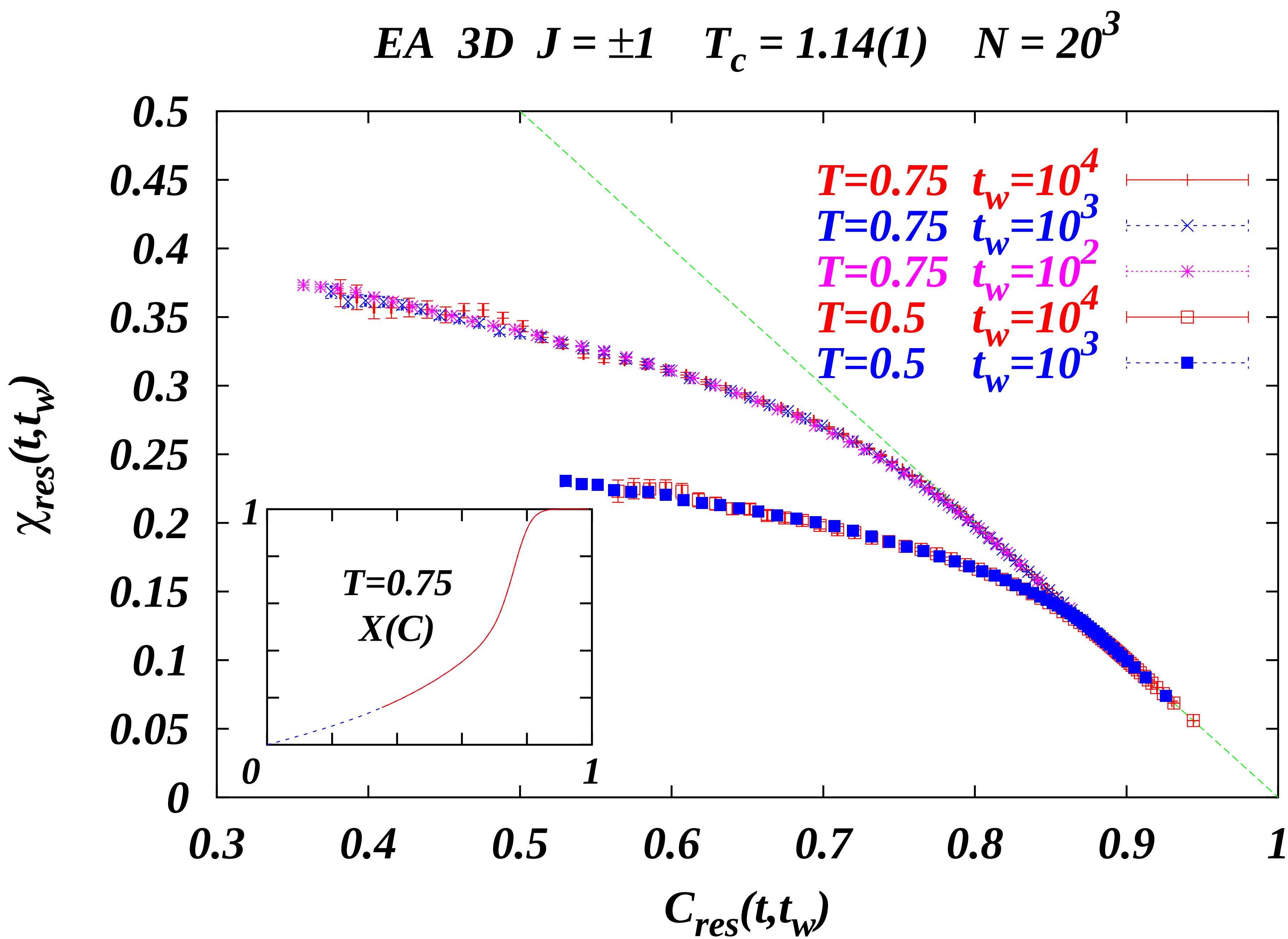
Rescaling

$$
\begin{aligned}
C_{\mathrm{res}}(t, t_w) &= \lambda \, \frac{C(t, t_w)}{q_{\mathrm{EA}}(t_w)} \\
\chi_{\mathrm{res}}(t, t_w) &= 1 - \lambda \, \frac{1 - \chi(t, t_w)}{q_{\mathrm{EA}}(t_w)}
\end{aligned}
$$

with an arbitrary λ

- $\lambda = q_{\mathrm{EA}}(10^4)$ is used

- $\lim_{t_w \to \infty} q_{\mathrm{EA}}(t_w) = q_{\mathrm{EA}} > 0$ is assumed


EA 3D J = ±1 T_c = 1.14(1) N = 20^3
T=0.75 t_w=10^4
T=0.75 t_w=10^3
T=0.75 t_w=10^2
T=0.5 t_w=10^4
T=0.5 t_w=10^3
T=0.75
X(C)
χ_res(t,t_w)
C_res(t,t_w)
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
0.45
0.5

Conclusions

Physical side

Stronger evidences for a non-trivial $X(C)$ in the 3D Edwards-Anderson model

Computational side

A priori no better method for measuring $\chi(C)$

- **small times** $\rightarrow$ new method
- **very large times** $\rightarrow$ old method

More awareness!