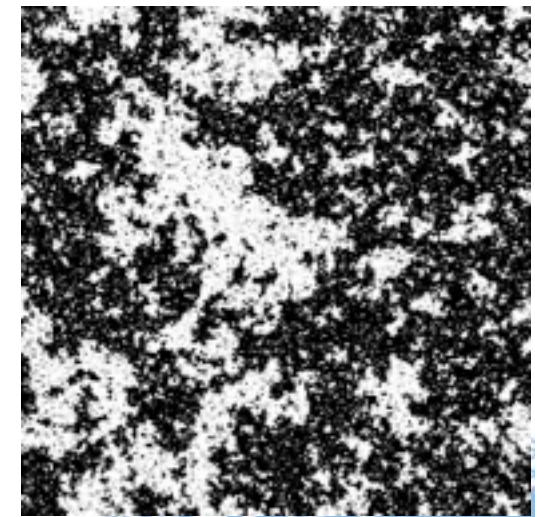
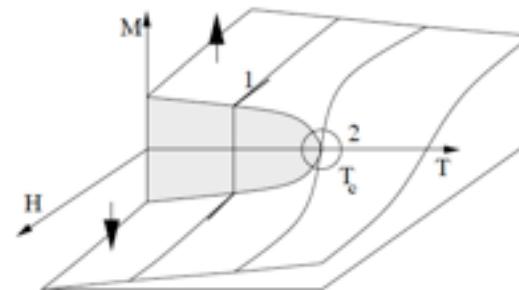
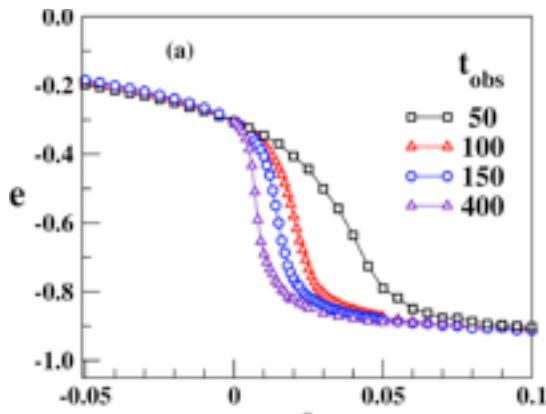
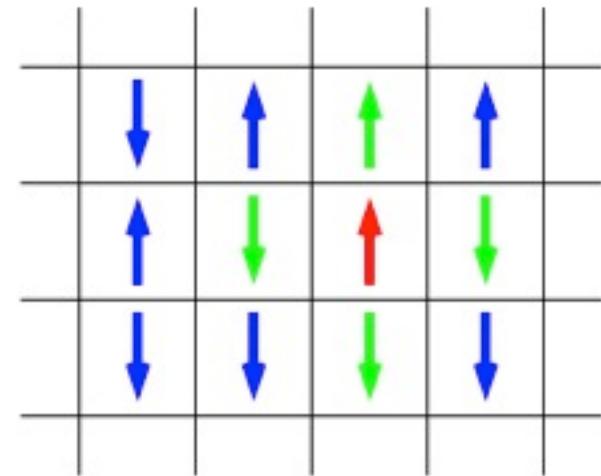




# Cálculos de Monte Carlo (I)

Prof. José Daniel Muñoz  
Grupo Simulación de Sistemas Físicos  
CEIBA-Complejidad  
Departamento de Física  
Universidad Nacional de Colombia, Bogotá

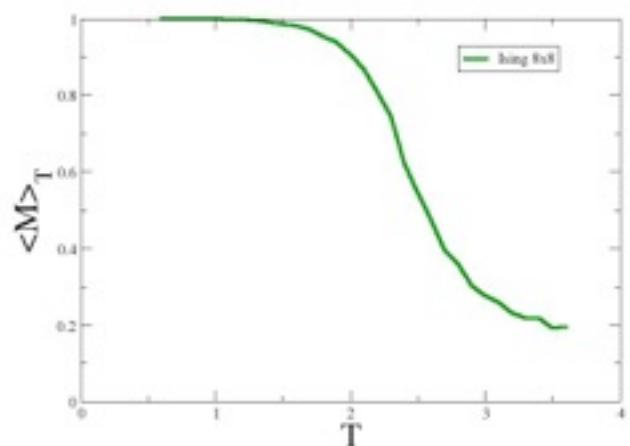
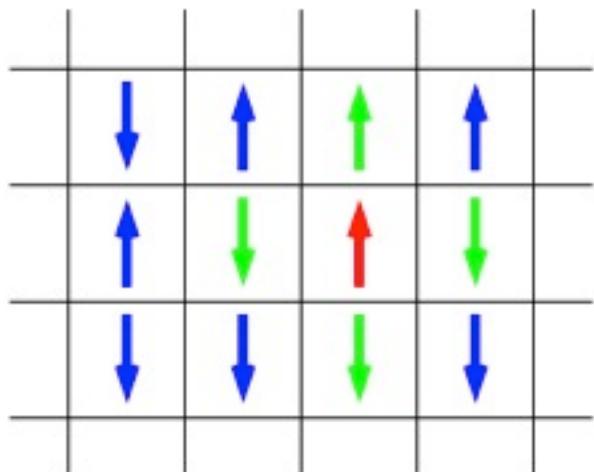


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DEPARTAMENTO DE FÍSICA

# El modelo de Ising



$$T_C = 2,269185$$

$$\mathcal{H} = - \sum_{\langle ij \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j$$

$$M := \left| \sum_{i=1} \sigma_i \right|$$

Distribución de Boltzmann

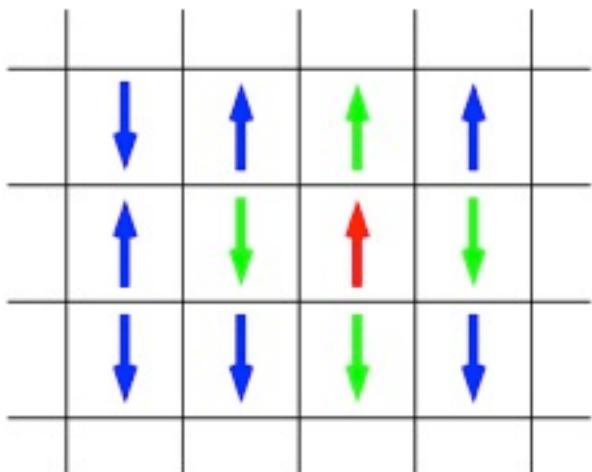
$$P_T(x) = \frac{1}{Z(T)} \exp(-E(x)/k_B T)$$

$$\langle M \rangle_T = \sum_x M(x) P_T(x)$$

$N_s$  muestras con probabilidad  $P_s = P_T$

$$\langle M \rangle_T = \frac{1}{N_s} \sum_{x \in s} M(x)$$

# El modelo de Ising



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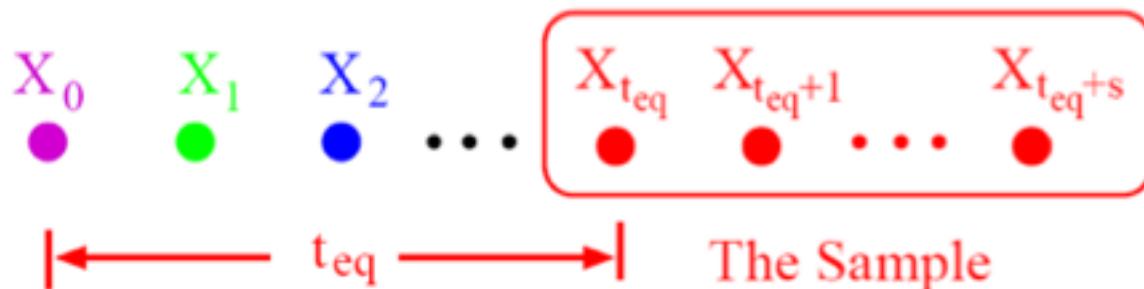
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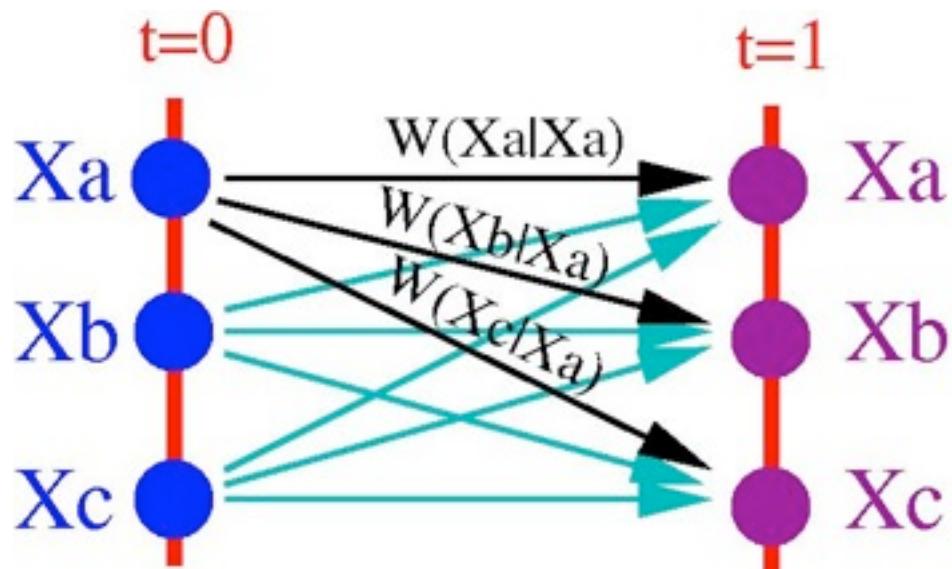
$$T_C = 2,269185$$

# Importance Sampling

En un proceso de Markov,



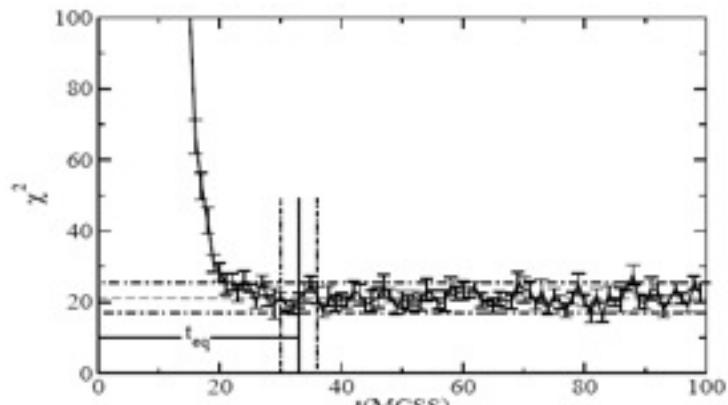
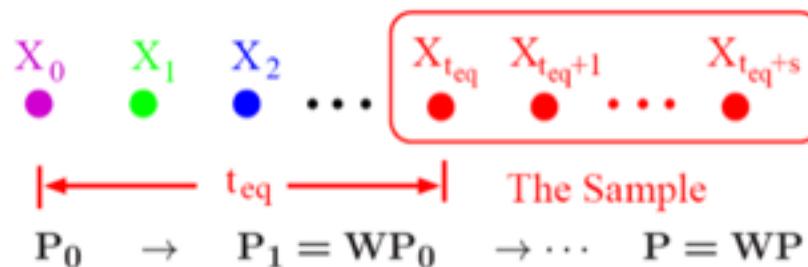
Matriz de transición  $W$



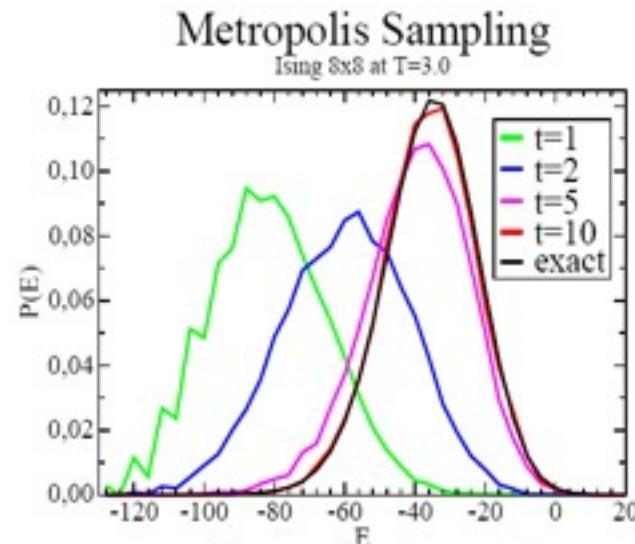
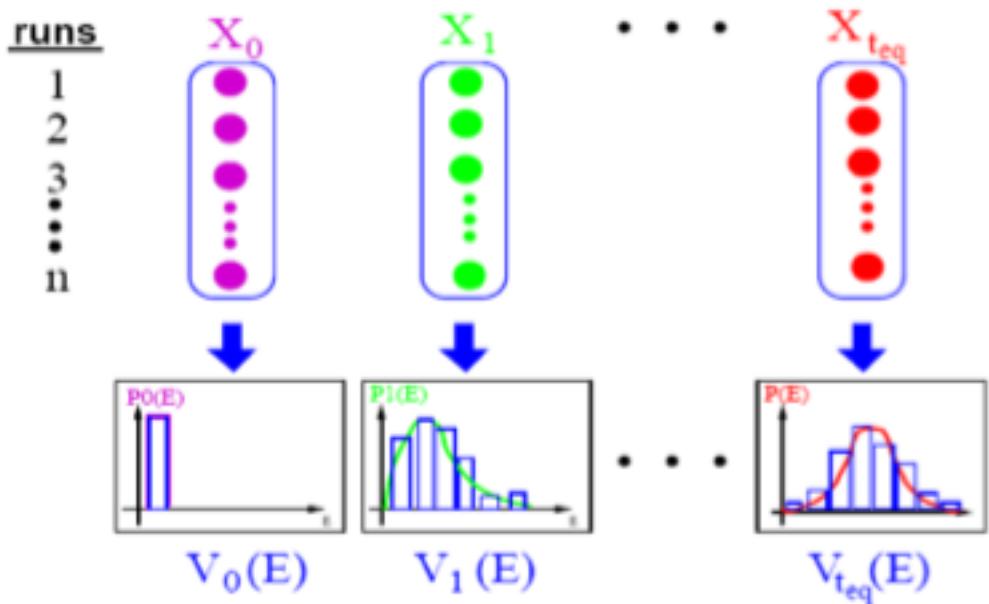
$$\sum_{x'} W(x'|x) = 1$$

# Importance Sampling

$P_n$  alcanza una distribución límite



Se necesita un  $t_{eq}$  para llegar a la distribución límite



Existe un  $P^\infty$  y Cualquier  $P_0$  va a  $P^\infty$

$= 1$

### Balance

$$W \cdot P^\infty = P^\infty$$

$$\sum_x W(x'|x)P^\infty(x) = P^\infty(x')$$

$$\sum_x W(x'|x)P^\infty(x) = P^\infty(x') \sum_x W(x|x')$$

$$\sum_x W(x'|x)P^\infty(x) = \sum_x W(x|x')P^\infty(x')$$

*Un teorema más sencillo: Si  $W$  es ergódica e irreducible y cumple balance detallado, entonces existe una única distribución límite  $P^\infty =$  la que cumple balance detallado.*

### Balance Detallado

$$W(x'|x)P^\infty(x) = W(x|x')P^\infty(x')$$

# Cómo lograr que $P_\infty = P$ deseado?

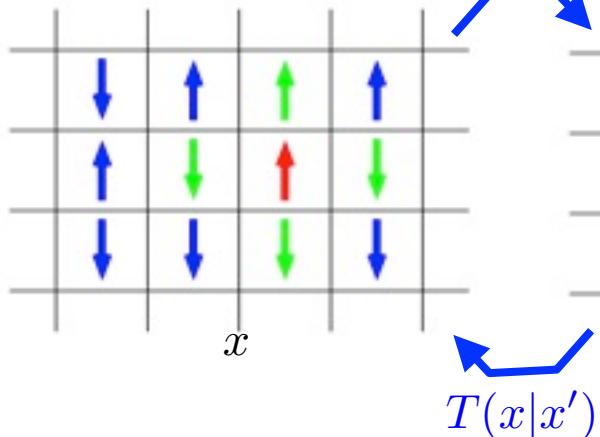
W se separa en dos pasos:

Simétrico:

$$T(x'|x) = T(x|x')$$

**Escoger**

$$T(x'|x)$$



$$W(x'|x) = T(x'|x)A(x'|x)$$

Balance Detallado:

$$A(x'|x)$$

**Aceptar**

$$A(x'|x)$$

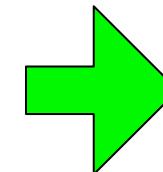
$$A(x|x')$$

$$P(x)$$

$$x$$

$$P(x')$$

$$x'$$



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W se separa en dos pasos:

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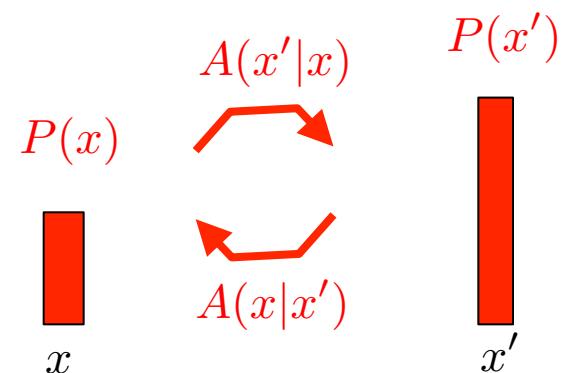
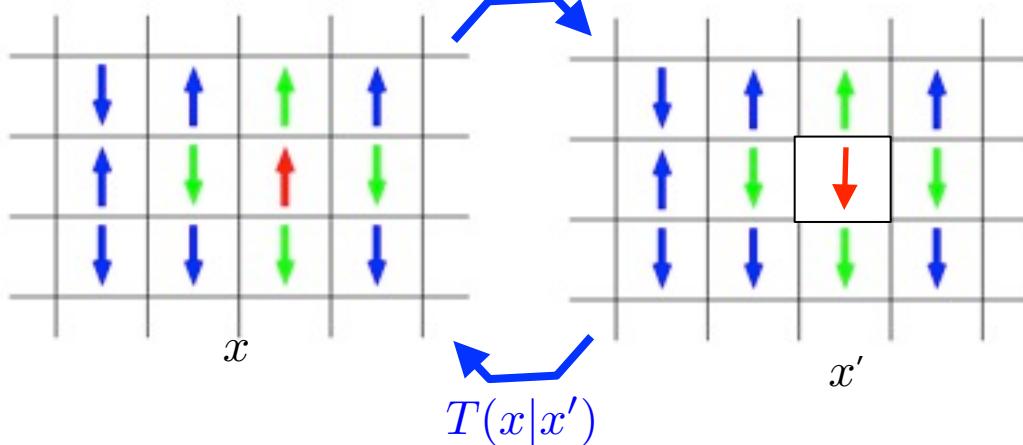
**Escoger**

$$W(x'|x) = T(x'|x)A(x'|x)$$

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**Aceptar**



Metropolis:  $A(x'|x) = \min \{1, P(x')/P(x)\}$

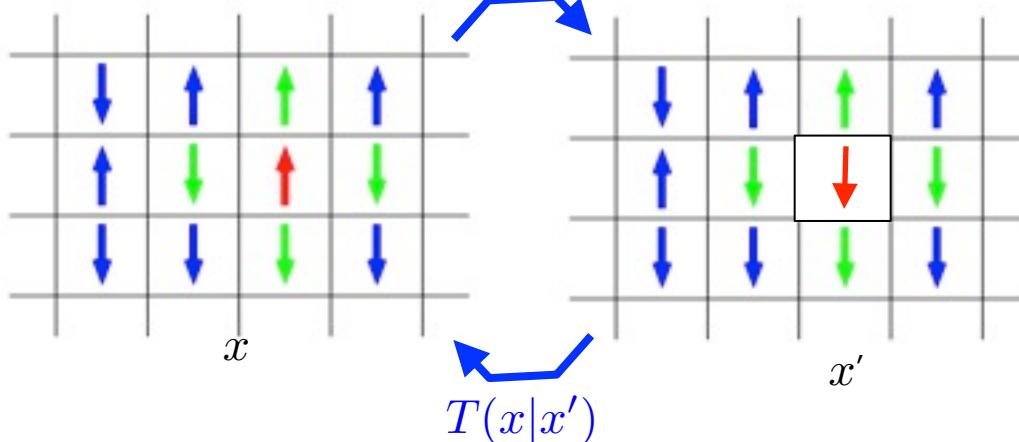
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$$A(x'|x)P(x) = A(x|x')P(x')$$

**Aceptar**

$$A(x'|x)$$

$$P(x')$$

$$P(x)$$

$$x$$

$$A(x|x')$$

$$x'$$

Ejemplo: Para Boltzmann:

$$P_T(x) = \frac{1}{Z(T)} \exp[-E(x)/k_B T]$$

$$A(x'|x) = \min\{1, \exp(-\Delta E/k_B T)\}$$

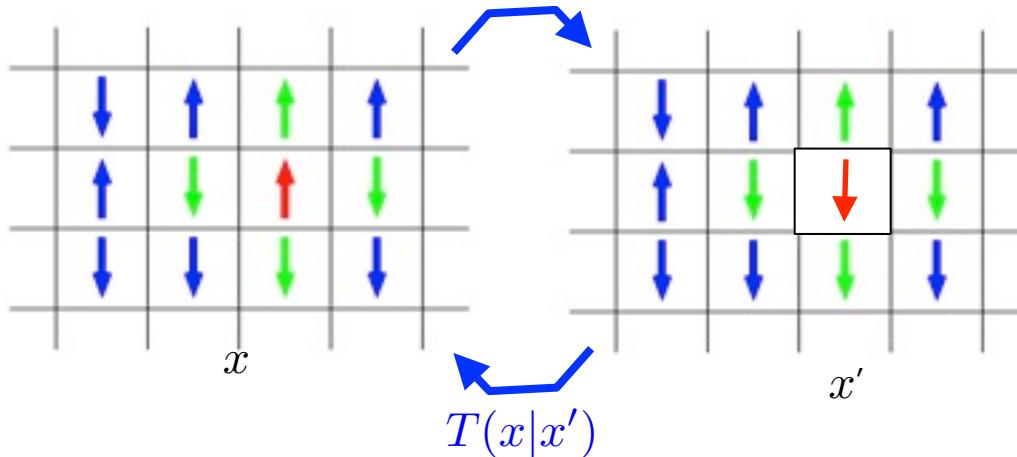
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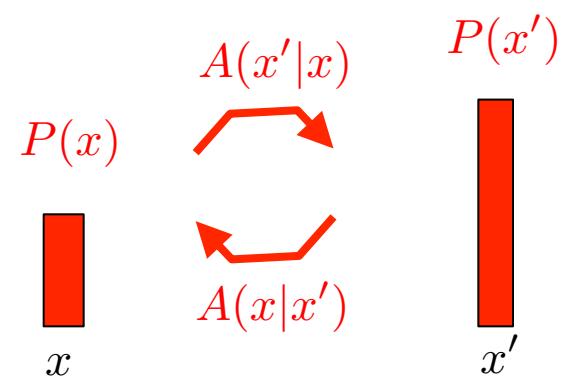


$$W(x'|x) = T(x'|x)A(x'|x)$$

Balance Detallado:

$$A(x'|x)P(x) = A(x|x')P(x')$$

Aceptar



Tres formas de hacerlo:

Metropolis:  $A(x'|x) = \min\{1, P(x')/P(x)\}$

Glauber:  $A(x'|x) = \frac{P(x')}{P(x) + P(x')}$

Heat Bath:  $A(x'|x) = \frac{1}{Z'}P(x')$

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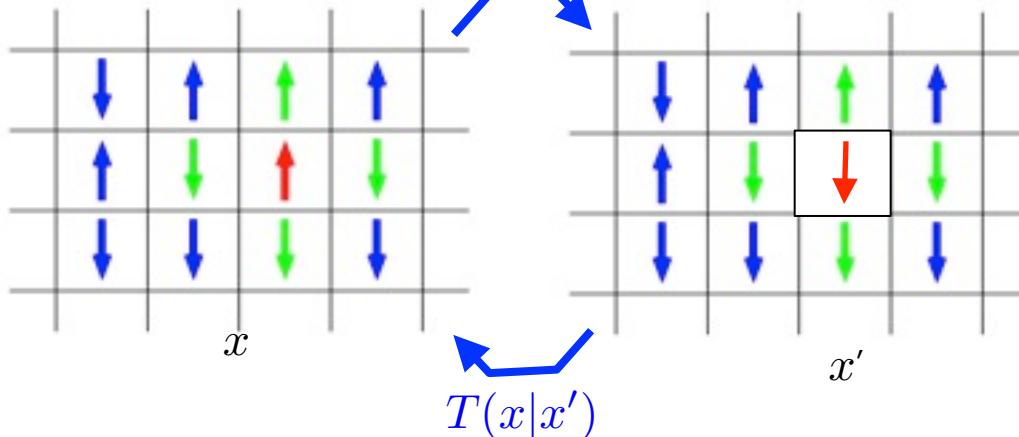
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Balance Detallado:

$$A(x'|x)P(x)$$

**Aceptar**

$$P(x)$$

$$A(x'|x)$$

$$P(x')$$

$$A(x|x')$$

$$x'$$

Ejemplo: Para Boltzmann:

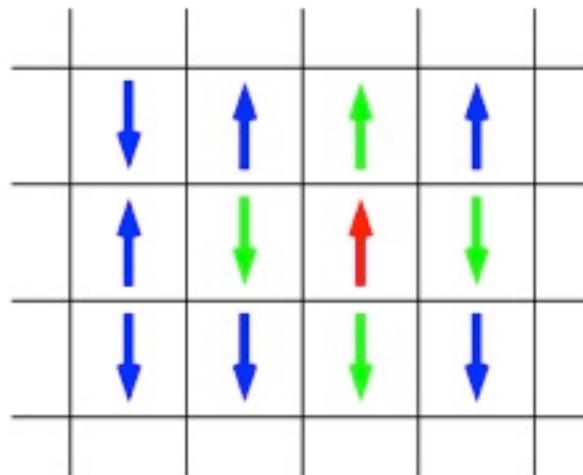
$$P_T(x) = \frac{1}{Z(T)} \exp[-E(x)/k_B T]$$

$$A(x'|x) = \min\{1, \exp(-\Delta E/k_B T)\}$$

$$A(x'|x) = \frac{1}{1 + \exp(-\Delta E/k_B T)}$$

$$A(x'|x) = \frac{1}{Z'} \exp [E(x')/k_B T]$$

# Ejemplo: Ising2D por Metrópolis



# Ejemplo: un programa de Metrópolis

```
class SpinSystem{  
private:  
    int s[L][L]; int E,M;  
public:  
    void InicieArriba(void);  
    void Muestre(void);  
    void MetropolisStep(Crandom & ran2,double T);  
    double GetE(void){return (double)E;};  
    double GetM(void){return fabs((double)M);};  
};  
...
```

# Ejemplo: un programa de Metrópolis

```
void SpinSystem::MetropolisStep(Crandom & ran2, double T){  
    int n,i,j,dE;  
    //Escojo un espin al azar;  
    n=(int) (L2*ran2.r()); i=n/L; j=n%L;  
    //Calculo el dE que habría si volteara ese espín;  
    dE=2*s[i][j]*(s[(i+L-1)%L][j]+s[(i+1)%L][j]+s[i][(j+L-1)%L]+s[i][(j+1)%L]);  
    //Implemento la rata de aceptación A(x'|x) de Metrópolis;  
    if(dE<0)  
        {s[i][j]*=-1; E+=dE; M+=2*s[i][j];}//volteo el espín;  
    else if((ran2.r())<exp(-dE/(k*T)))  
        {s[i][j]*=-1; E+=dE; M+=2*s[i][j];}//volteo el espín;  
}
```

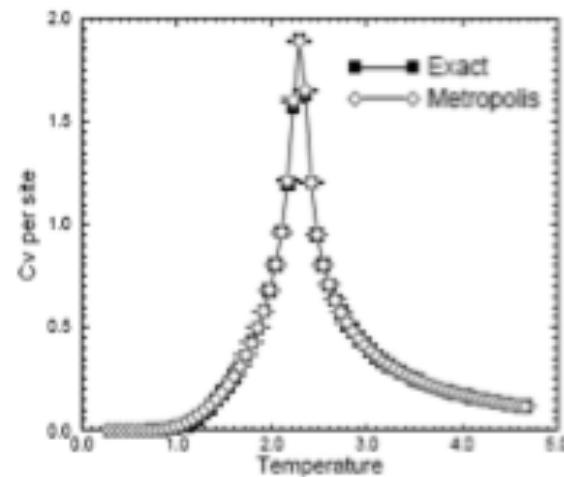
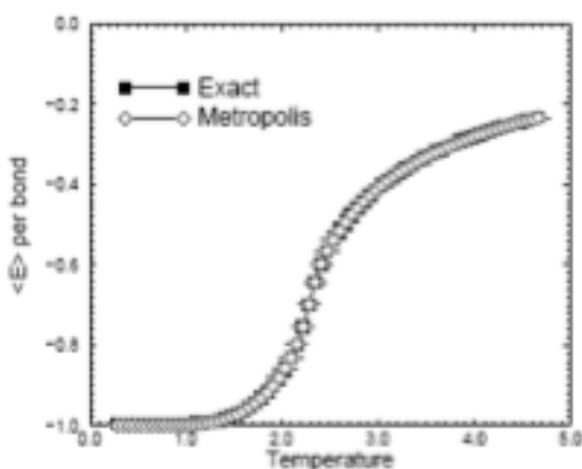
# Ejemplo: un programa de Metrópolis

```
for(T=2.0;T<3.0;T+=0.02){  
    //Inicio el sistema  
    Ising.InicieArriba();  
    //Equilibrio  
    for(t=0;t<teq;t++){  
        for(mcs=0;mcs<L2;mcs++) //Un MCSS  
            Ising.MetropolisStep(ran2,T);  
    }  
    //Inicio Acumuladores en cero  
    Mprom=M2prom=M4prom=Eprom=E2prom=0;  
    //Tomo muestras  
    for(t=0;t<Nmuestras;t++){  
        E=Ising.GetE(); M=Ising.GetM();  
        Mprom+=M; M2prom+=M*M; M4prom+=M*M*M*M; Eprom+=E; E2prom+=E*E;  
        for(ccorr=0;ccorr<tcorr;ccorr++)  
            for(mcs=0;mcs<L2;mcs++) //Un MCSS  
                Ising.MetropolisStep(ran2,T);  
    }  
}
```

# Ejemplo: un programa de Metrópolis

```
//Normalizo los acumuladores  
Mprom/=Nmuestras; M2prom/=Nmuestras; M4prom/=Nmuestras;  
Eprom/=Nmuestras; E2prom/=Nmuestras;  
//Calculo lo que me interesa  
Cv=1/(k*T*T)*(E2prom-Eprom*Eprom);  
Xs=1/(k*T)*(M2prom-Mprom*Mprom);  
Ub=1.0-1.0/3.0*(M4prom/(M2prom*M2prom));  
//Imprimo  
cout<<T<<" "<<Eprom<<" "<<Mprom<<" "<<Cv<<" "<<Xs<<" "<<Ub<<endl;  
}
```

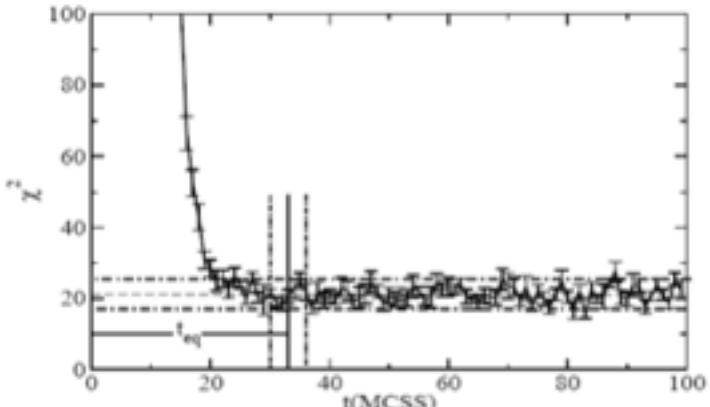
## Ej: Metrópolis para el modelo de Ising



En general, para cualquier proceso de Markov,

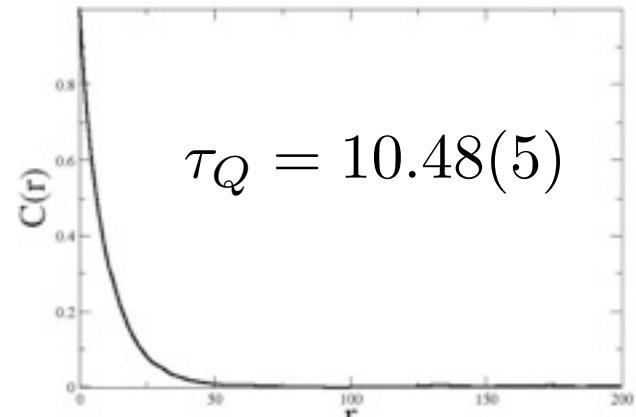
**t Equilibrio:**  $\chi^2(t) = \sum_E \frac{[V_t(E) - nP(E)]^2}{nP(E)}$

$$\begin{aligned} \mu &= r \\ \sigma &= 2r \end{aligned} \rightarrow \text{average } m \text{ times} \rightarrow \begin{aligned} \mu &= r \\ \sigma &= 2r/\sqrt{m} \end{aligned}$$

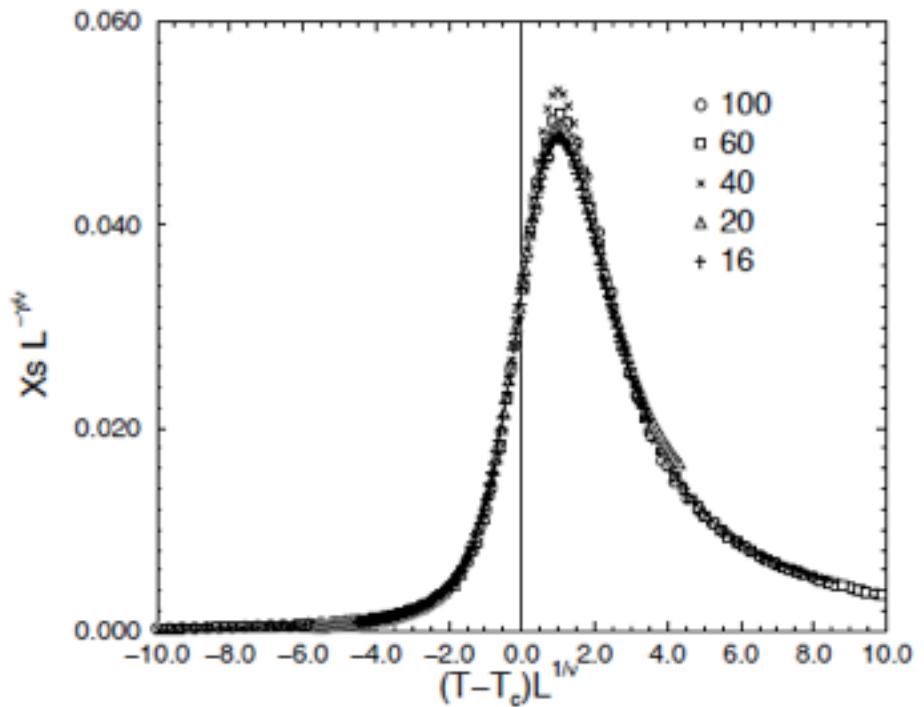
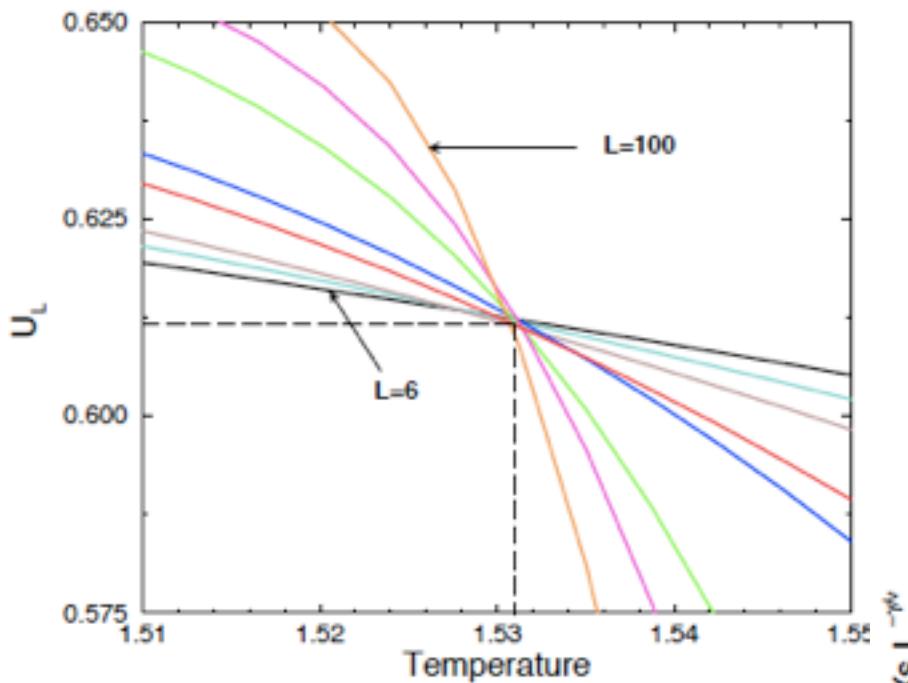


**t Correlación:**

$$\langle (\delta Q)^2 \rangle = \frac{1}{n} [\langle Q^2 \rangle - \langle Q \rangle^2] \left( 1 + 2 \frac{\tau_Q}{\delta t} \right)$$



# Escalamiento Finito



# ¿Cómo Hallar los Exponentes Críticos?

Cerca de la transición de fase, todas las cantidades se comportan como leyes de potencias:

H=0

$$\langle M \rangle_T \sim |T - T_C|^\beta$$

$$\chi_s = \frac{1}{k_B T} \left( \langle M^2 \rangle_T - \langle M \rangle_T^2 \right) \sim \frac{1}{|T - T_C|^\gamma}$$

$$C_v = \frac{1}{k_B T^2} \left( \langle E^2 \rangle_T - \langle E \rangle_T^2 \right) \sim \frac{1}{|T - T_C|^\alpha}$$

$$\xi \sim \frac{1}{|T - T_C|^\nu}$$

T=Tc

$$\langle M \rangle_{T_C, H} \sim |H - H_C|^\delta \quad \langle M(0)M(r) \rangle_{H_C, T_C} \sim r^{-d+2-\eta}$$

Scaling laws

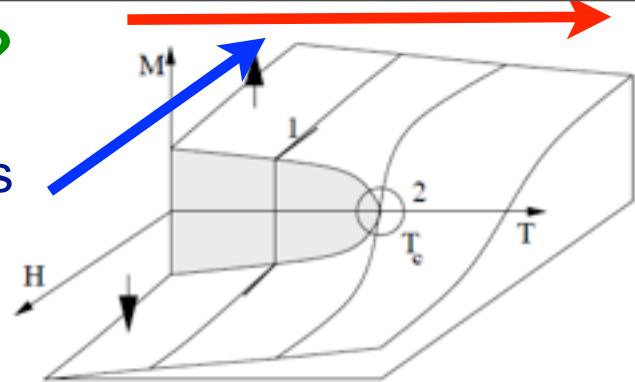
$$\alpha + 2\beta + \gamma = 2$$

Hyperscaling laws

$$d\nu = 2 - \alpha$$

$$\beta\delta = \beta + \gamma$$

$$2 - \eta = d \frac{(\delta - 1)}{(\delta + 1)}$$



$d$	2	3	4
$\alpha$	0	0.110(1)	0
$\beta$	1/8	0.3265(3)	1/2
$\gamma$	7/4	1.2372(5)	1
$\delta$	15	4.789(2)	3
$\eta$	1/4	0.0364(5)	
$\nu$	1	0.6301(4)	1/2
$\omega$	2	0.84(4)	

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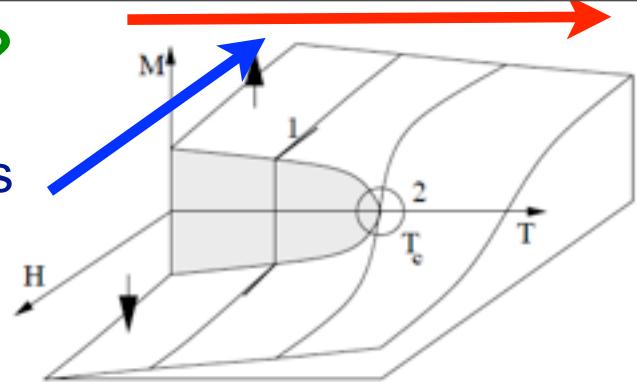
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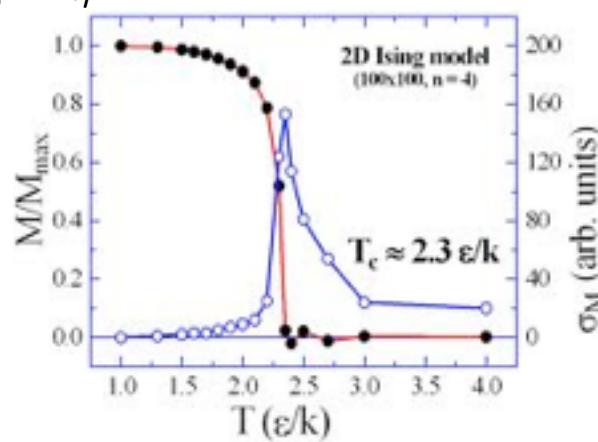
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# Longitud de Correlación

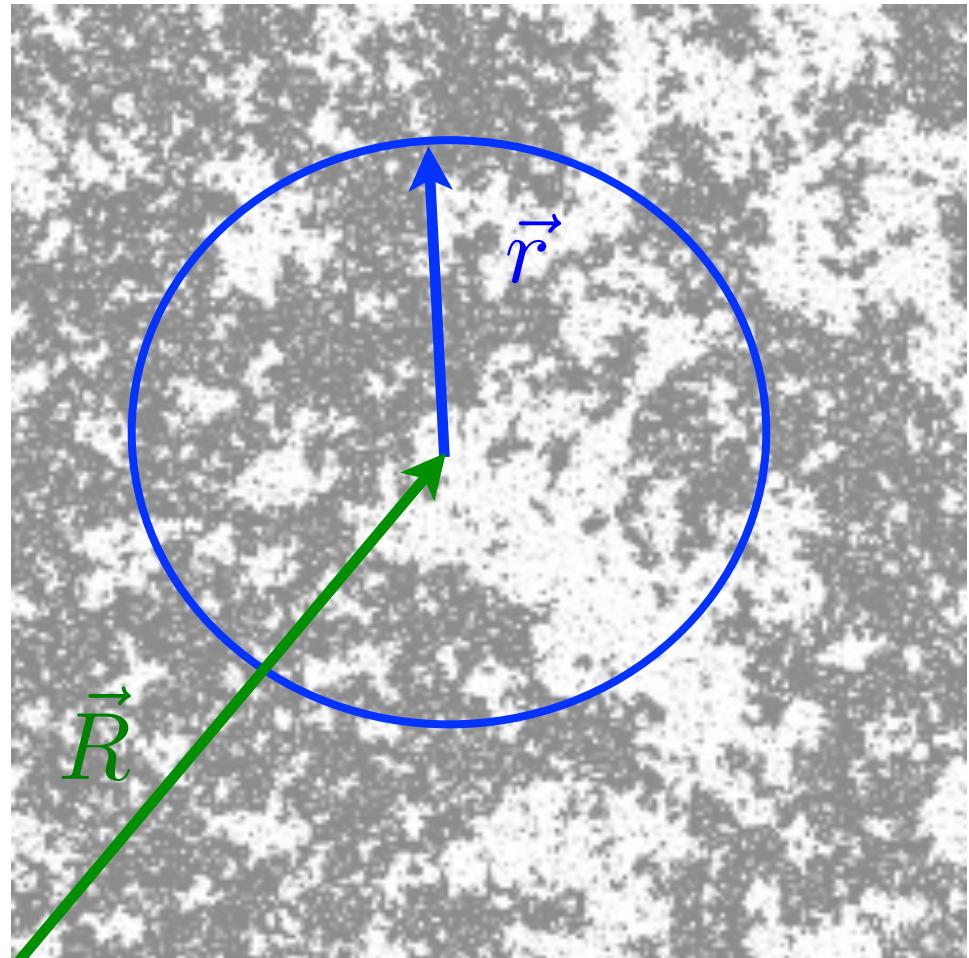
Se define como

$$G(r) = \langle \mathbf{s}(R) \cdot \mathbf{s}(R + r) \rangle - \langle \mathbf{s} \rangle^2$$

Dentro de cada fase,

$$G(r) \approx \frac{1}{r^{d-2+\eta}} \exp\left(\frac{-r}{\xi}\right)$$

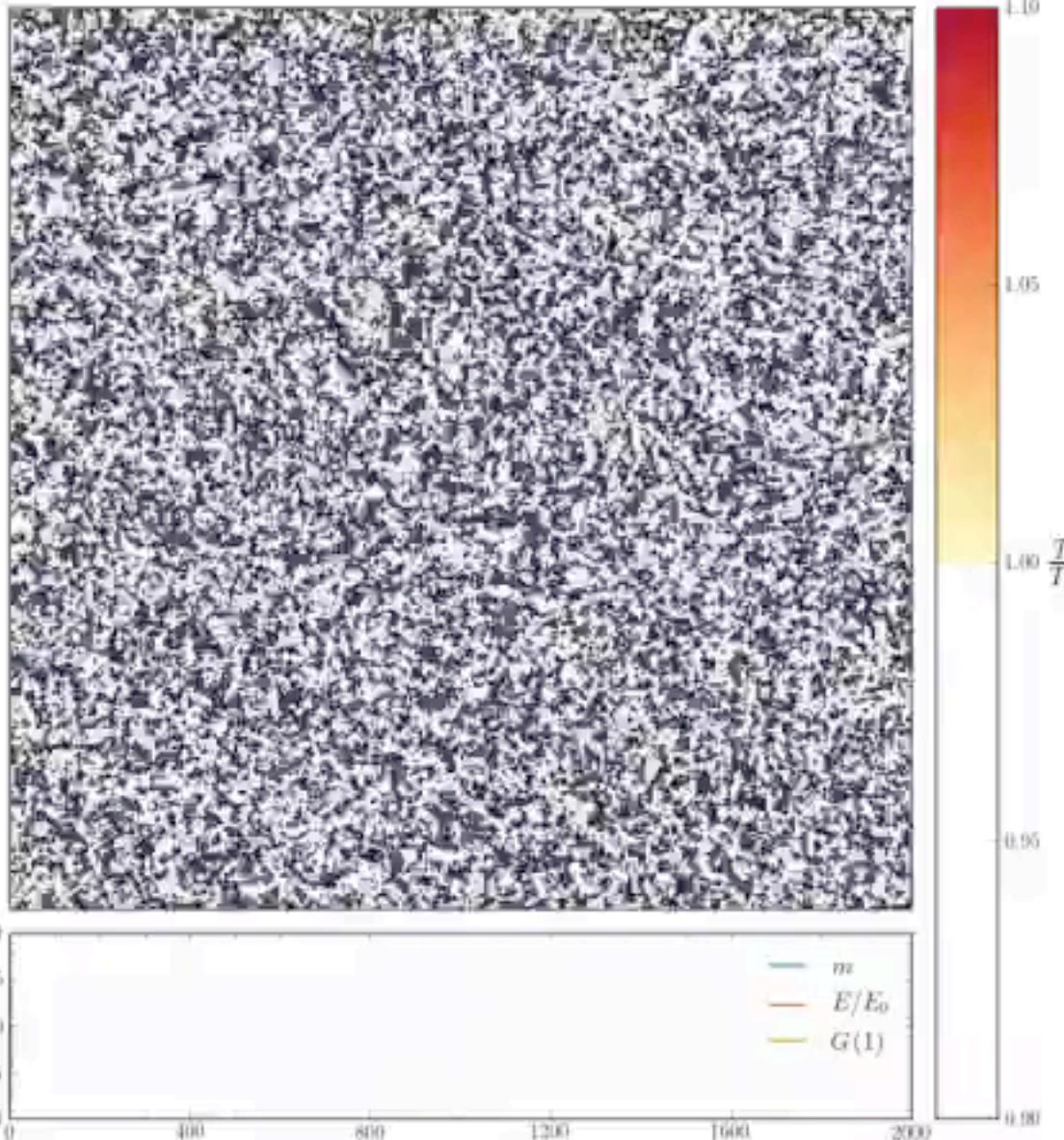
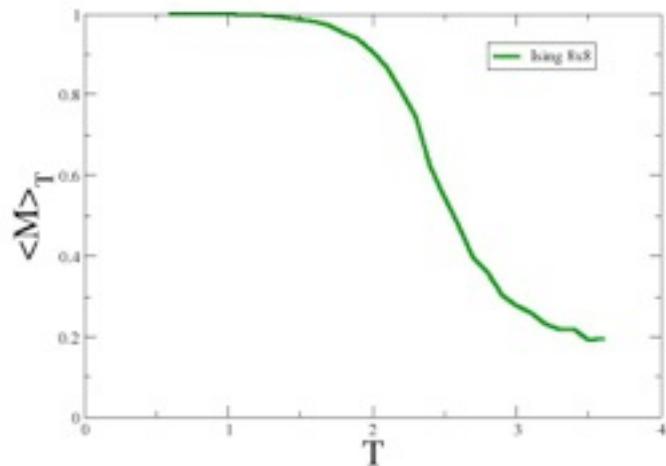
$\xi$  = El tamaño característico  
de los clusters



En la transición

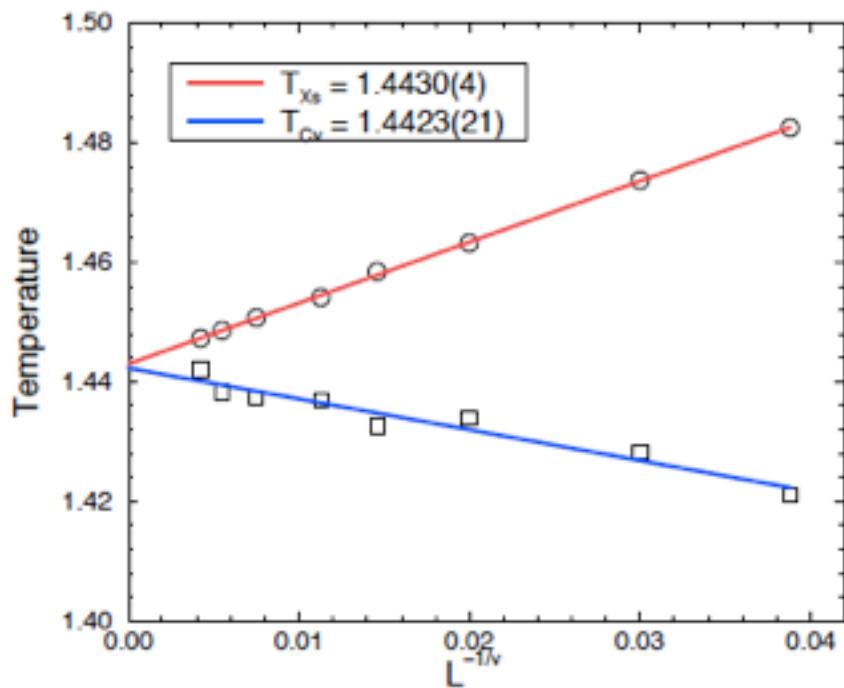
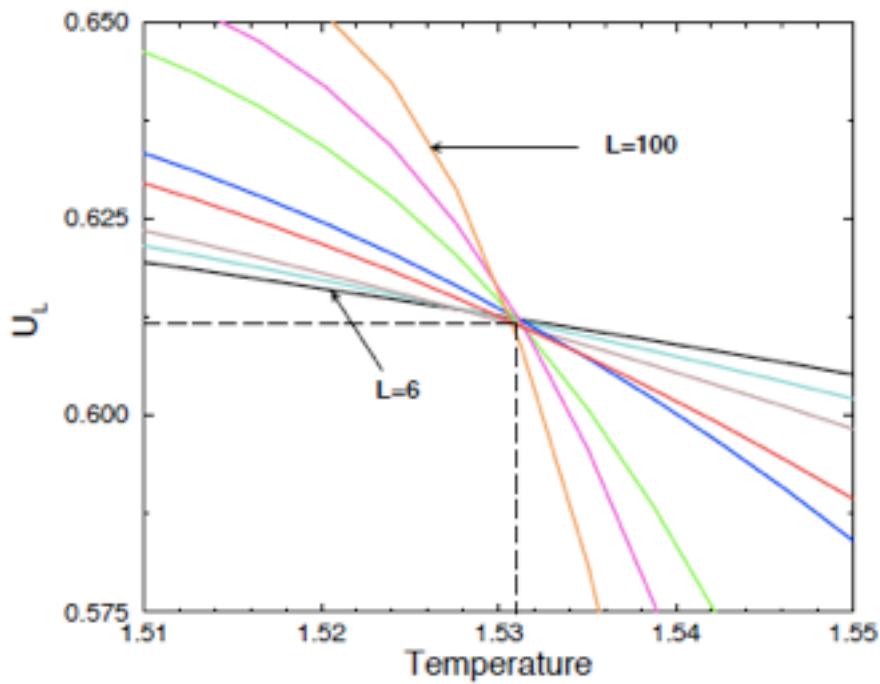
$$\xi \propto |T - T_c|^{-\nu}$$

# Un muestreo por diferentes configuraciones a temperatura fija



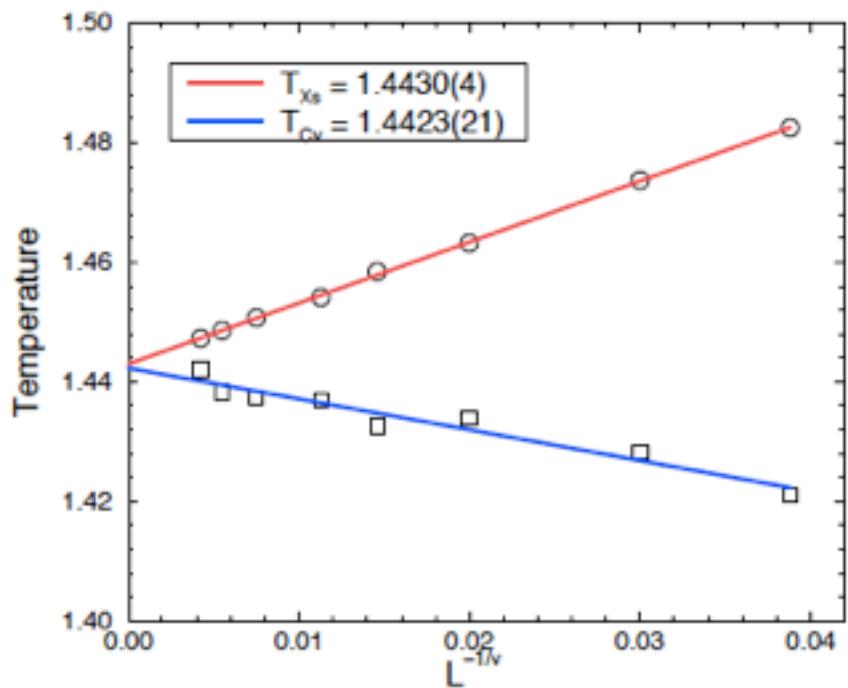
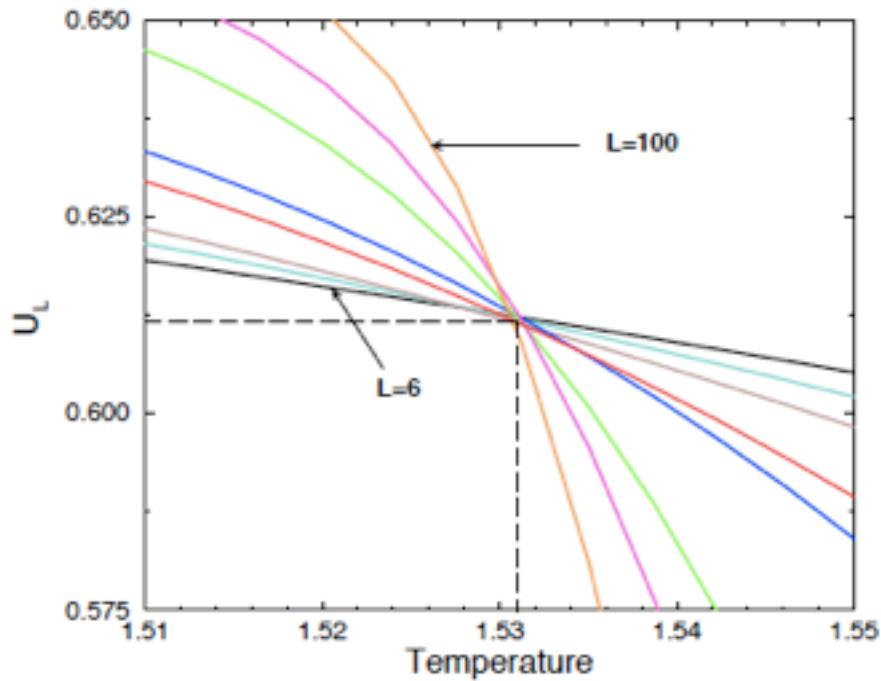
- A temperaturas altas, cada espín se orienta al azar (fase paramagnética)
- A temperaturas bajas, escoge una orientación (fase ferromagnética)

# Paso 1: Determine la temperatura crítica



$$U_B(T) = 1 - \frac{1}{3} \frac{\langle M^4 \rangle_T}{\langle M^2 \rangle_T^2}$$

## Paso 2: Hallar $\nu$



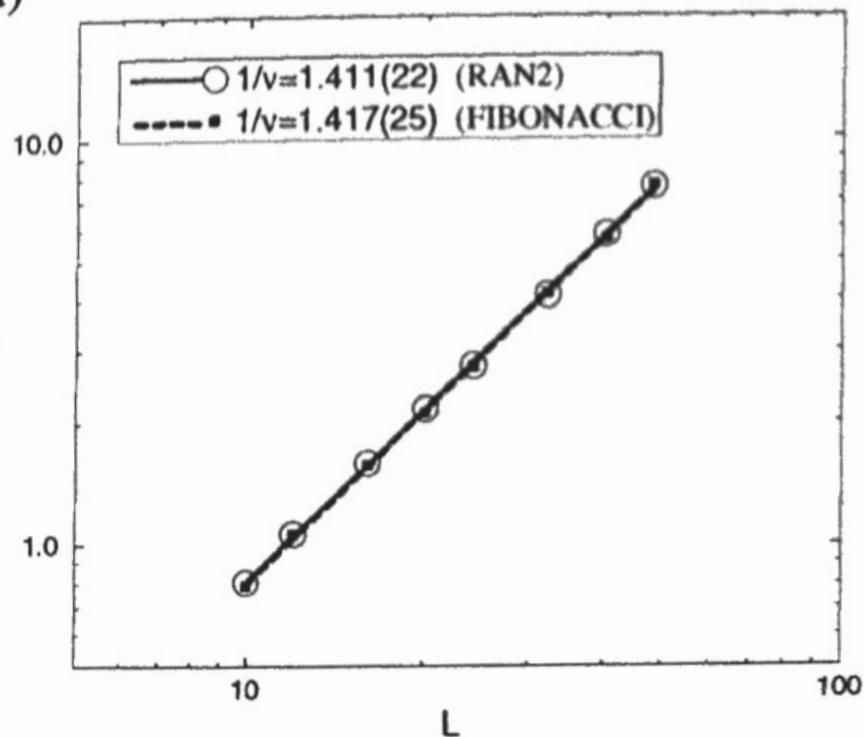
$$-\left. \frac{\partial U_B}{\partial T} \right|_{T_C} \sim L^{1/\nu}$$

$$T_{Xs_{\max}} \sim T_C + aL^{-1/\nu}$$

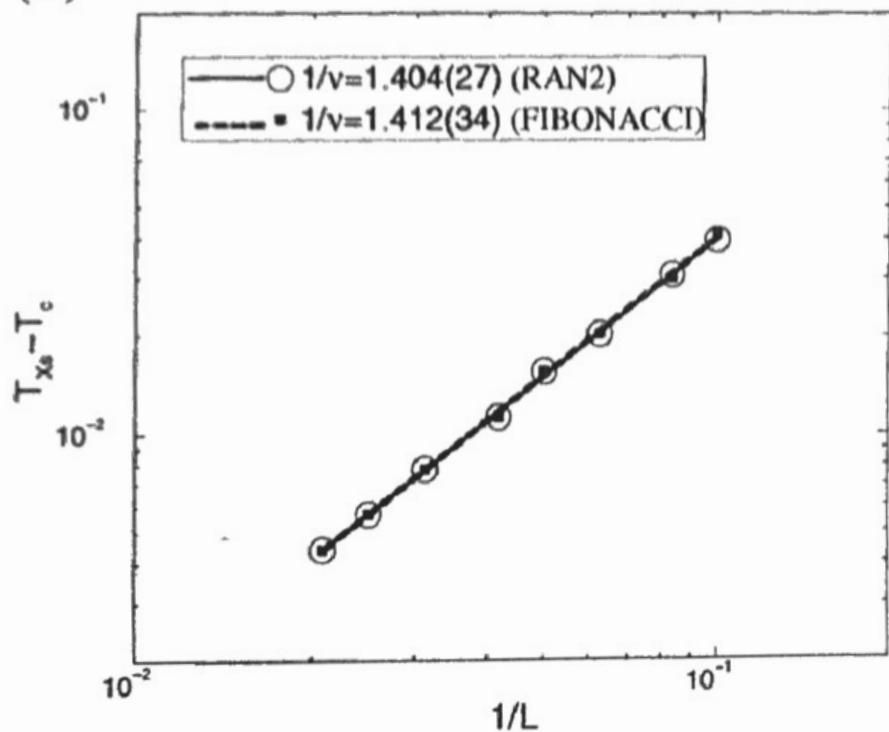
$$T_{C_{v \max}} \sim T_C + bL^{-1/\nu}$$

## Paso 2: Hallar $\nu$

(a)



(b)

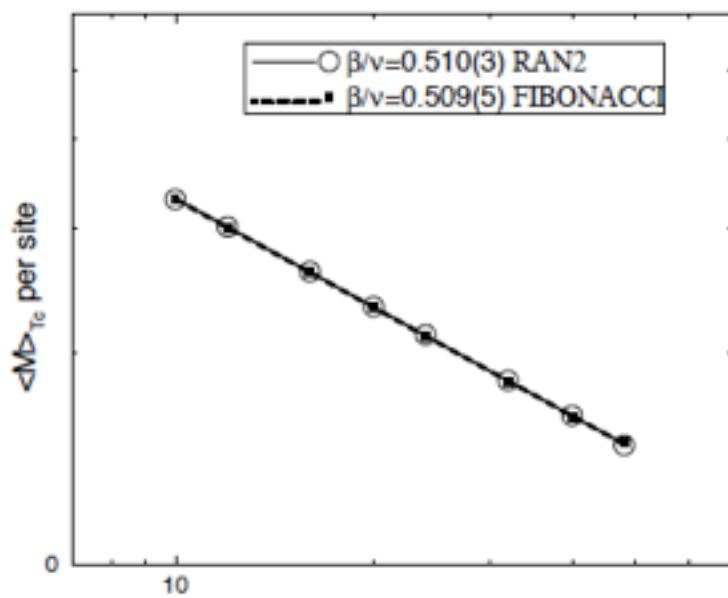
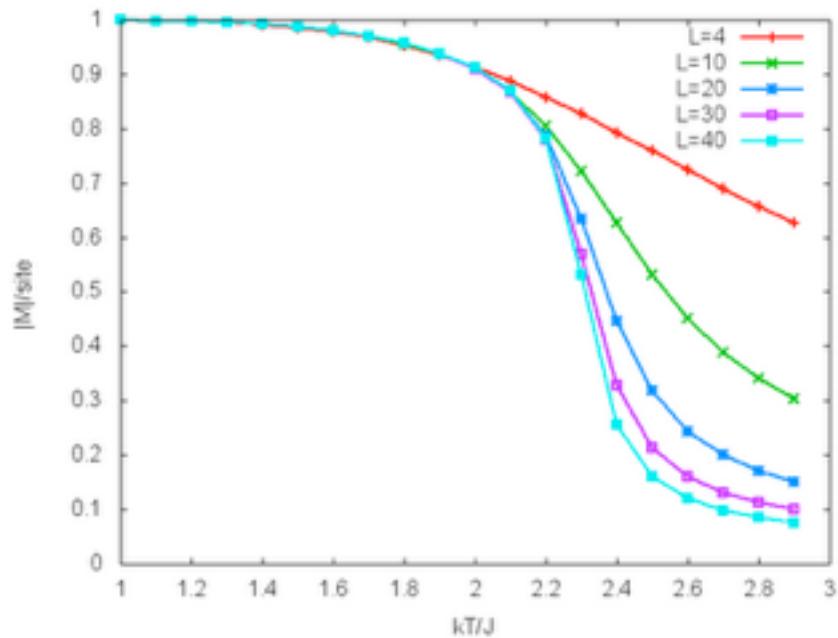


$$-\left. \frac{\partial U_B}{\partial T} \right|_{T_C} \sim L^{1/\nu}$$

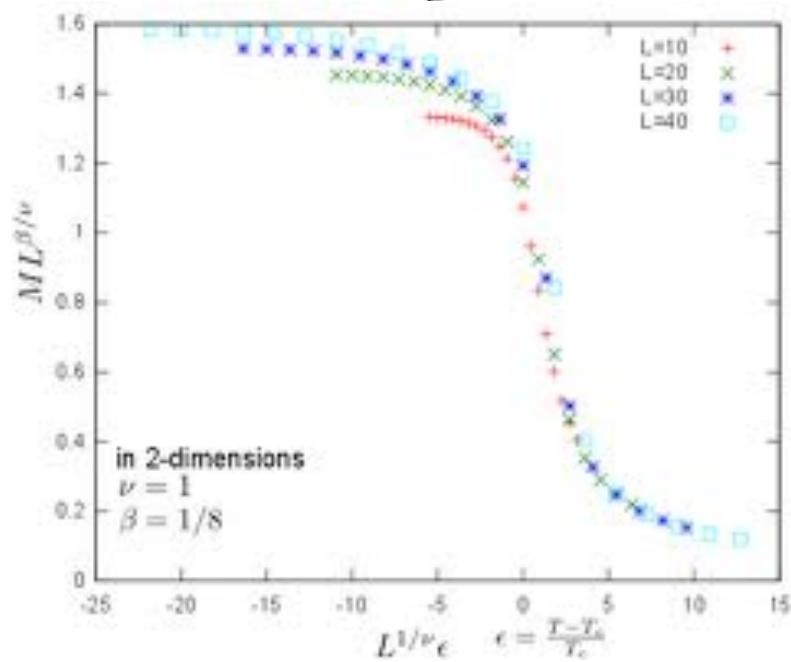
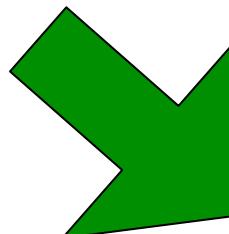
$$T_{X_{s_{\max}}} \sim T_C + aL^{-1/\nu}$$

$$T_{C_{v \max}} \sim T_C + bL^{-1/\nu}$$

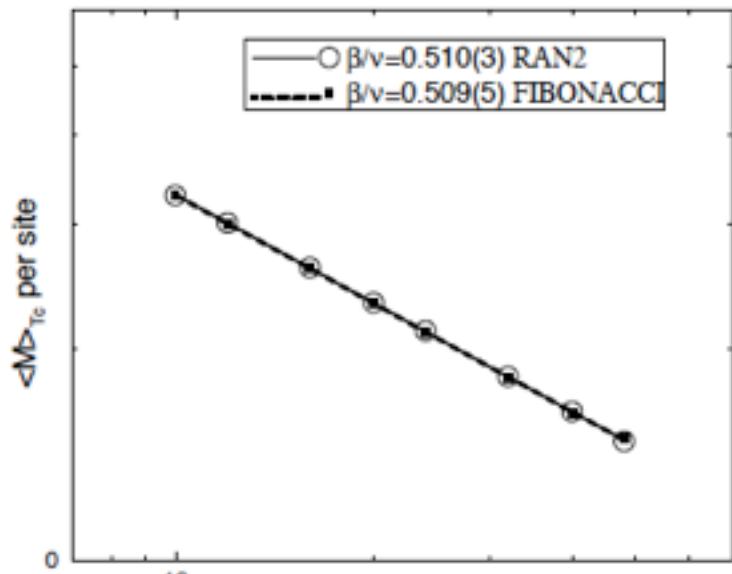
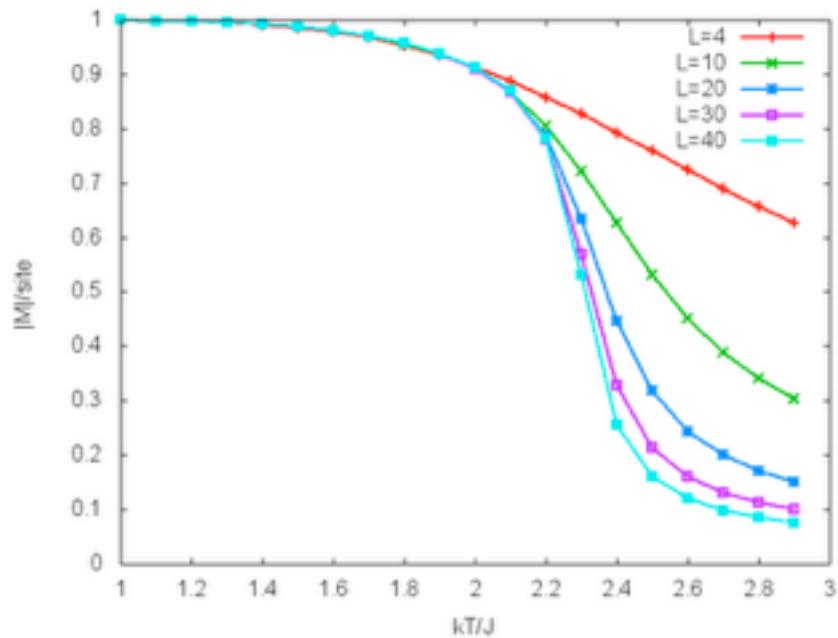
## Paso 3: Medir $\langle M \rangle$ a $T=T_c$ y escalar



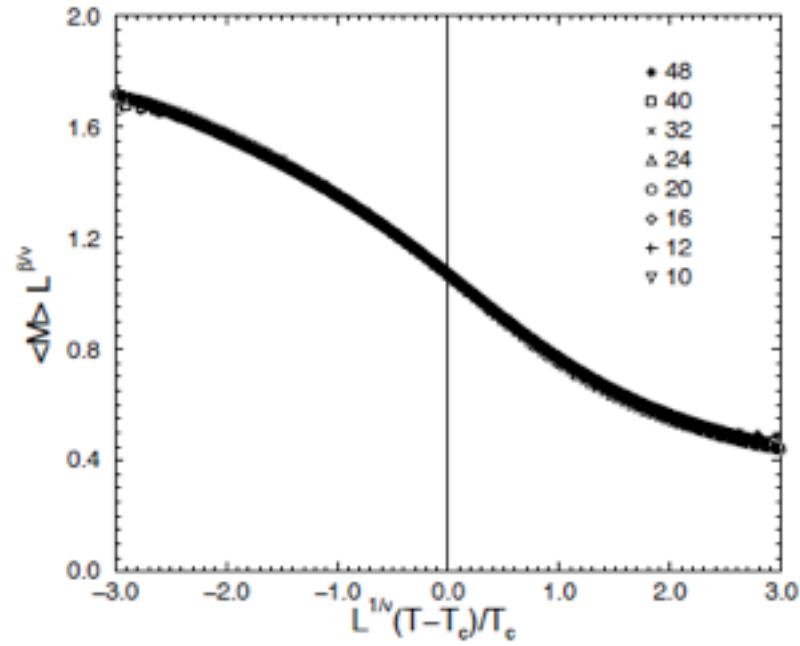
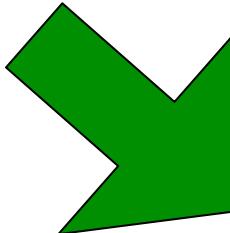
$$\frac{1}{L^d} \langle M \rangle_{T_C} \sim L^{-\beta/\nu}$$



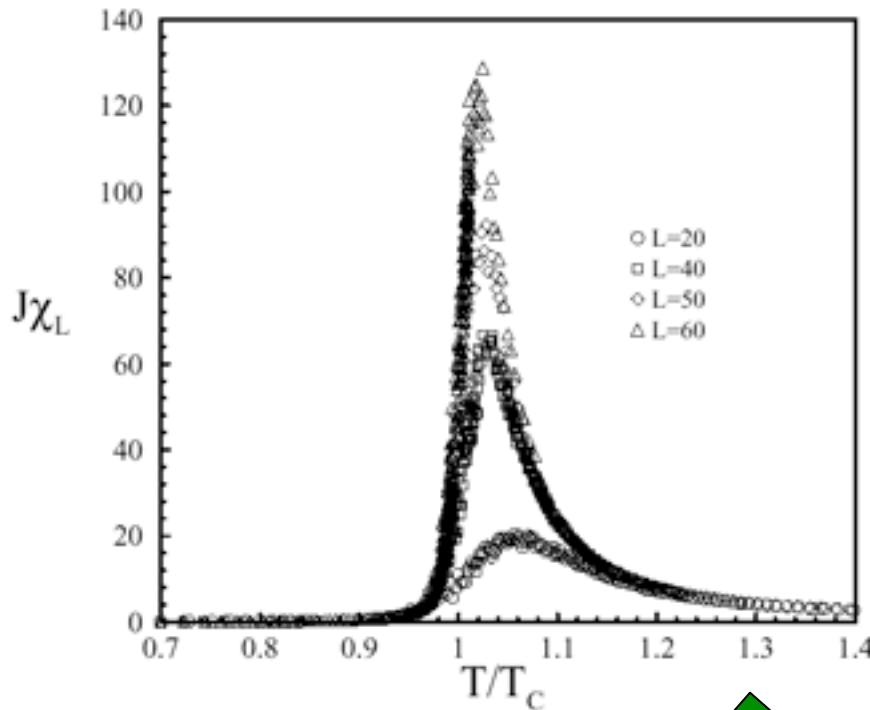
## Paso 3: Medir $\langle M \rangle$ a $T=T_c$ y escalar



$$\frac{1}{L^d} \langle M \rangle_{T_C} \sim L^{-\beta/\nu}$$



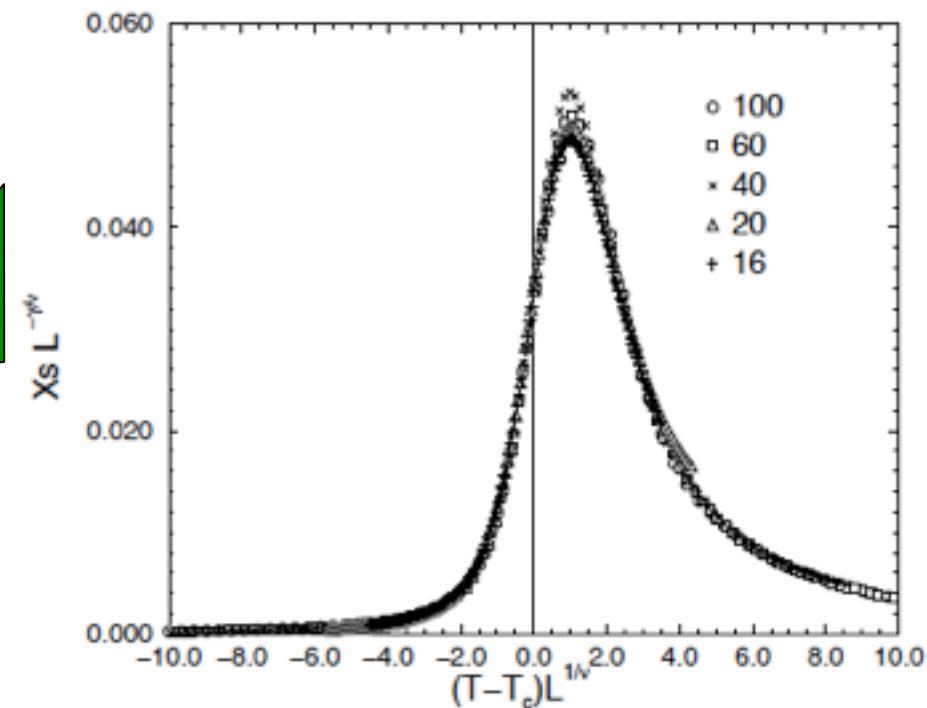
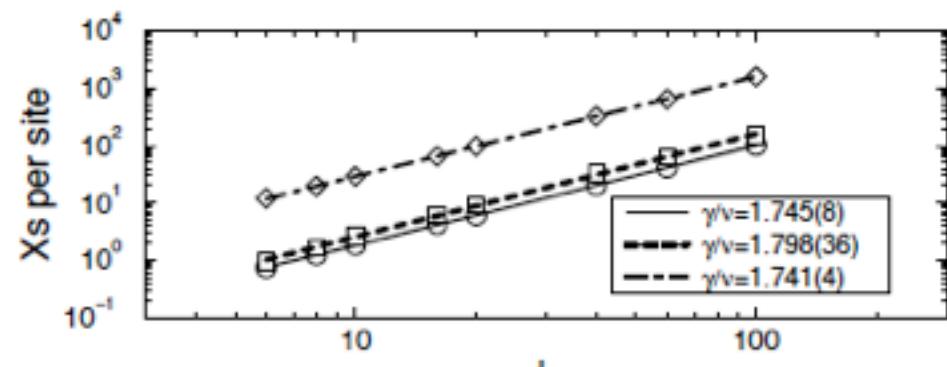
## Paso 4: Medir $X_s$ a $T=T_c$ y escalar



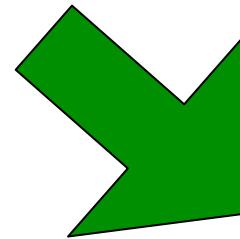
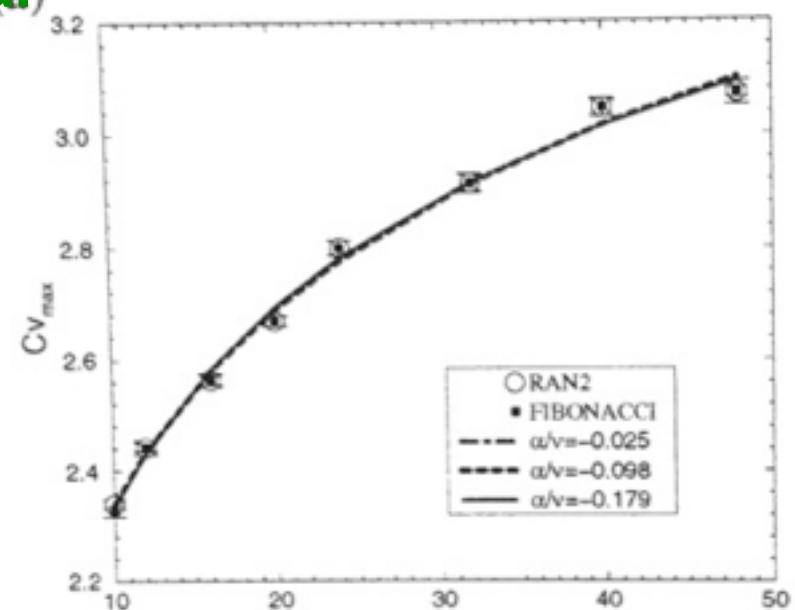
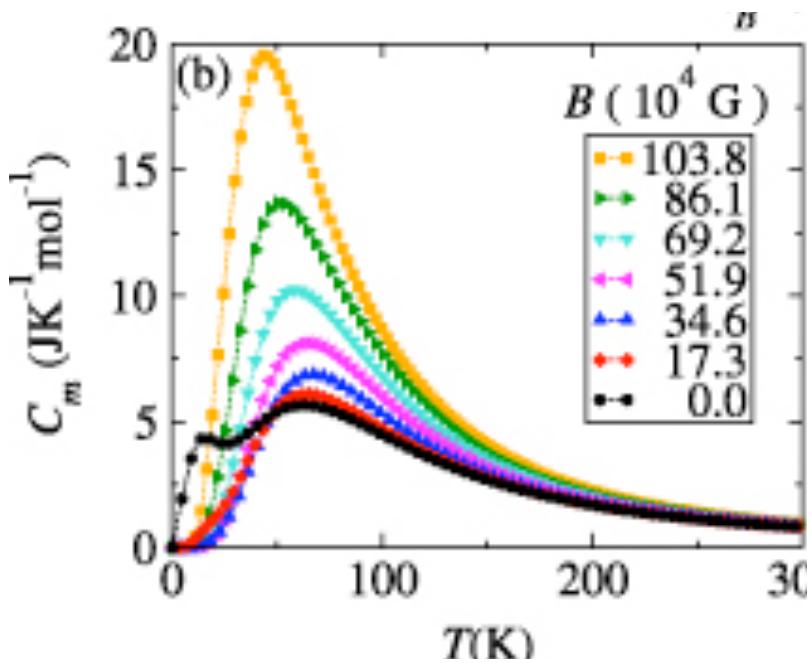
$$\frac{1}{L^d} X_s(T_c) \sim L^{\gamma/\nu}$$

$$\frac{1}{L^d} X_{s_{\max}} \sim L^{\gamma/\nu}$$

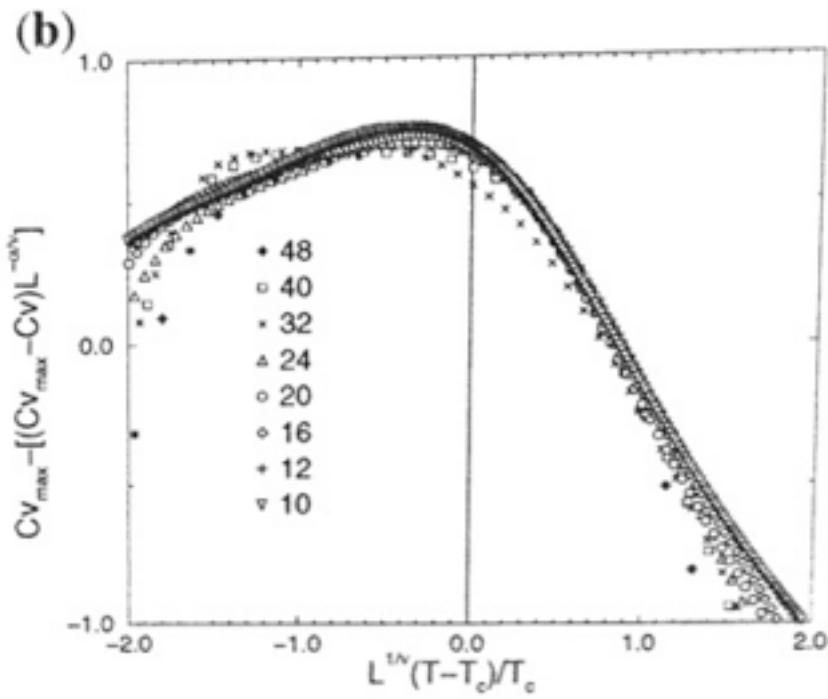
$$\frac{1}{L^d} \langle M^2 \rangle_{T_c} \sim L^{\gamma/\nu}$$



## Paso 4: Medir Cv a T=Tc y escalar



$$Cv_{\max}(L) = Cv_{\max}(\infty) - a \sim L^{\alpha/\nu}$$



Parameter	Monte Carlo Study		
	PFL	HJ	This Study
$\beta_{T_c}$	0.6929(1)	0.6930(1)	0.69303(4)
$U^*$	-	0.6217(8)	0.62145(8)

Exponent	Monte Carlo Study		
	PFL	HJ	This Study
$\nu$	0.706(9)	0.704(6)	0.709(6)
$\beta/\nu$	0.516(3)	0.514(1)	0.510(3)
$\gamma/\nu$	1.969(7)	1.9729(17)	1.982(3)
$\alpha$	-0.118(18)	-0.112(18)	-0.127(18)



COMISIÓN  
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# ¡ Muchas Gracias !

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