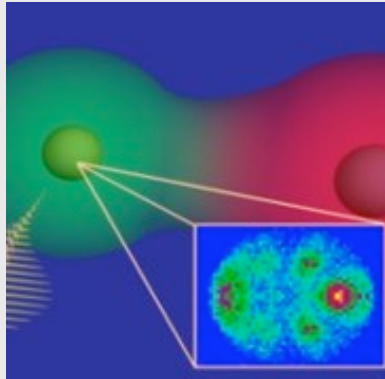
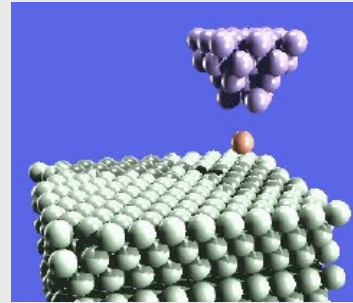


KSU Ph.D. Program

Atomic, Molecular, Optical



Condensed Matter



Physics Education



High Energy



www.phys.ksu.edu

graduate@phys.ksu.edu

Full financial support to all students

Research in first summer

27 Faculty and 60 Graduate students

Cosmology

Efeitos de vacâncias de spin nos magnetos bi-dimensionais de plano fácil

Gary M. Wysin
Kansas State University
Manhattan, Kansas, U.S.A.

Onde é Kansas State University?



KSU



Os assuntos principais

- **modelos** de magnetismo
- propriedades de **vórtices**
- **transição de fase** via pares de vórtices
- efeitos de **vacâncias** (vagos na rede dos spins) nos vórtices e na transição de fase

um vortice

Wichita, KS



Materiais magnéticos

- elétron spins num átomo quer alinhar em pares: $\uparrow\downarrow$
- $S = \text{spin}$ do átomo = \sum (spins sem pares)
- exemplo: átomos Fe, Co, Ni, Mn, Cr podem ter $S \neq 0$
- Material é **magnetizado** quando muitos spins ficam alinhados, sendo um estado de baixa energia.
- **Calor/temperatura** diminui o alinhamento dos spins.

Modelos de 2D de plano fácil

- átomos com $S > 0$, situados numa **rede regular**
- spins ou de 2 componentes (rotor planar) ou de **3 componentes (XY, Heisenberg)**
- intercâmbio **anisotrópico** entre vizinhos, spins preferem ficar dentro do **plano fácil (xy)**
- **ferromagnets:** tendência de spins alinhados
antiferromagnets: tendência de spins opostos
- **transição de fase via nucleação de vórtices (Berezinskii-Kosterlitz-Thouless)**

modelo de Heisenberg com anisotropia

Hamiltoniana

$$H = \frac{-J}{2} \sum_{\mathbf{n}, \mathbf{a}} \left[S_{\mathbf{n}}^x S_{\mathbf{n}+\mathbf{a}}^x + S_{\mathbf{n}}^y S_{\mathbf{n}+\mathbf{a}}^y + \lambda S_{\mathbf{n}}^z S_{\mathbf{n}+\mathbf{a}}^z \right]. \quad (1)$$

parâmetro de
anisotropia

$$0 \leq \lambda < 1$$

XY ----- isotropic

ângulos dos spins

It is convenient to write the spins of length S in terms of in-plane angles $\phi_{\mathbf{n}} \equiv \tan^{-1}(S_{\mathbf{n}}^y/S_{\mathbf{n}}^x)$ and scaled out-of-plane component $m_{\mathbf{n}} \equiv S_{\mathbf{n}}^z/S$,

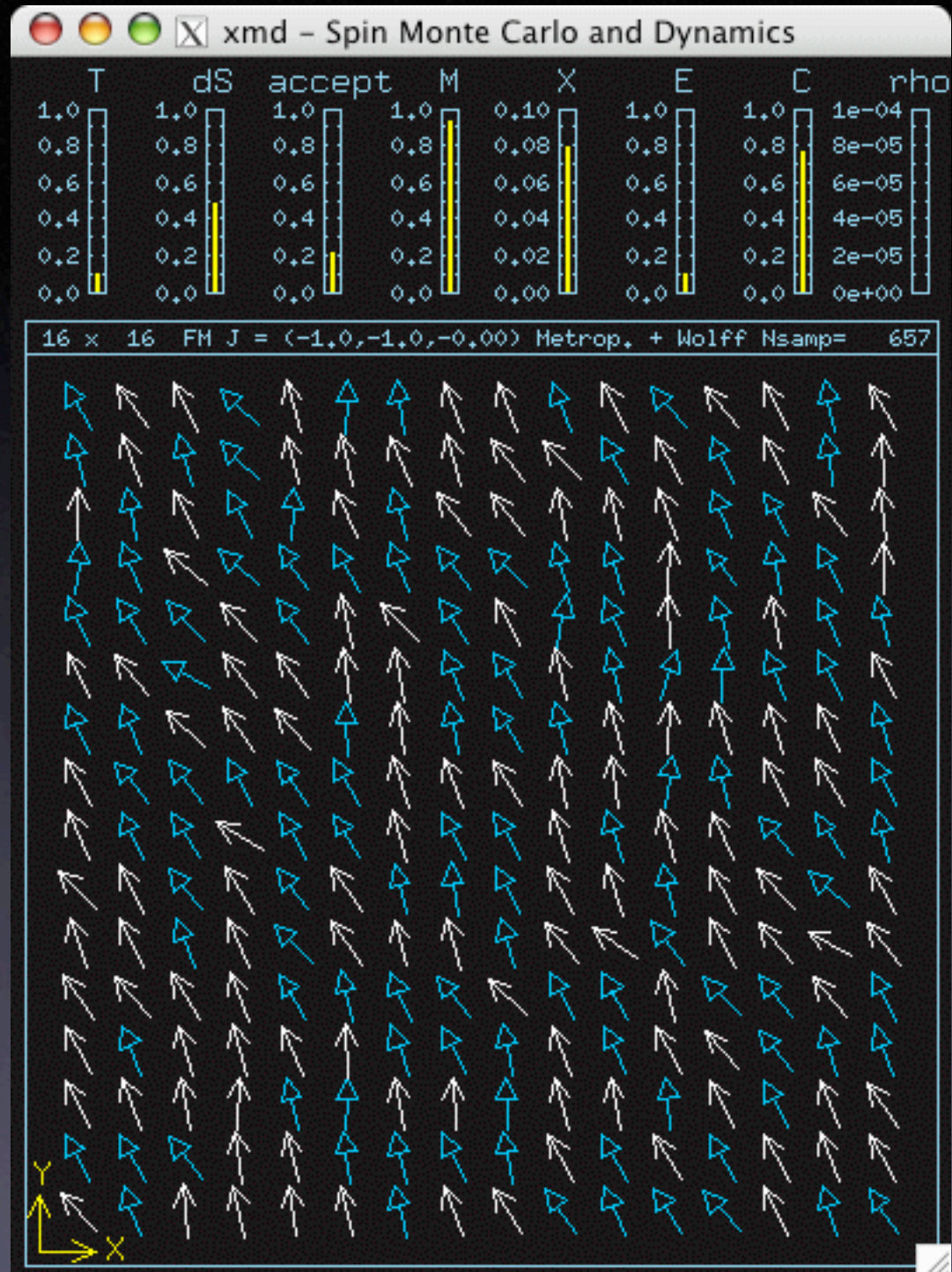
$$\vec{S}_{\mathbf{n}} = S(\sqrt{1 - m_{\mathbf{n}}^2} \cos \phi_{\mathbf{n}}, \sqrt{1 - m_{\mathbf{n}}^2} \sin \phi_{\mathbf{n}}, m_{\mathbf{n}}). \quad (2)$$

Modelo de XY ($\lambda=0$)

temperatura
muito baixa
 $T/J = 0.1$

ondas de spin
longas

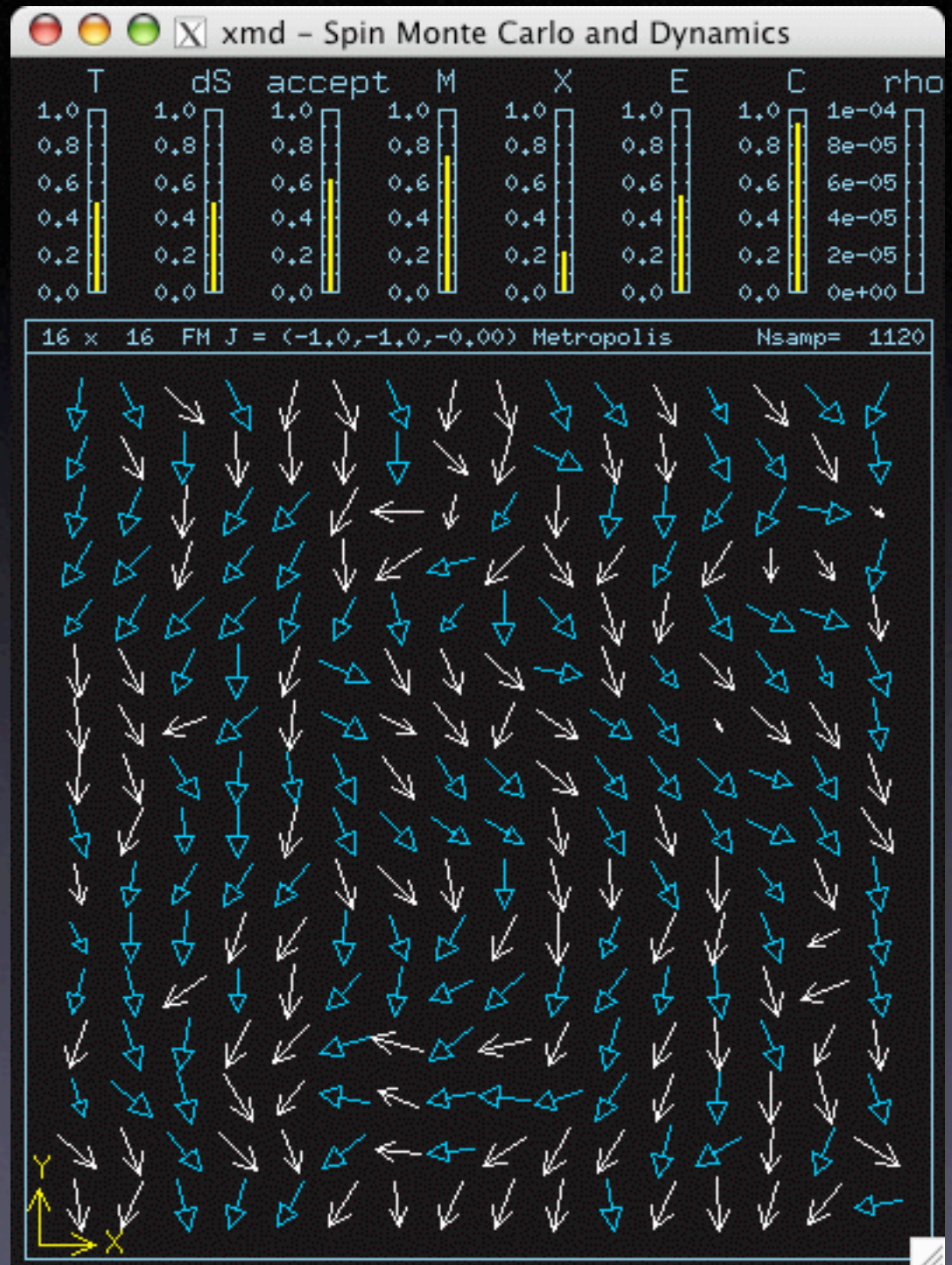
a fase de baixa
temperatura,
ordenada



Modelo de XY ($\lambda=0$)

temperatura baixa
 $T/J = 0.5$

ondas de spin
longas e curtas

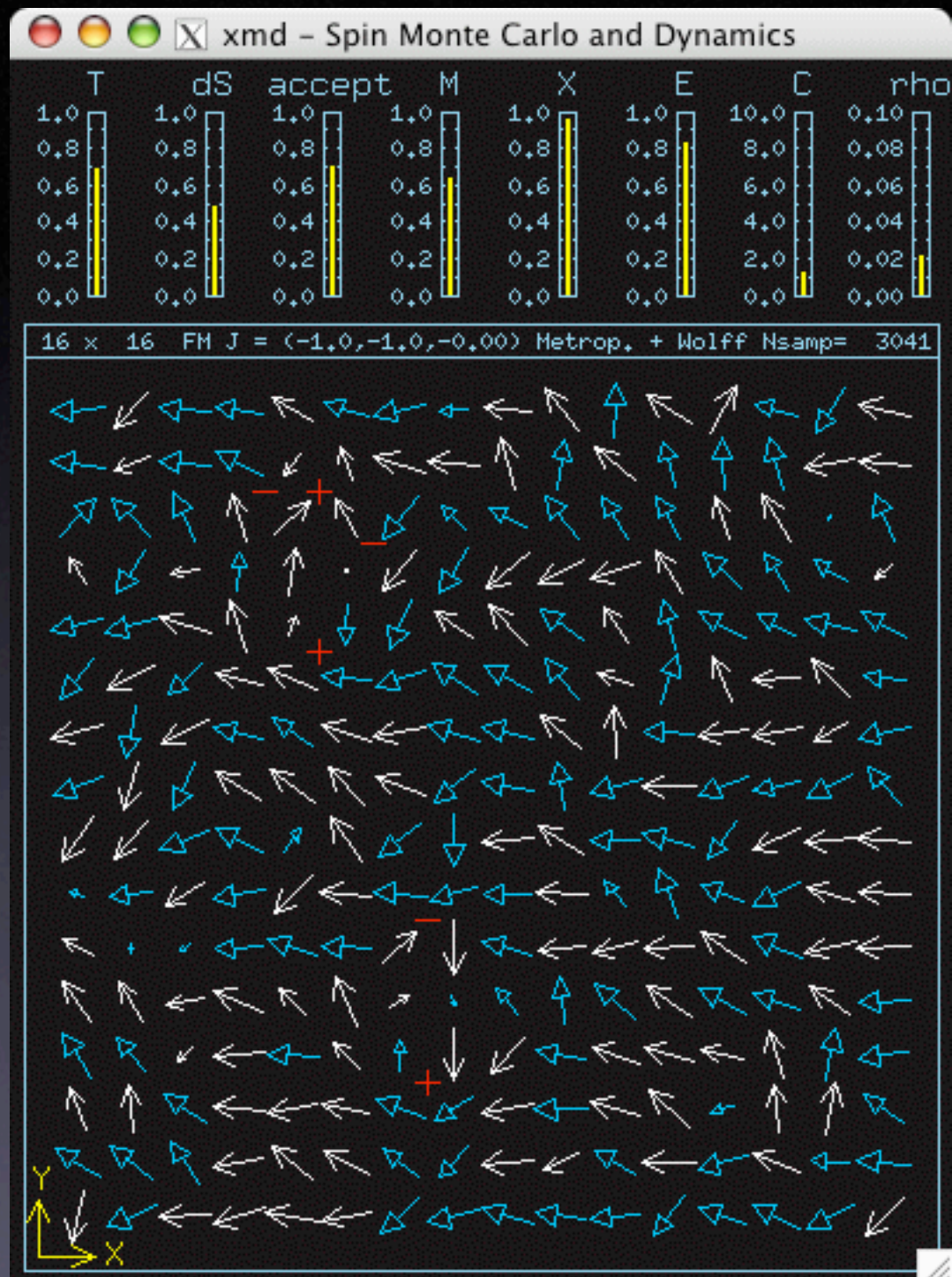


Modelo de XY ($\lambda=0$)

temperatura crítica
 $T_c / J = 0.7$

desordem associado
com nucleação de
vórtices

a transição de fase
acontece

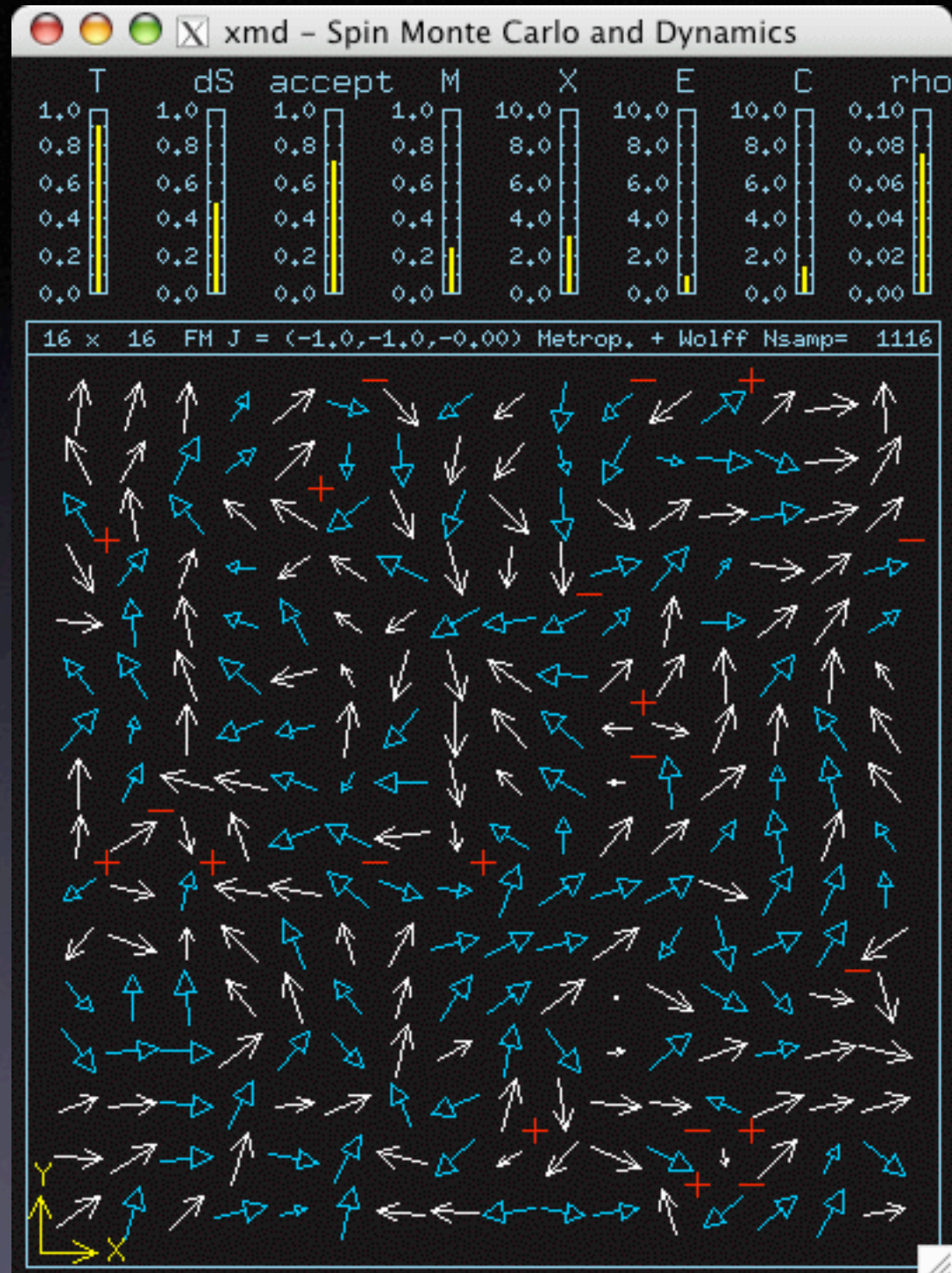


Modelo de XY ($\lambda=0$)

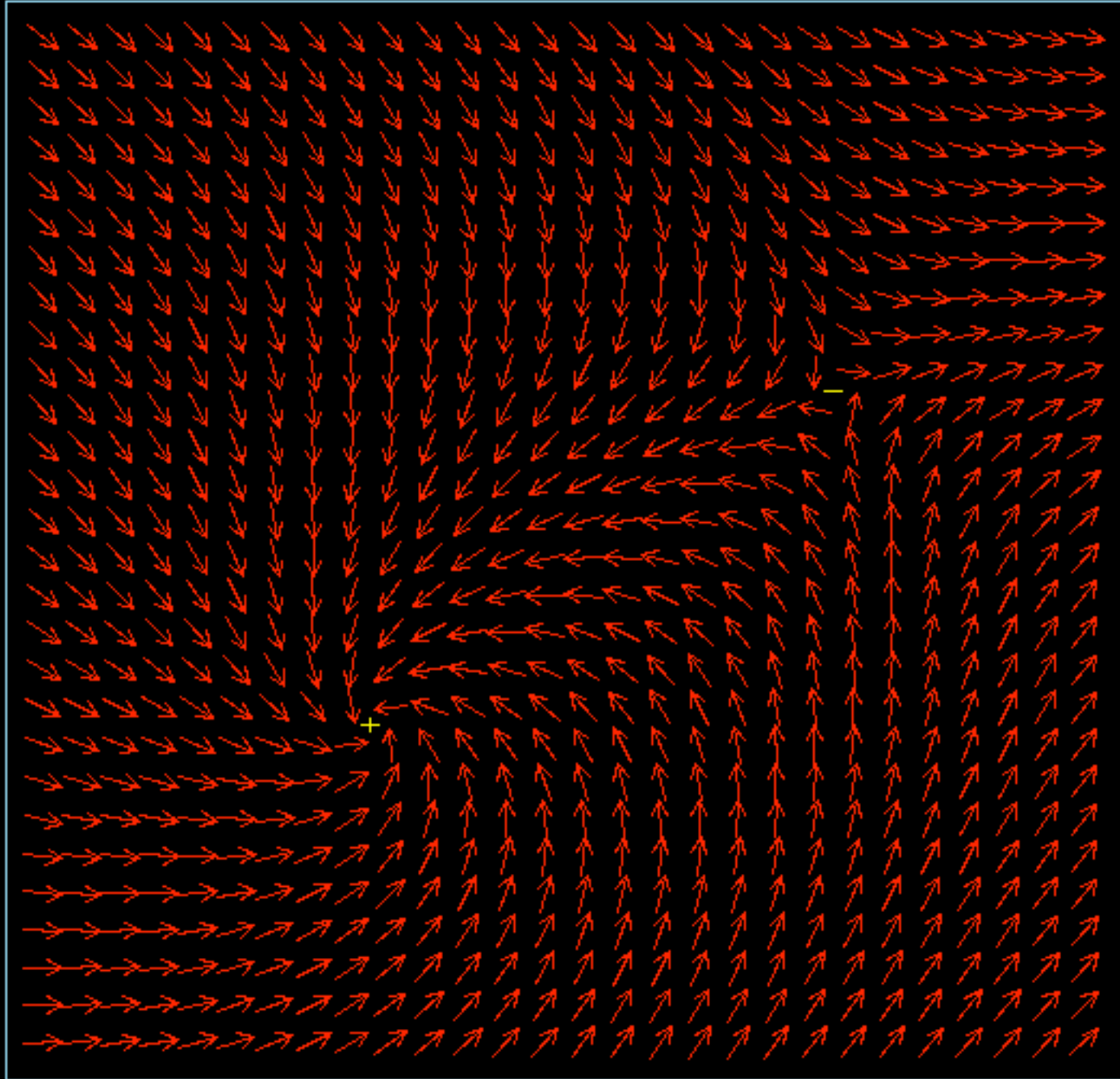
temperatura
alta
 $T/J = 0.9$

densidade de
vórtices subindo
alinhamento dos
spins diminuindo

fase de alta
temperatura,
desordenada



t= 0.00 e= 48.11 m= 1792.20 -100.45 4.00



vórtice
 $q=1$

antivórtice
 $q=-1$

Propriedades dos vórtices

- uma carga topológica integral: $q = \oint d\Phi / 2\pi$
- criados em +q/-q pares
- ângulo dos spins dentro do plano:

$$\phi(x, y) = q \tan^{-1} \left(\frac{y - y_v}{x - x_v} \right) + \phi_0.$$

- energia de um vórtice: $E \approx \pi JS^2 q^2 \ln(R/a)$
- energia de um +q/-q par: $E \approx \pi JS^2 q^2 \ln(d/a)$

R=raio do sistema, d=separação do par,
a=constante da rede

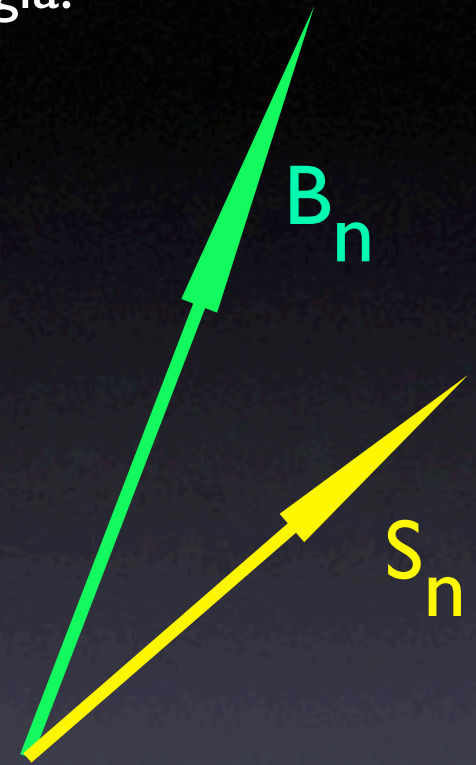
Cálculos de estados de spins via

Relaxação para um estado mínimo local de energia:

campo efetivo dos vizinhos =

$$\vec{B}_n = J \sum_{\mathbf{a}} p_{n+\mathbf{a}} [S_{n+\mathbf{a}}^x \hat{x} + S_{n+\mathbf{a}}^y \hat{y} + \lambda S_{n+\mathbf{a}}^z \hat{z}],$$

$p_n = 0/1$ (sítio vazio/ocupado)



Escolha um estado inicial
(por exemplo, parecido com um vórtice).

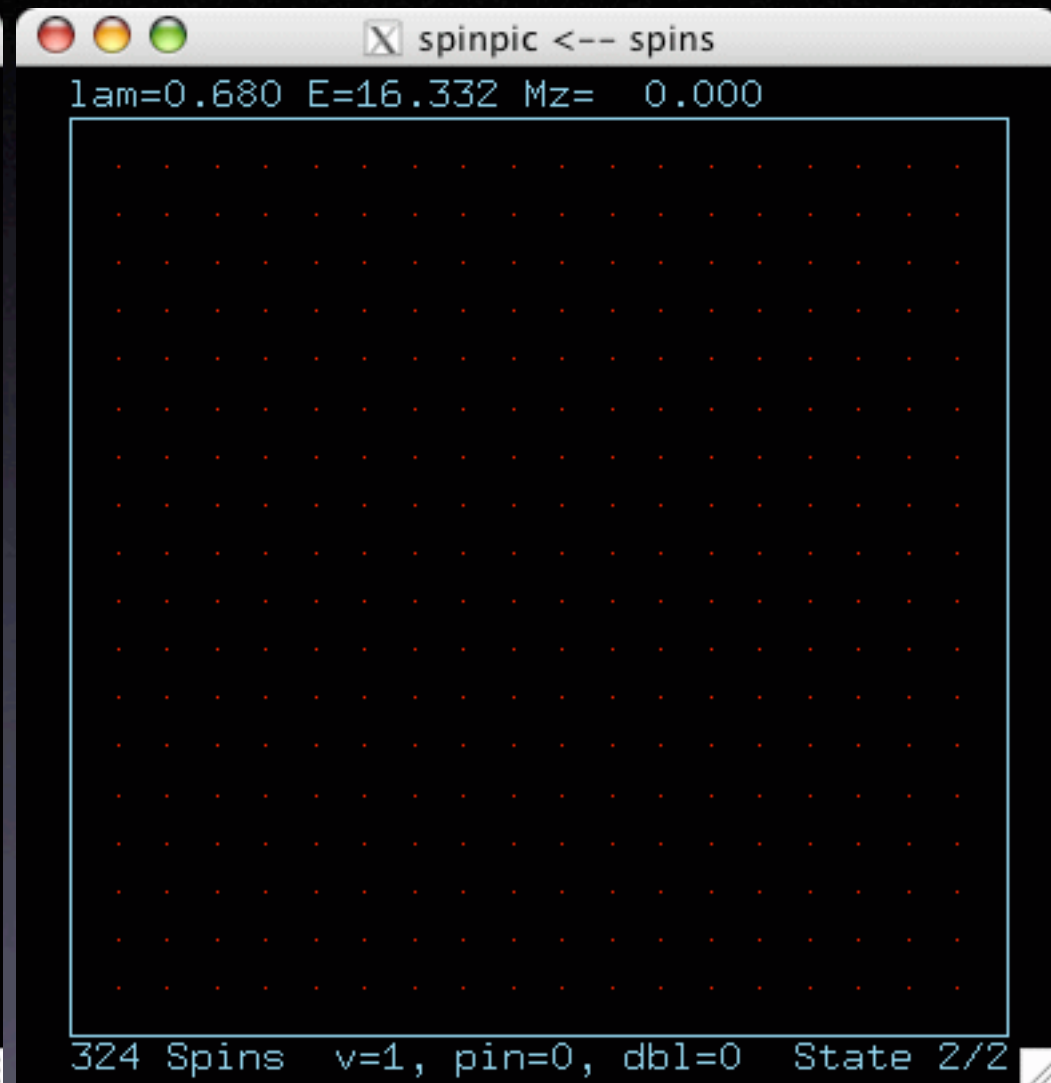
Iteração: Coloque cada spin da rede paralelo ao campo efetivo dos vizinhos, até não há mais mudanças no sistema.

Vórtice **planar** ($\lambda=0.68$) (R=50a)

estável só com $\lambda < \lambda_c \approx 0.7$ (anisotropia forte)



(S_x, S_y)

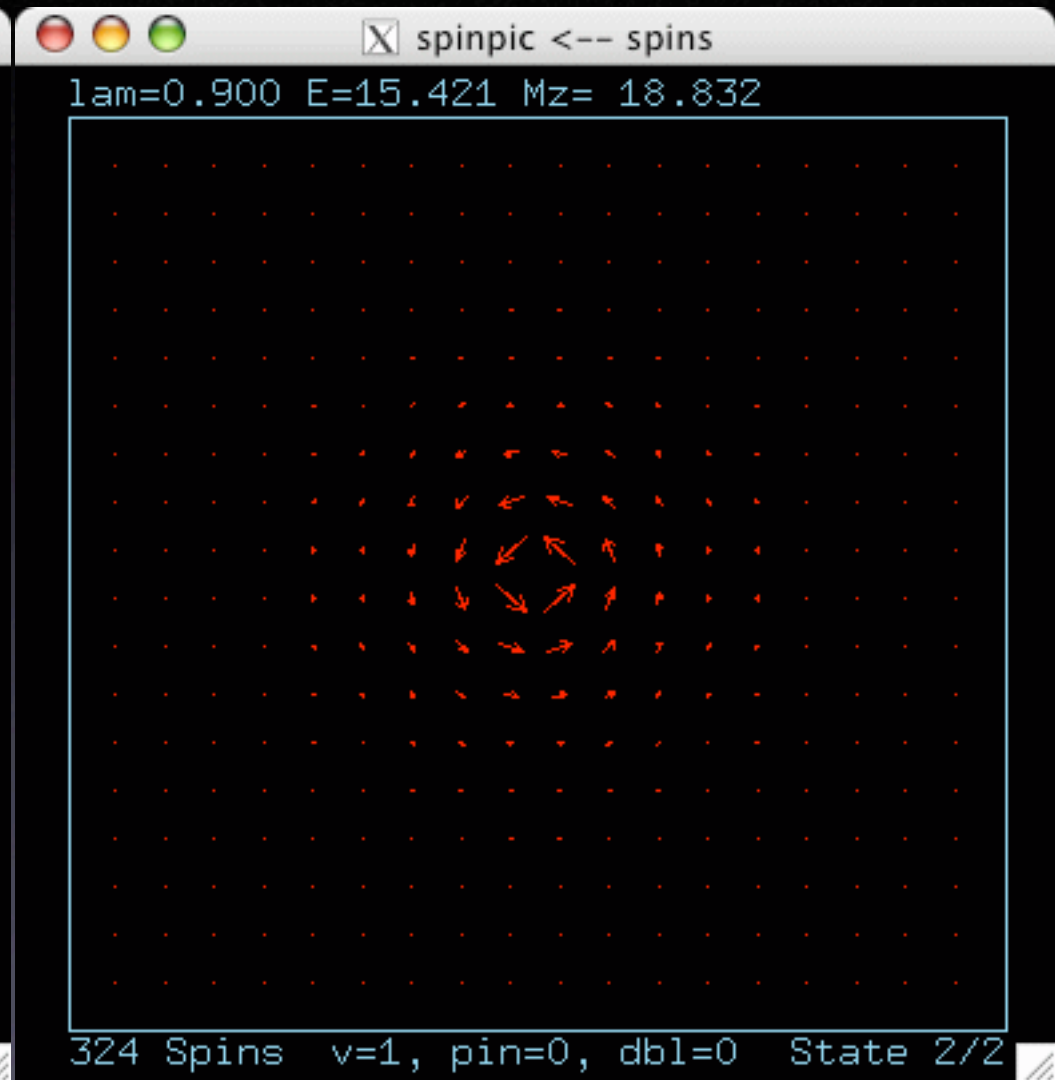


S_z

Vórtice **fora do plano** ($\lambda=0.9$) ($R=50a$)
estável só com $\lambda > \lambda_c \approx 0.70$ (anisotropia fraca)

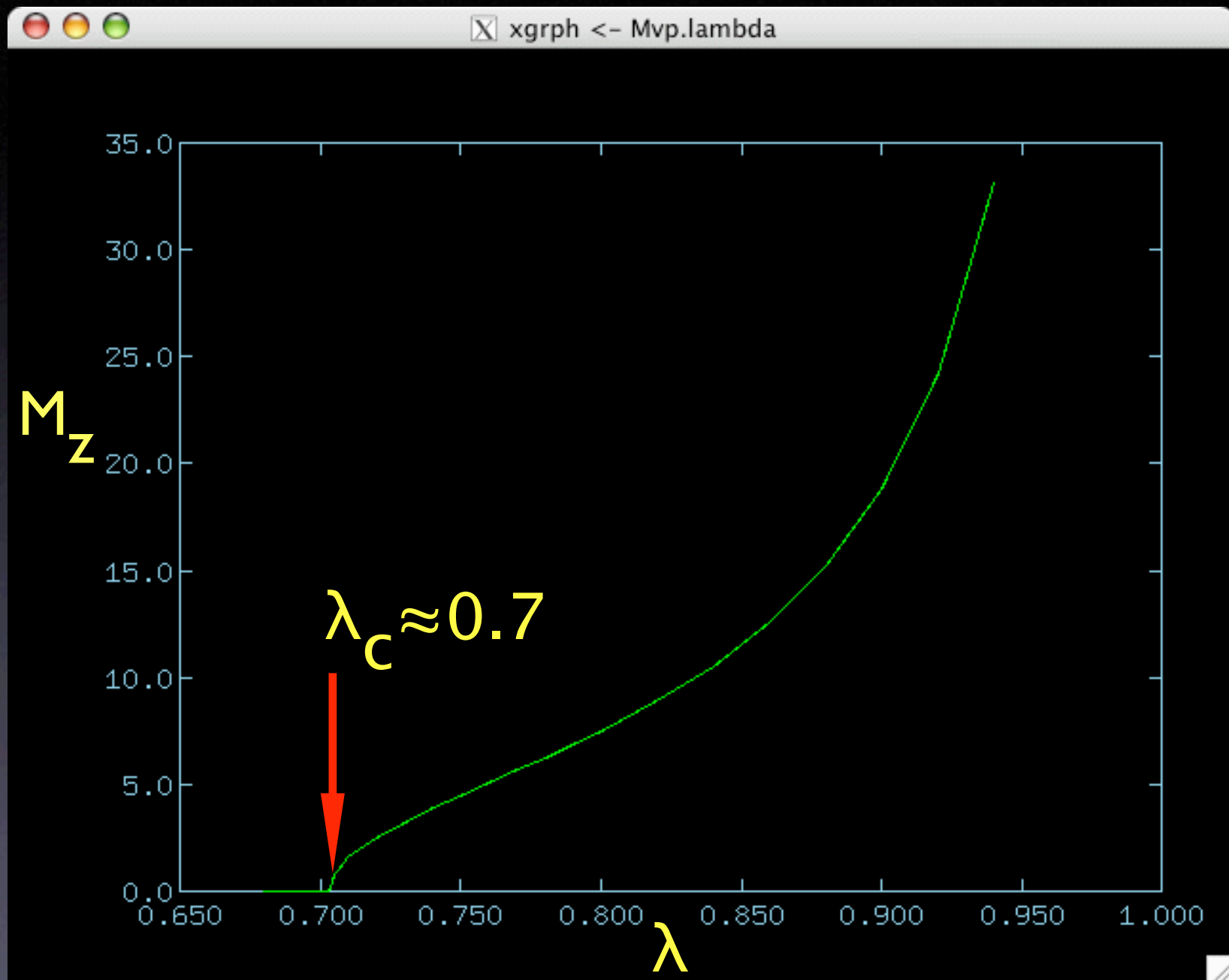


(S_x, S_y)



S_z

M_z do vórtice fora do plano



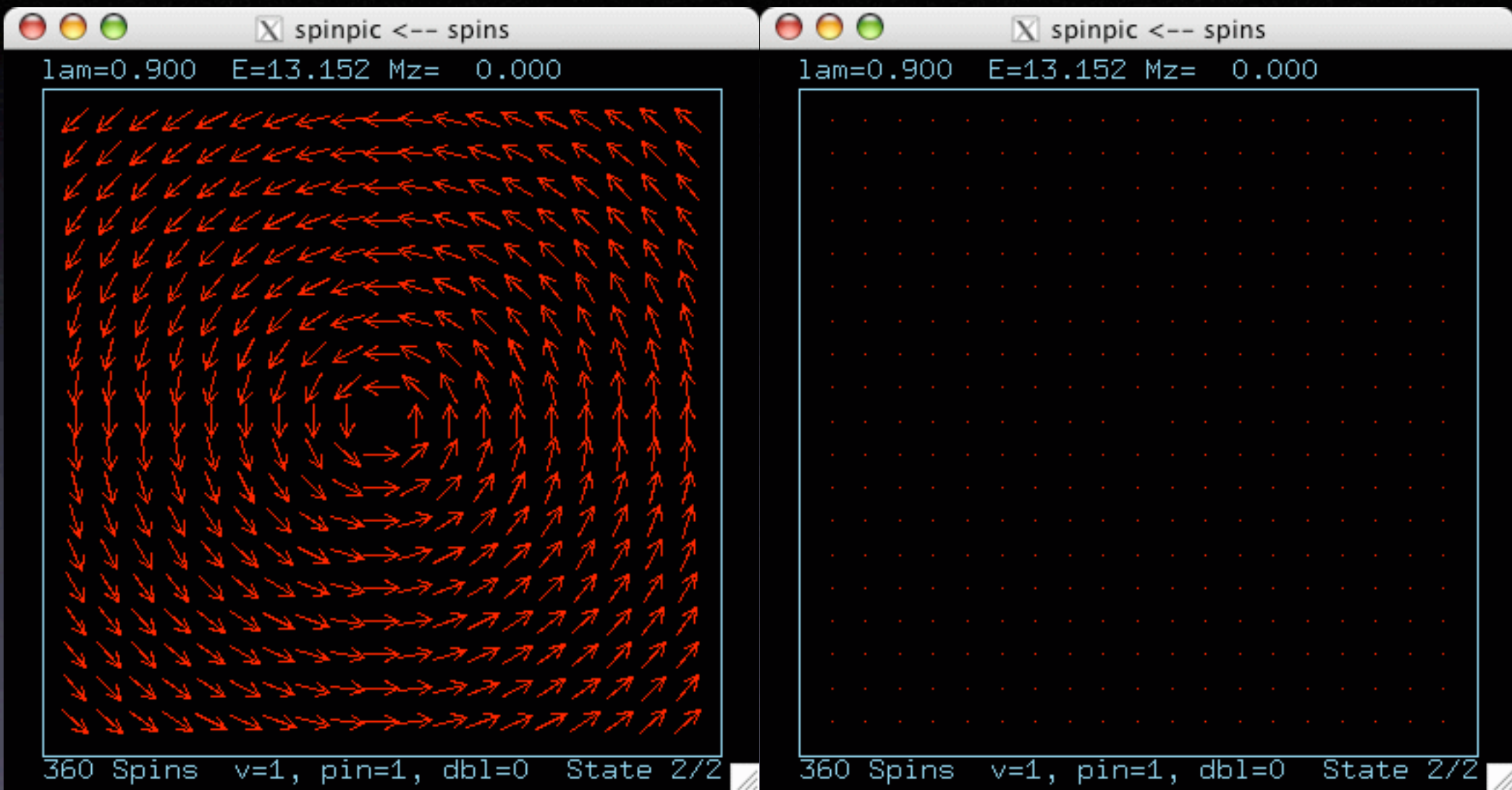
vortex motion...

$$\lambda=0.95$$

Quais são as mudanças quando um vórtice localiza numa vacância?

- a **energia** fica menor.
- o valor critical, $\lambda_c \approx 0.7$,
aumenta para $\lambda_{cv} \approx 0.9545$.
- vórtices **planares** ficam mais estáveis.
- o vórtice é **atraído** pela vacância.
- a carga de vórtice pode ser $q = \pm 2$.

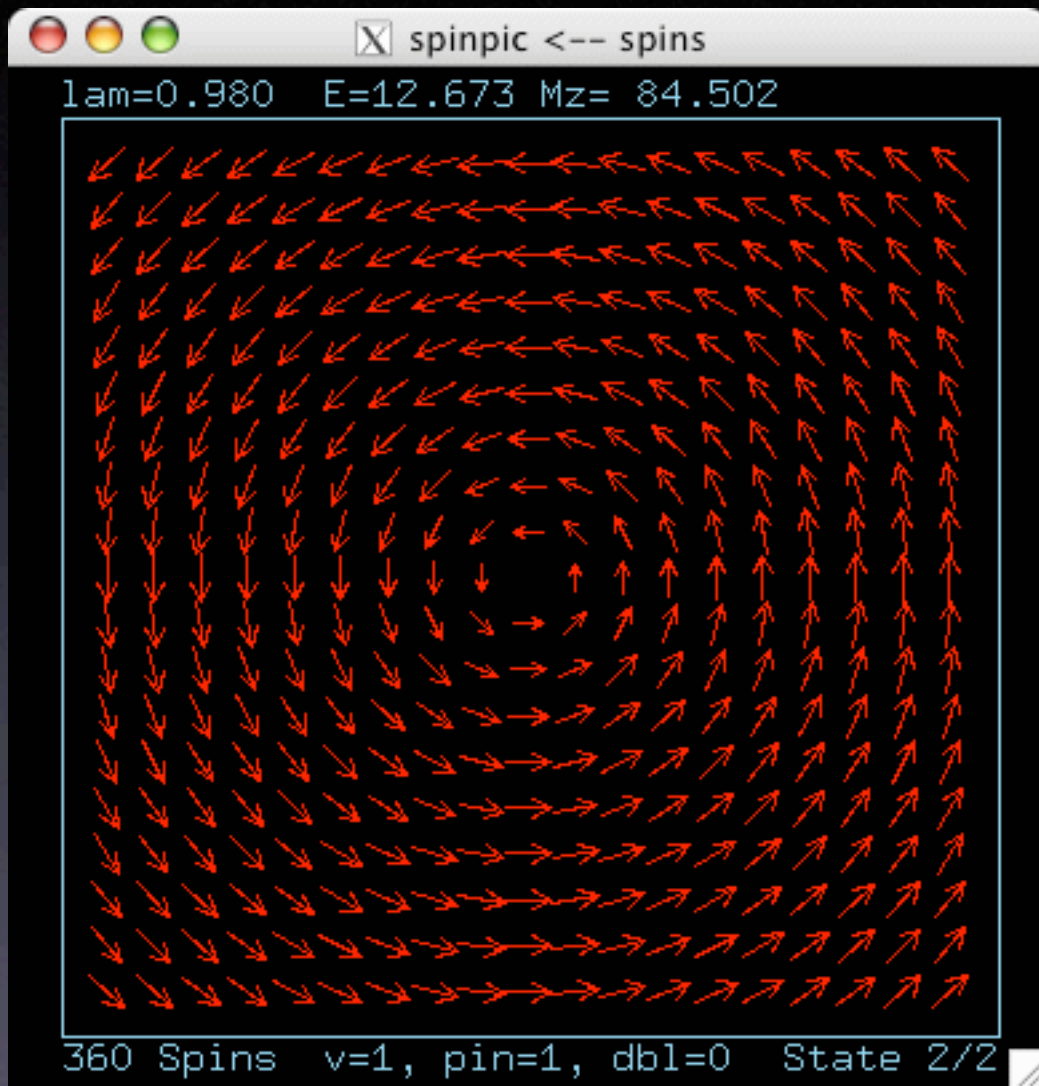
Vórtice **planar**, numa vacância ($\lambda=0.9$) ($R=50a$)
estável só com $\lambda < \lambda_{cv} \approx 0.95$ (anisotropia forte)



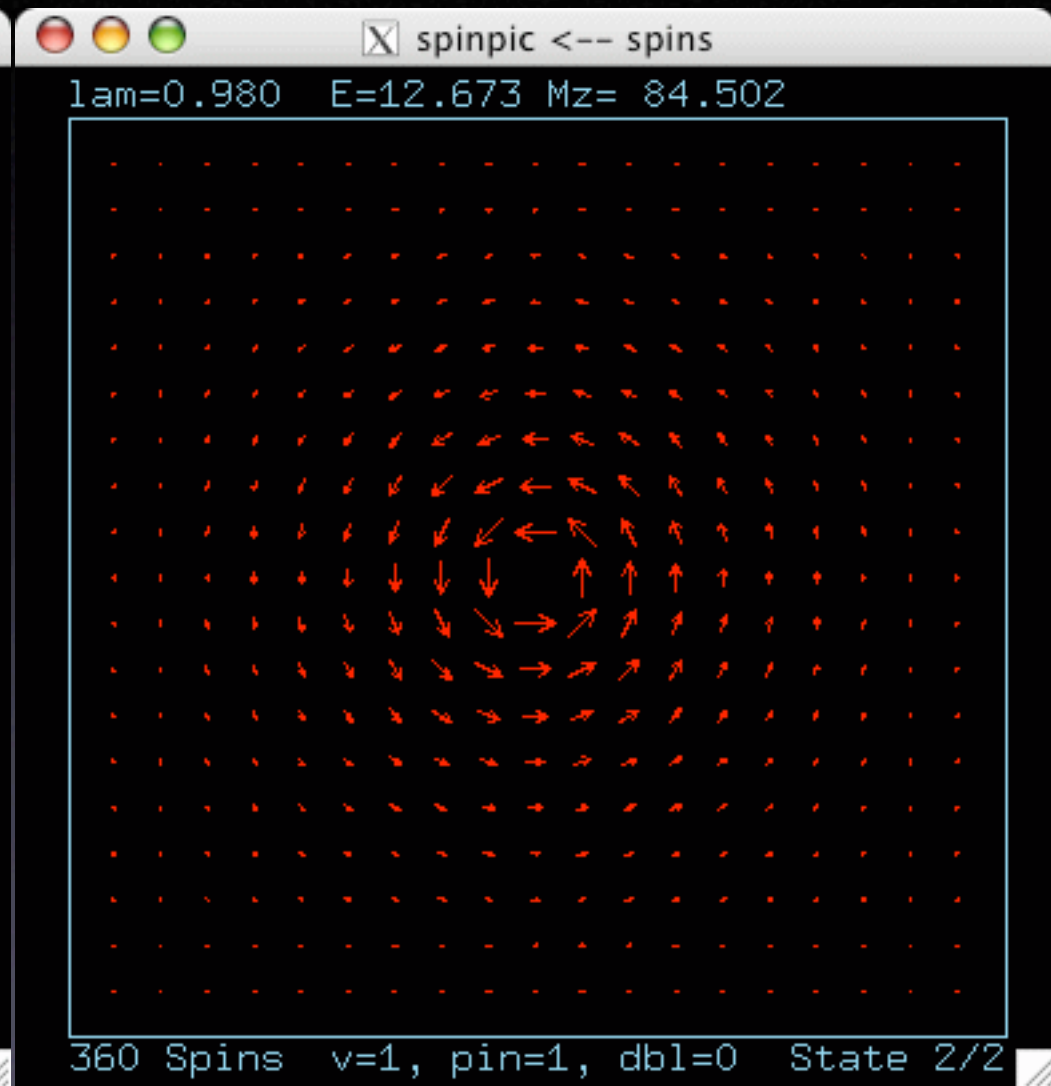
(S_x, S_y)

S_z

Vórtice **fora do plano**, numa vacância ($\lambda=0.98$)
estável só com $\lambda > \lambda_{cv} \approx 0.95$ (anisotropia fraca)



(S_x, S_y)



S_z

$M=M_z$, fora
do plano,
vórtice numa
vacância,
redes
hexagonal,
quadrada,
triangular

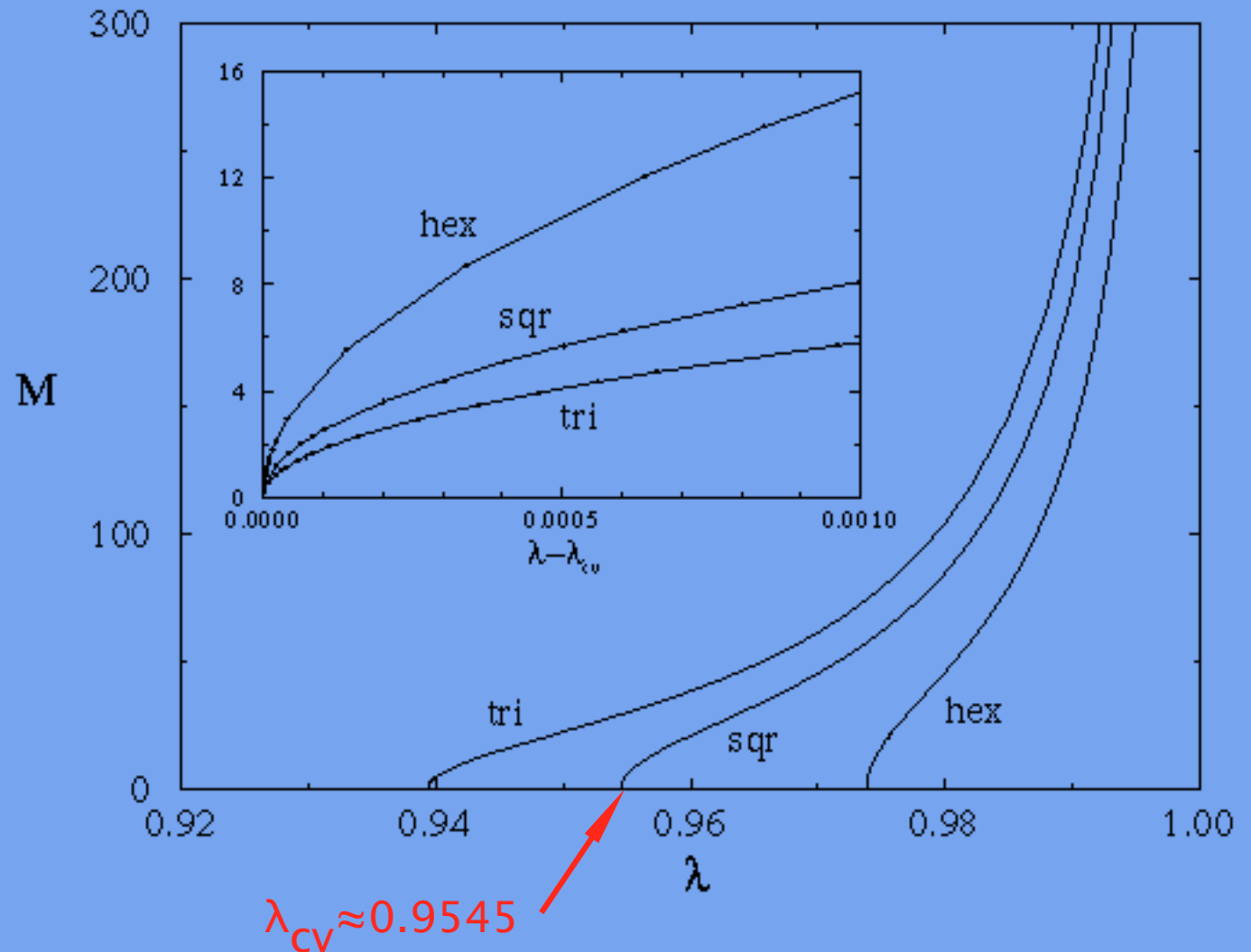
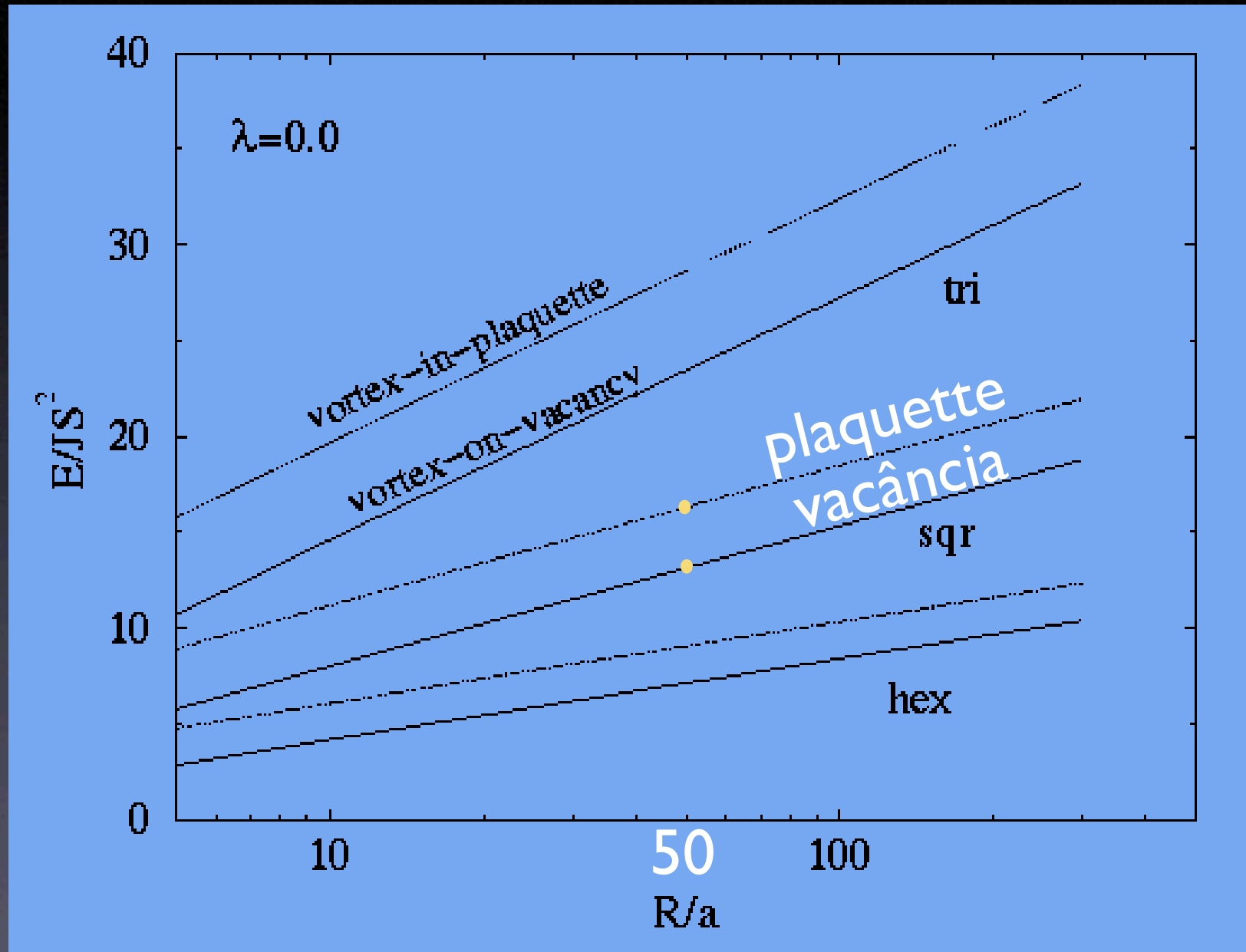
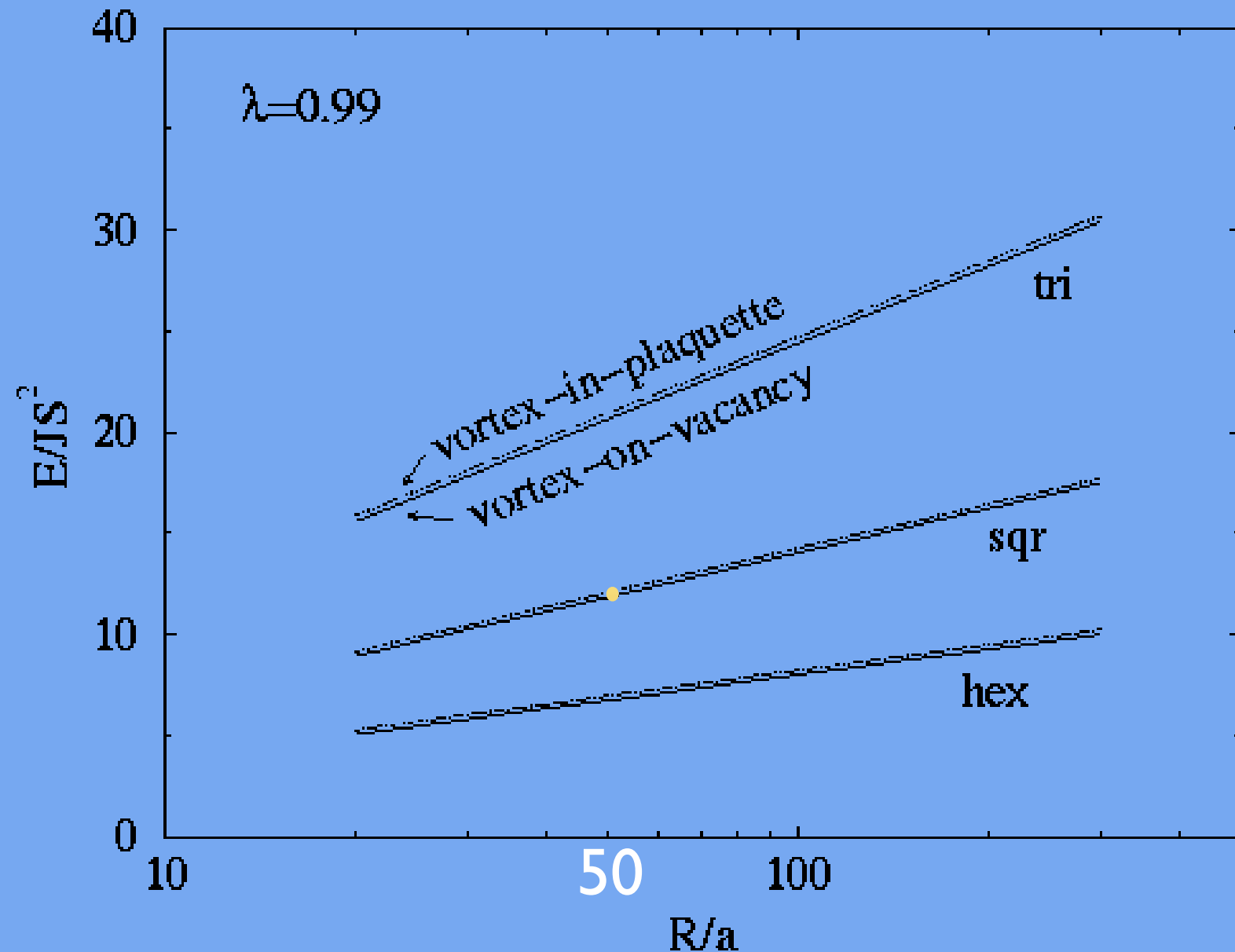


FIG. 4: Total out-of-plane magnetization of a numerically relaxed vortex-on-vacancy versus exchange anisotropy constant λ , for hexagonal, square and triangular lattice systems of radius $R = 50a$ with free boundaries. The inset shows the same data versus shifted exchange anisotropy constants $\lambda - \lambda_{cv}$ near the critical points.

Energia de vórtices **planares**, sistema circular, $\lambda=0$



Energia de vórtices **fora do plano**, $\lambda=0.99$



energia de ligação de um vórtice numa vacância

$$\Delta E = E_{(\text{vórt. no plaquette})} - E_{(\text{vórt. na vacância})}$$

TABLE IV: Some vortex-on-vacancy binding energies (in units of JS^2) and magnetization reductions (in units of S) estimated by comparing to the vortices-in-plaquette structures ($d = 0$), using circular systems of radius $R \leq 300a$.

λ	ΔE_{hex}	ΔM_{hex}	ΔE_{sqr}	ΔM_{sqr}	ΔE_{tri}	ΔM_{tri}
0.0	1.937	0.0	3.178	0.0	5.174	0.0
0.93	1.486	21.31	1.807	28.05	2.45	32.42
0.99	0.224	24.63	0.232	17.27	0.310	14.85

potencial entre
vacância e um
vórtice

r_{vv} = separação
entre vórtice e
vacância

a vacância atrai
o vórtice

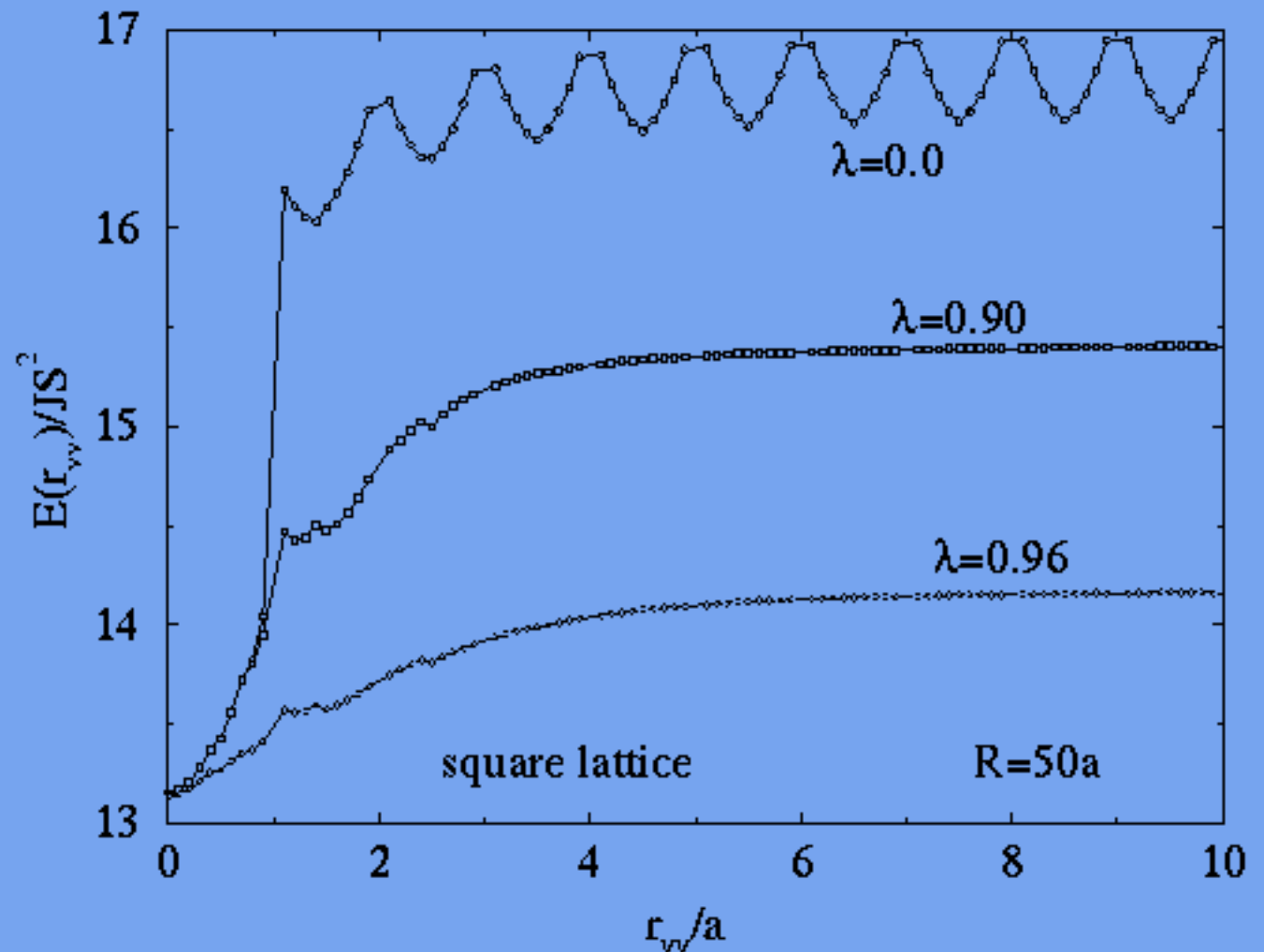


FIG. 10: Vortex–vacancy total energy as a function of their separation r_{vv} , calculated on a square lattice system of radius $R = 50a$ for indicated exchange anisotropies ($\lambda = 0$, in-plane; $\lambda = 0.90$, transition from in-plane to out-of-plane with increasing r_{vv} ; $\lambda = 0.96$, out-of-plane vortices). With the vortex at the origin $(0,0)$, the vacancy was placed at a sequence of positions in the (10) direction.

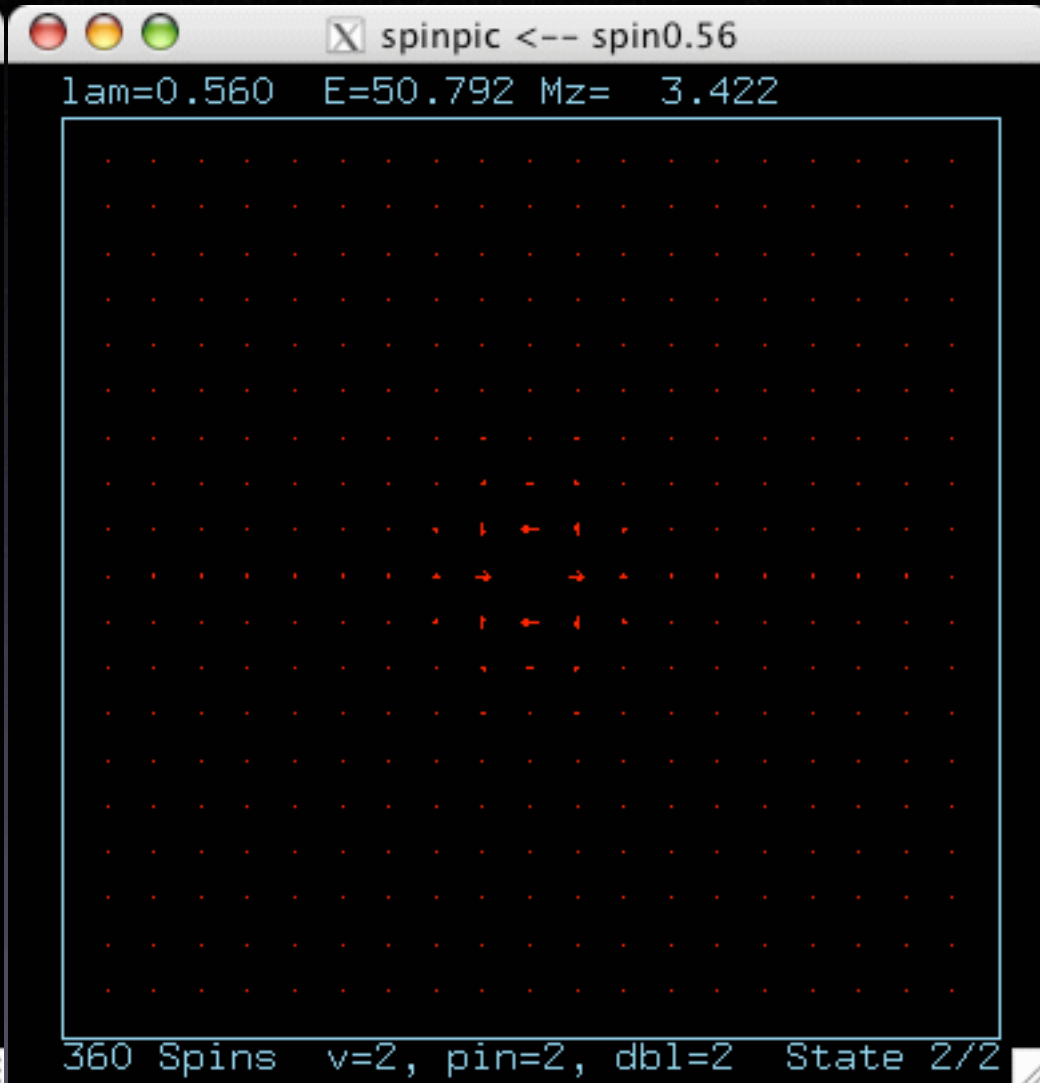
Vórtices de carga dupla, $q=\pm 2$

Sempre localizados numa vacância.

$\lambda=0.56$, $R=50a$, $q=2$ fora do plano

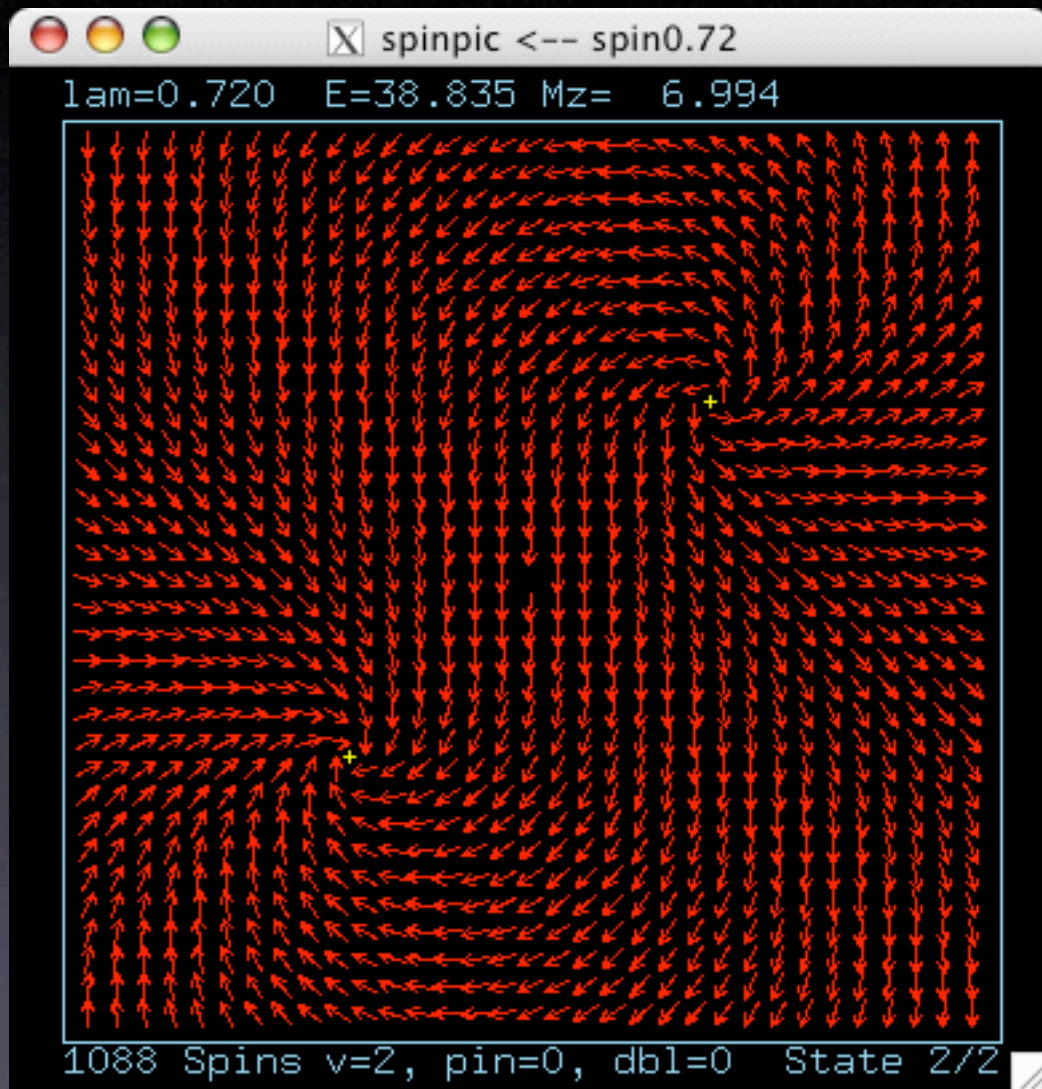


(S_x, S_y)

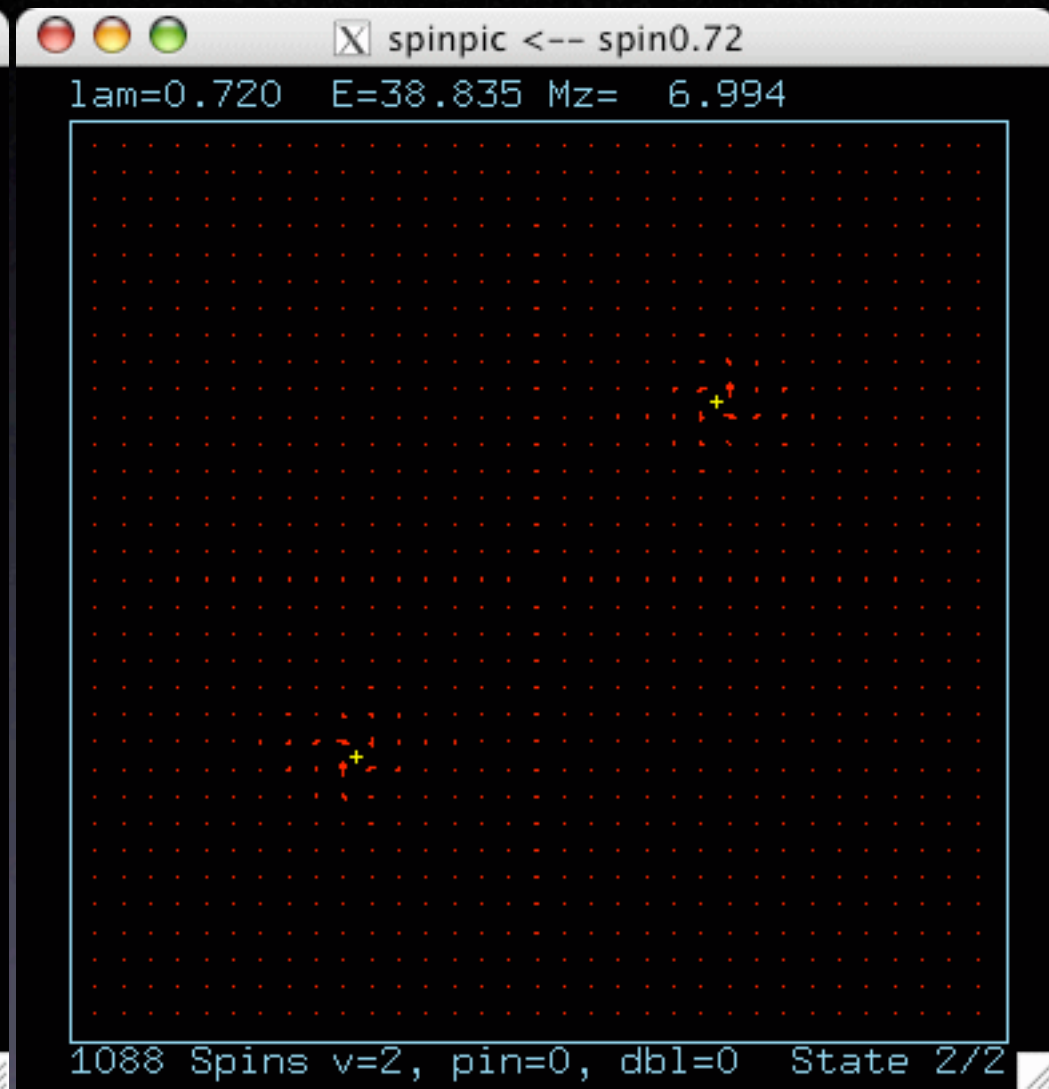


S_z

Relaxação de $q=2$, $\lambda=0.72$, $R=50a$
 $q=2$ é instável para $\lambda > 0.57$



(S_x, S_y)



S_z

P_2 :
q=2 planar
na vacância

O_2 :
q=2 fora do plano
na vacância

PP:
dois q=1 planar

PO:
q=1 planar, na vacância
q=1 fora do plano

∞ :
dois q=1 fora do plano,
livre da vacância

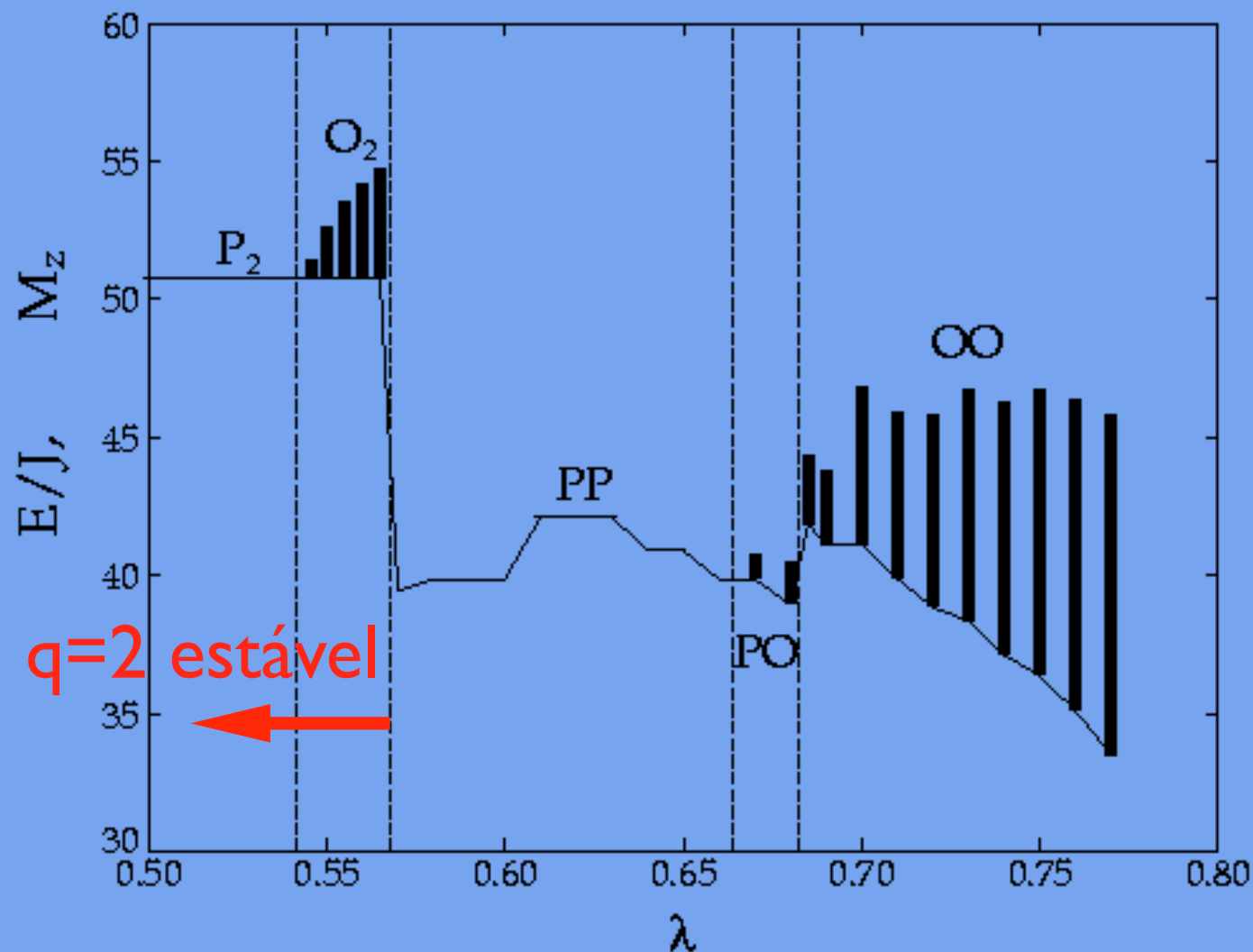


FIG. 12: After relaxation of a $q = 2$ vortex initially centered on an isolated vacancy in a circular system of radius $R = 50$, the total system energy (solid curve) is shown as a function of the anisotropy constant λ . The vertical bars indicate the net out-of-plane magnetization of the relaxed configuration, on the same numerical scale.

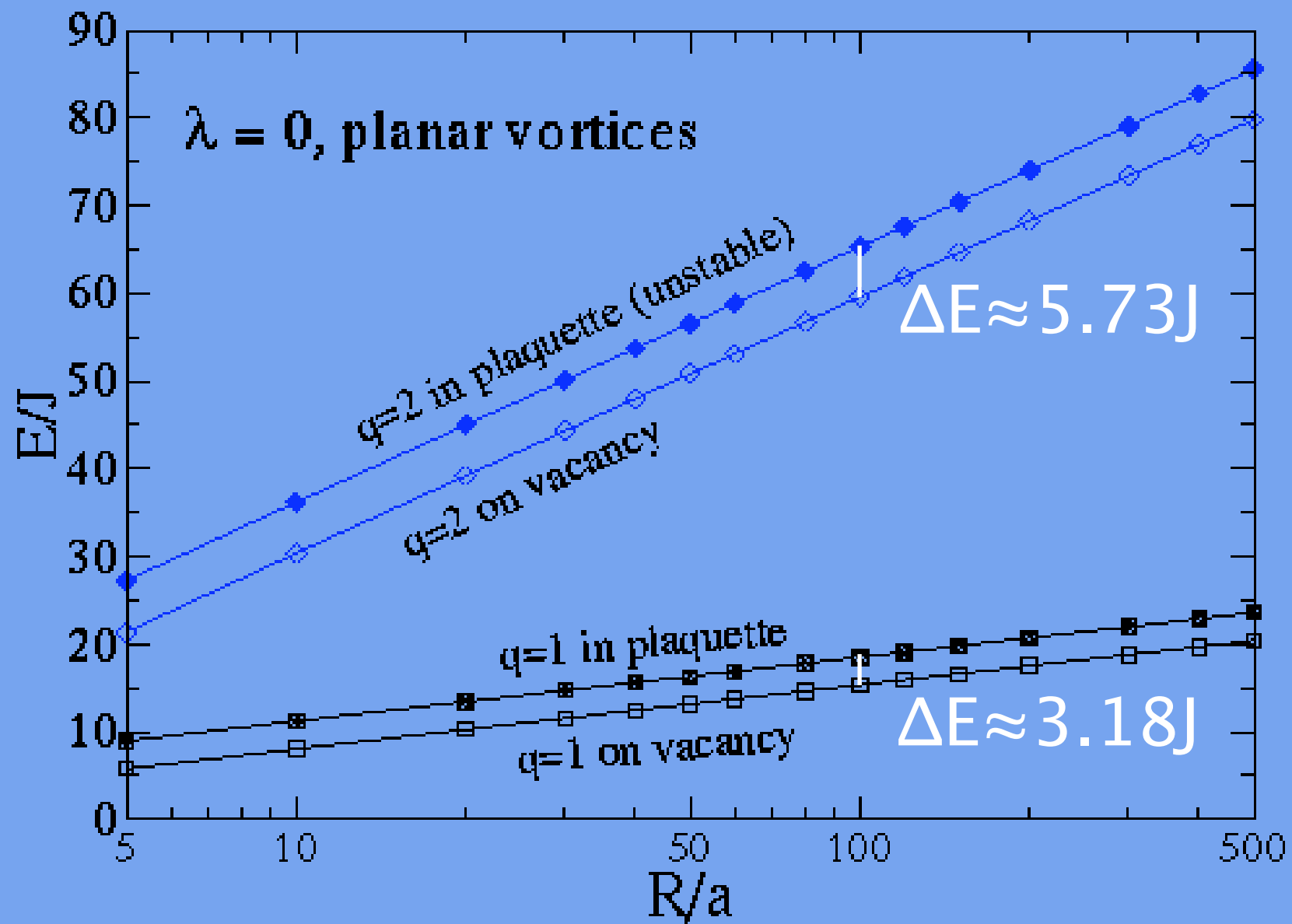


FIG. 11: Various total system energies with a vortex present versus system radius R . (rede quadrada)

Simulações de Monte Carlo

- sistemas $L \times L$, condições de contorno **periódica**
- ρ_{vac} = densidade de vacâncias = 0 ou 0.16
- mudanças dos spins via técnicas de **Metropolis**, **over-relaxation**, e **Wolff cluster**, todos juntos.
- localização de T_c = temperatura crítica, usando **susceptibilidade** dentro do plano (χ) e **finite size scaling**.

simulations.....

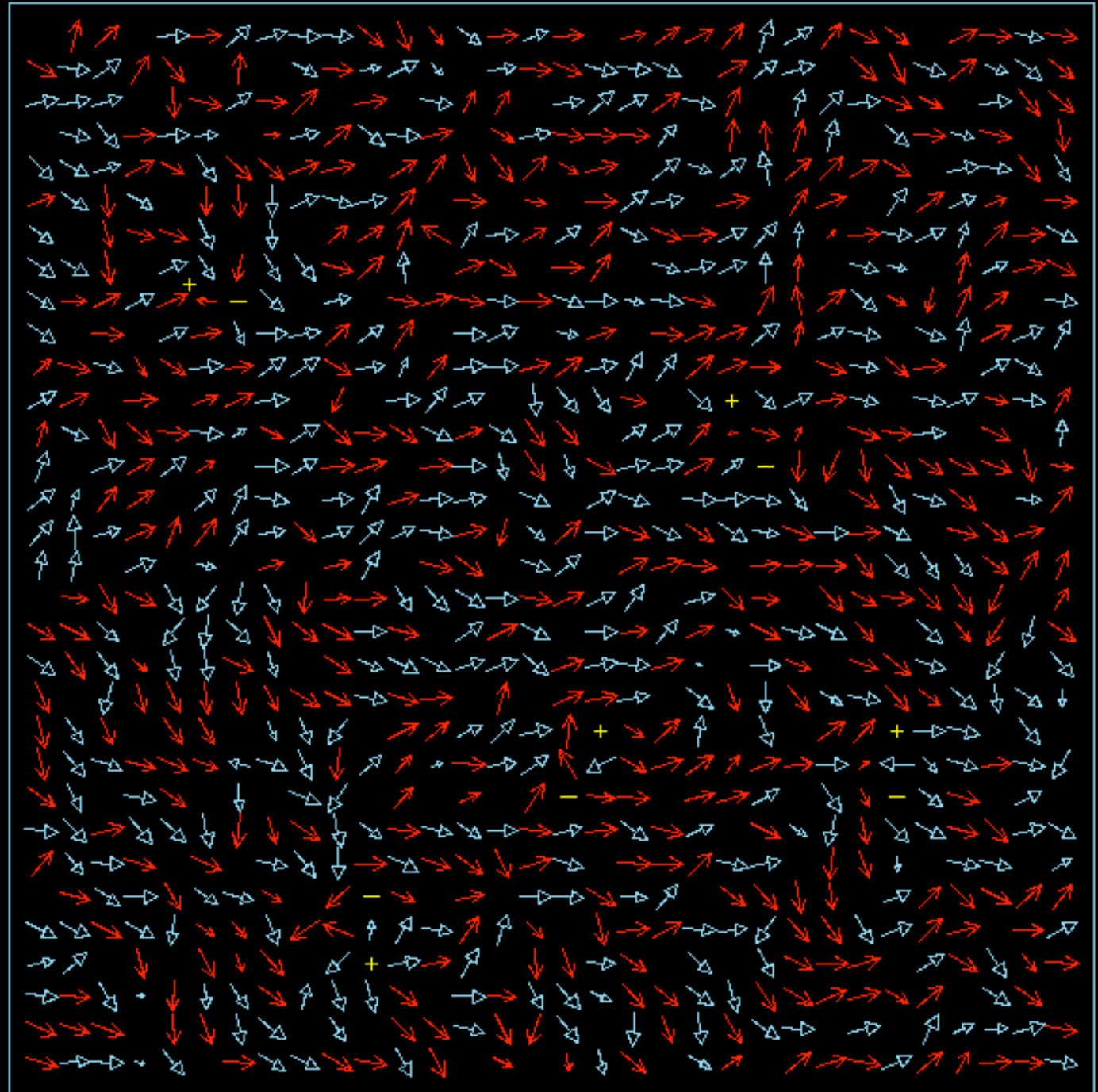
$$\lambda=0$$

$$@ T_c/J \approx 0.48$$

$$\rho_{\text{vac}} = 0.16$$

pequeno
número de
vórtices de
 $q = \pm 1$,

maioria ligados
nas vacâncias

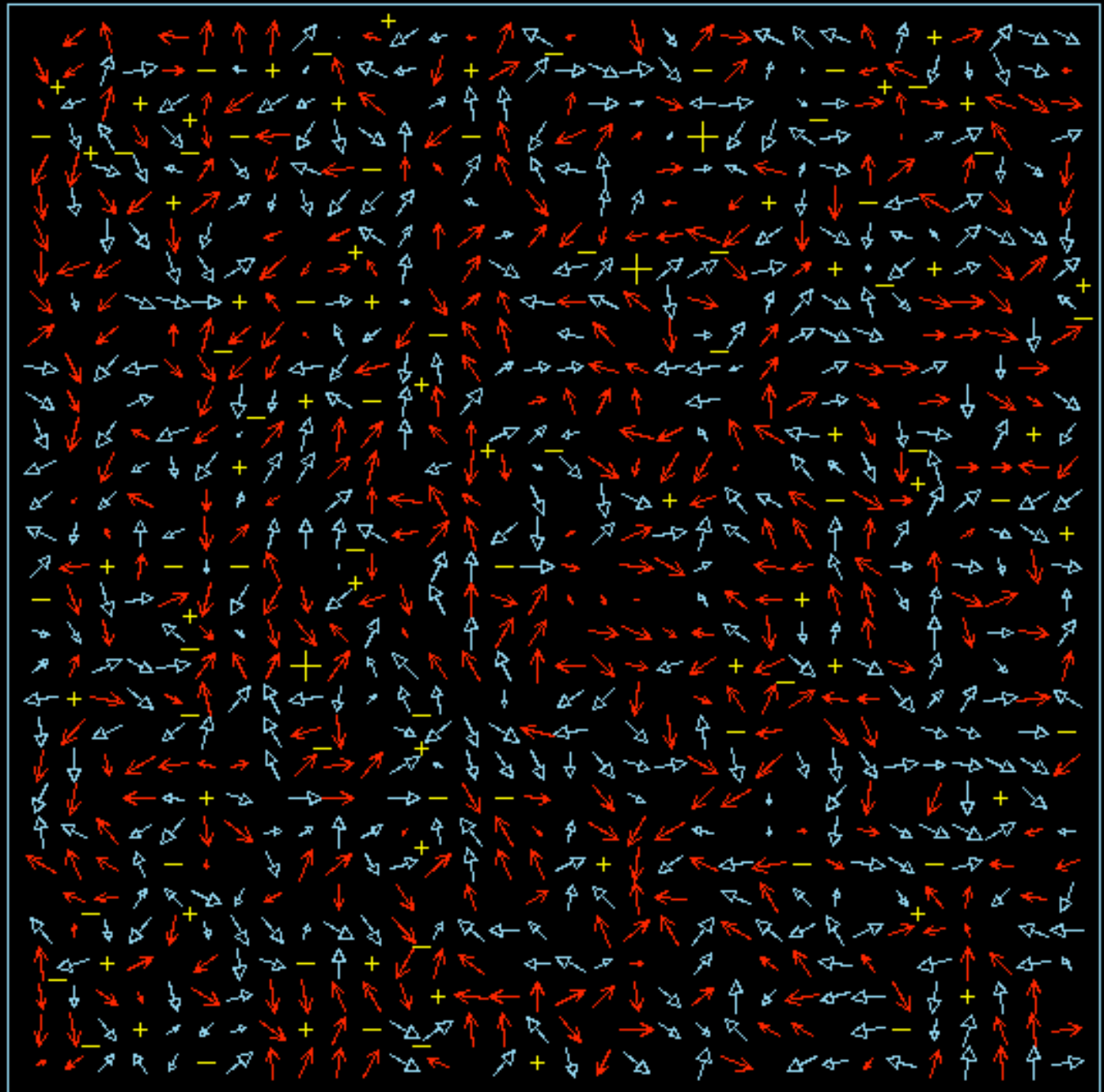


$\lambda=0$

@ T/J=0.85

$\rho_{vac}=0.16$

presença de
vórtices de
 $q=\pm 2$



B. MC Measurements

In terms of temperature T and Boltzmann's constant k , the system's thermodynamic energy E and heat capacity C are defined via usual relations,

$$E = \langle H \rangle, \quad C = k[\langle H^2 \rangle - \langle H \rangle^2]/T^2. \quad (4)$$

The instantaneous total magnetization of the system is the sum over all spins

$$\vec{M} = \sum_{\mathbf{n}} p_{\mathbf{n}} \vec{S}_{\mathbf{n}}. \quad (5)$$

For purposes of finding T_c , it is important to calculate the associated per-spin susceptibility $\chi^{\alpha\alpha}$ of any component α , derived from the magnetization fluctuations,

$$\chi^{\alpha\alpha} = (\langle M_{\alpha}^2 \rangle - \langle M_{\alpha} \rangle^2)/(NT). \quad (6)$$

Both χ^{xx} and χ^{yy} were computed by (6) and then averaged to get the in-plane susceptibility,

$$\chi = (\chi^{xx} + \chi^{yy})/2. \quad (7)$$

parâmetro
de ordem 

the system's total in-plane absolute valued magnetic moment (order parameter M^*), which only tends to zero in the high-temperature phase, and its associated per-spin susceptibility χ^* ,

$$M^* = \langle \sqrt{M_x^2 + M_y^2} \rangle, \quad \chi^* = [\langle M_x^2 + M_y^2 \rangle - M^{*2}] / (NT). \quad (8)$$

Related per-spin energy, specific heat, and order parameter (e, c, m^*), are obtained by dividing each by the number of occupied sites, N .

Quantidades calculados por spin:
(N=número dos sítios ocupados)

energia, $e = E/N$

calor específico, $c = C/N$

parâmetro de ordem, $m^* = M^*/N$

Fez médias com 300,000 passos de MC.

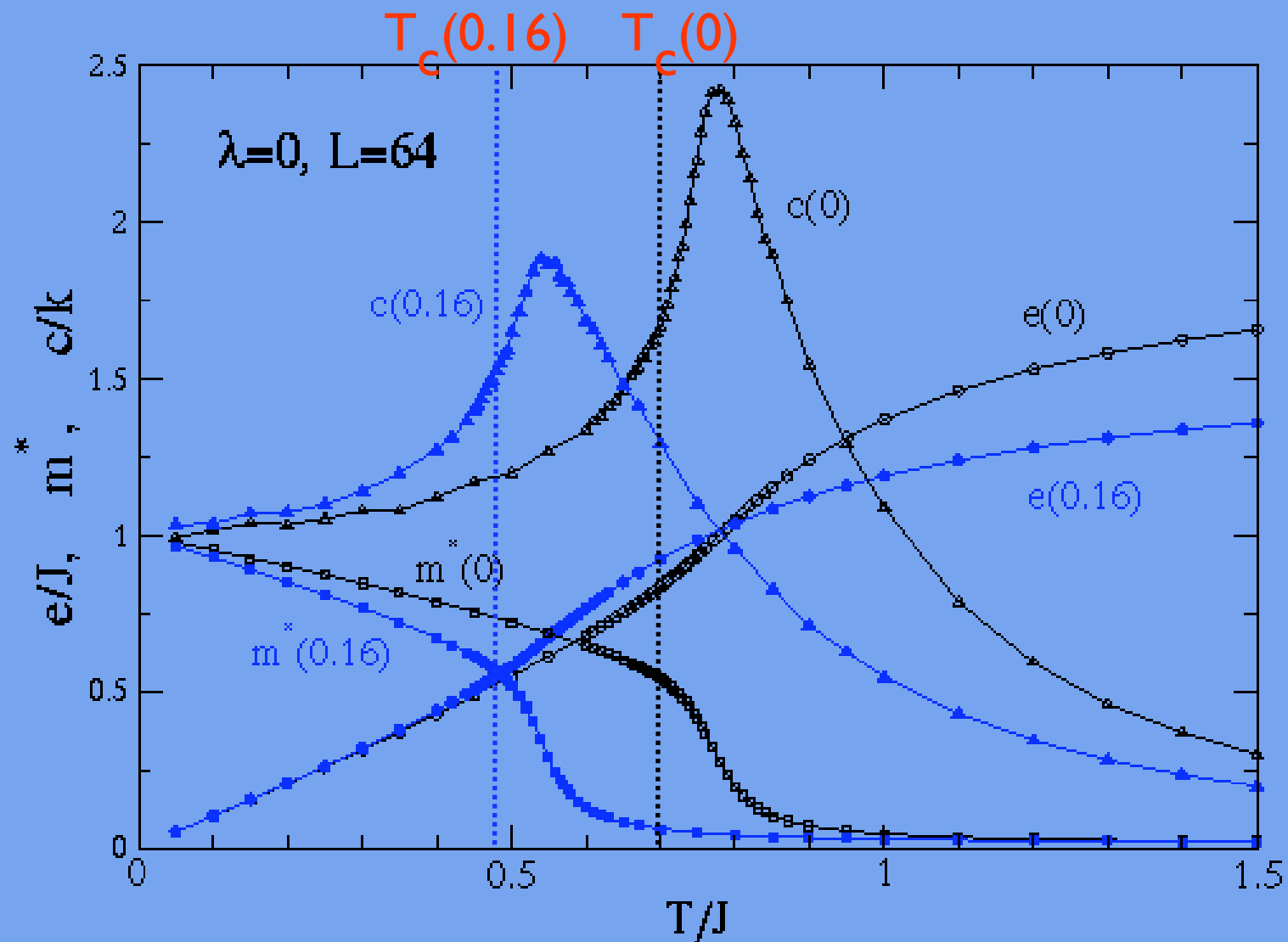
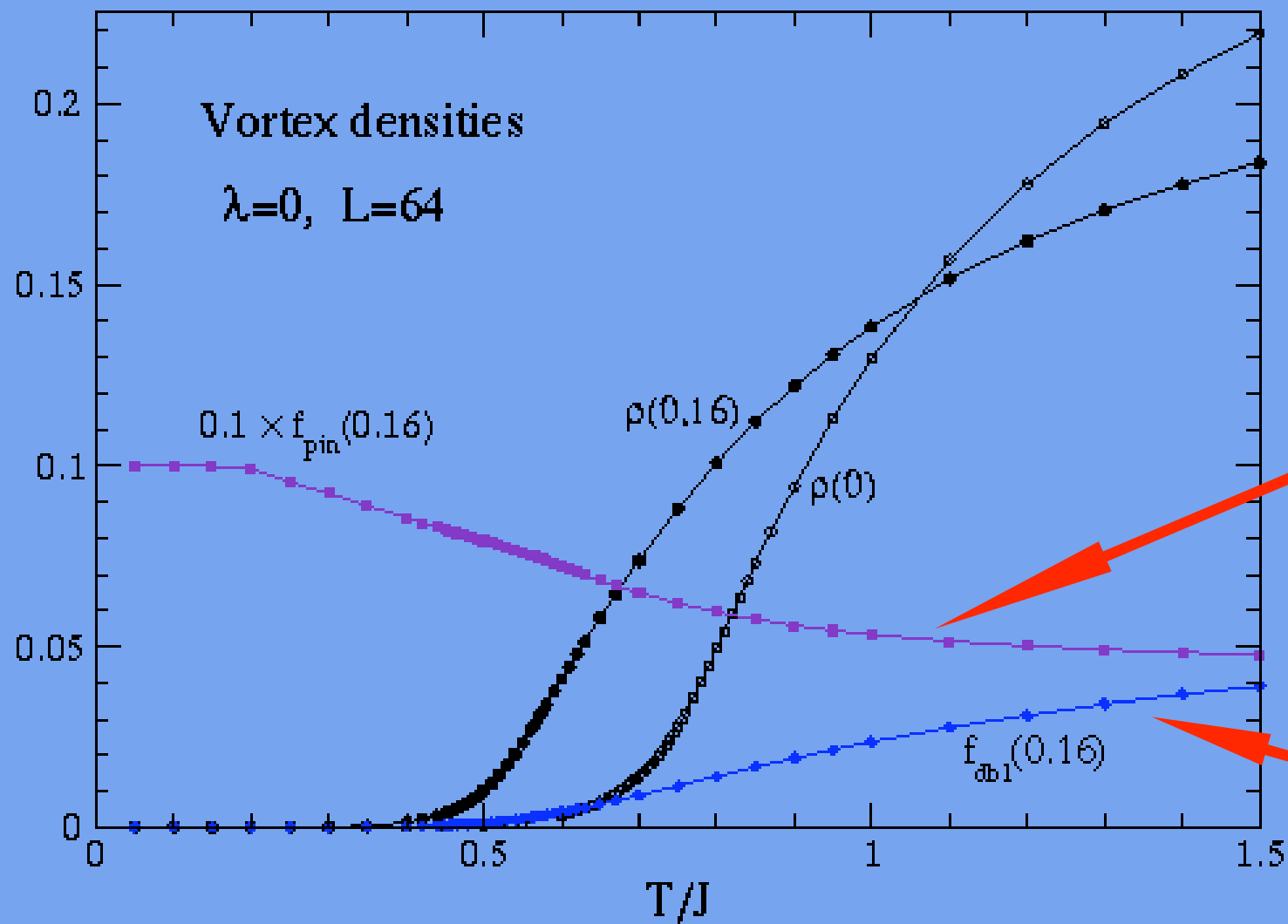


FIG. 1: For the model with edge $L = 64$, at the XY limit, the internal energy, absolute magnetization, and specific heat per spin for the uniform system and with 16% vacancy density.



$f_{\text{pin}} =$
 % vórtices
 localizados
 nas vacâncias

$f_{\text{dbl}} =$
 % vórtices
 de $q = \pm 2$

FIG. 5: Thermally induced vorticity density for the uniform XY model [$\rho(0)$] and at 16% vacancy density [$\rho(0.16)$]. Also displayed are the vorticity fraction pinned on vacancies [f_{pin}] and the fraction with doubled charges [f_{dbl}], both when $\rho_{\text{vac}} = 0.16$.

finite size
scaling

$$\chi \propto L^{2-\eta}$$

$$\eta = 1/4$$

$$@ T = T_c$$

localiza T_c

usando sistemas

de vários

tamanhos

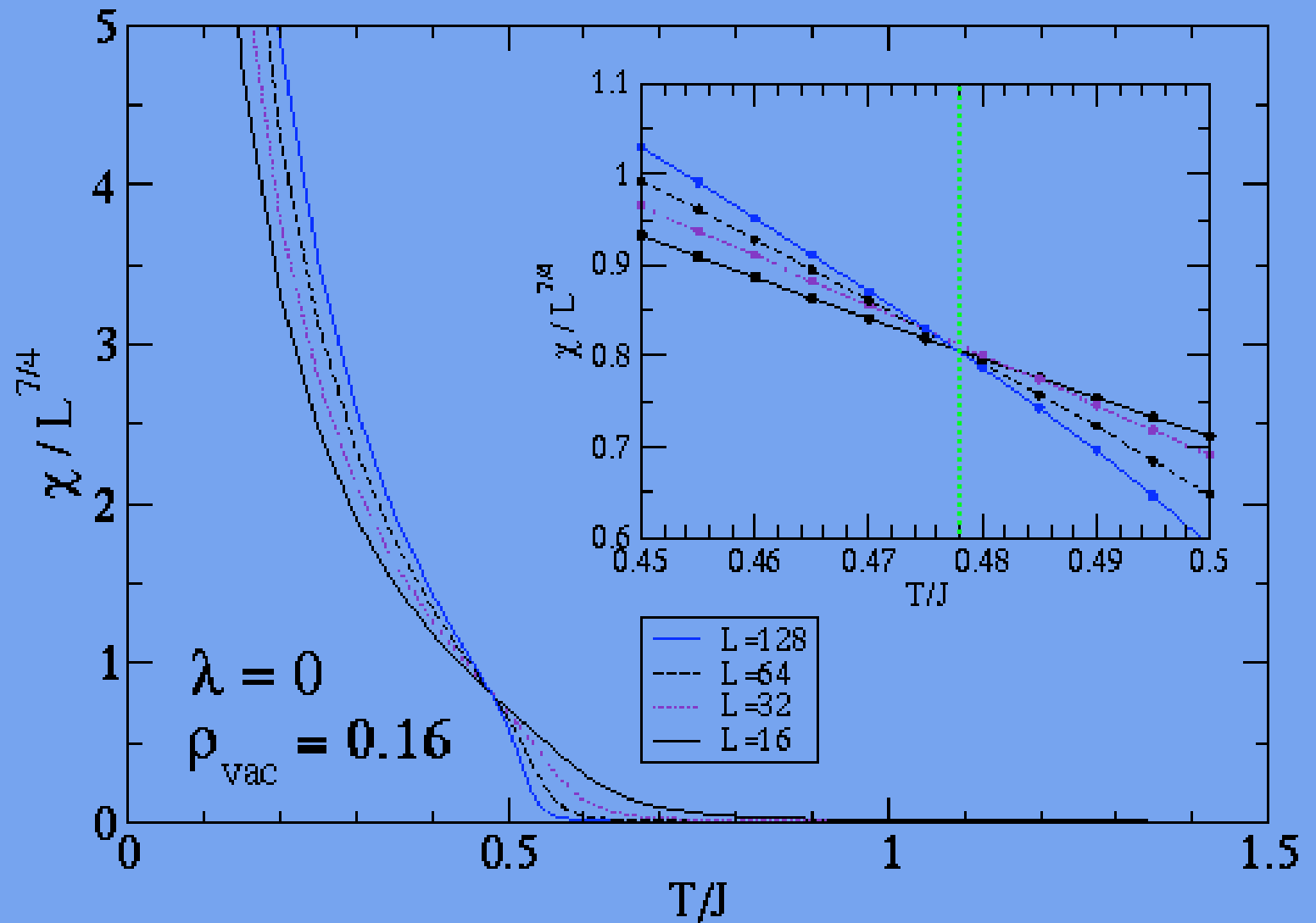
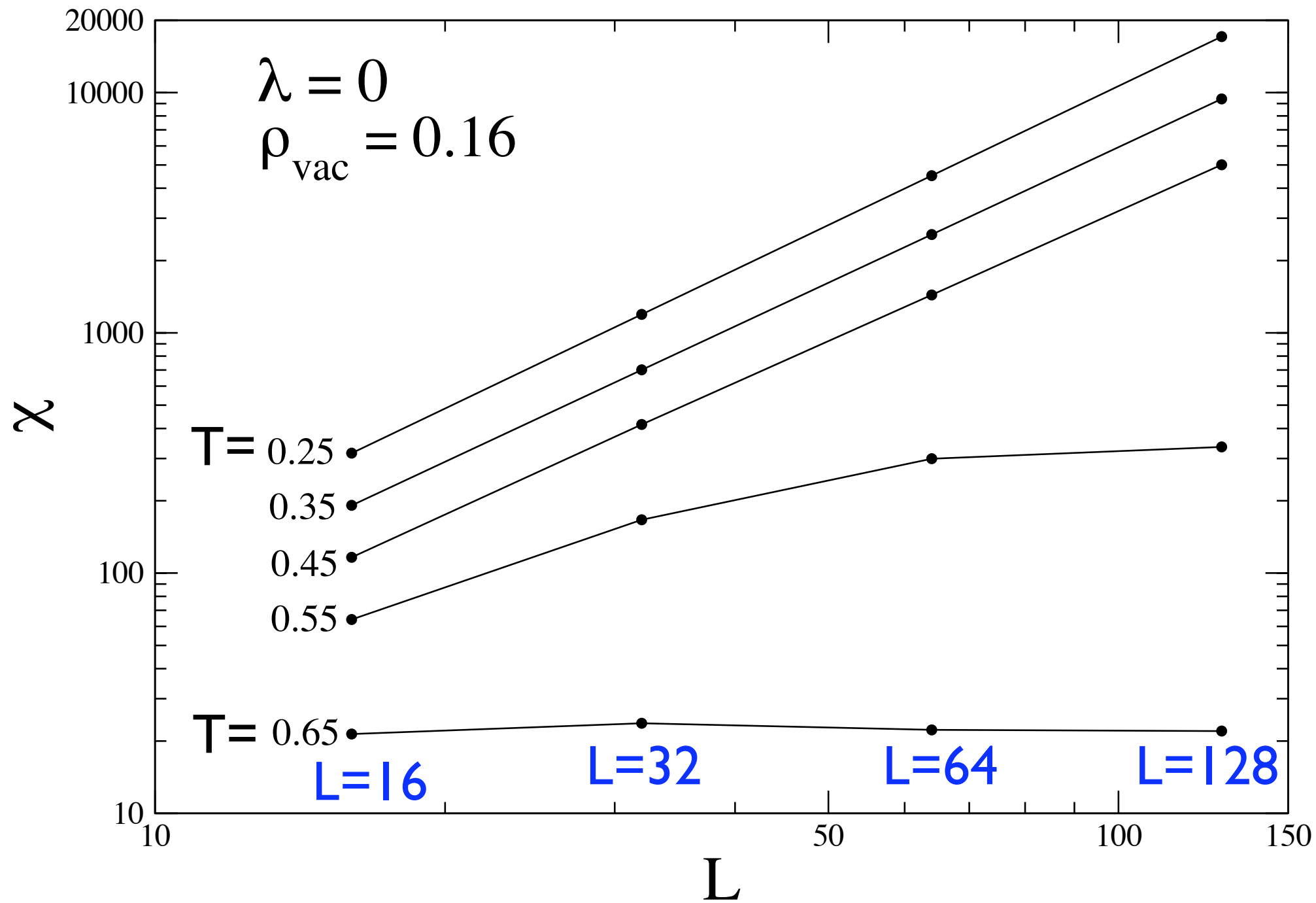
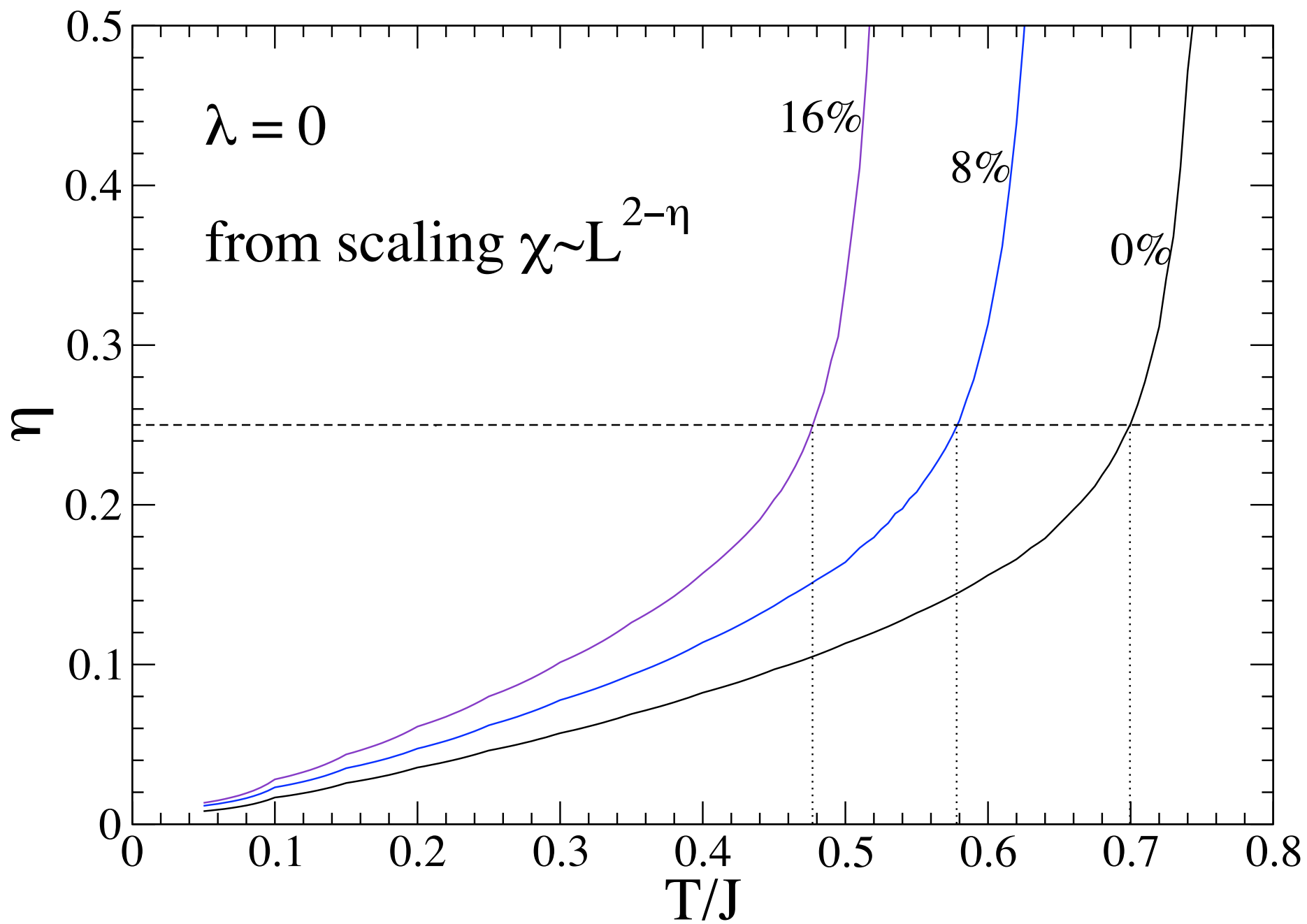


FIG. 3: Application of the finite-size scaling of in-plane susceptibility to estimate $T_c/J \approx 0.478$ (common crossing point of the data) at 16% vacancy density in the XY model, using exponent $\eta = 1/4$.





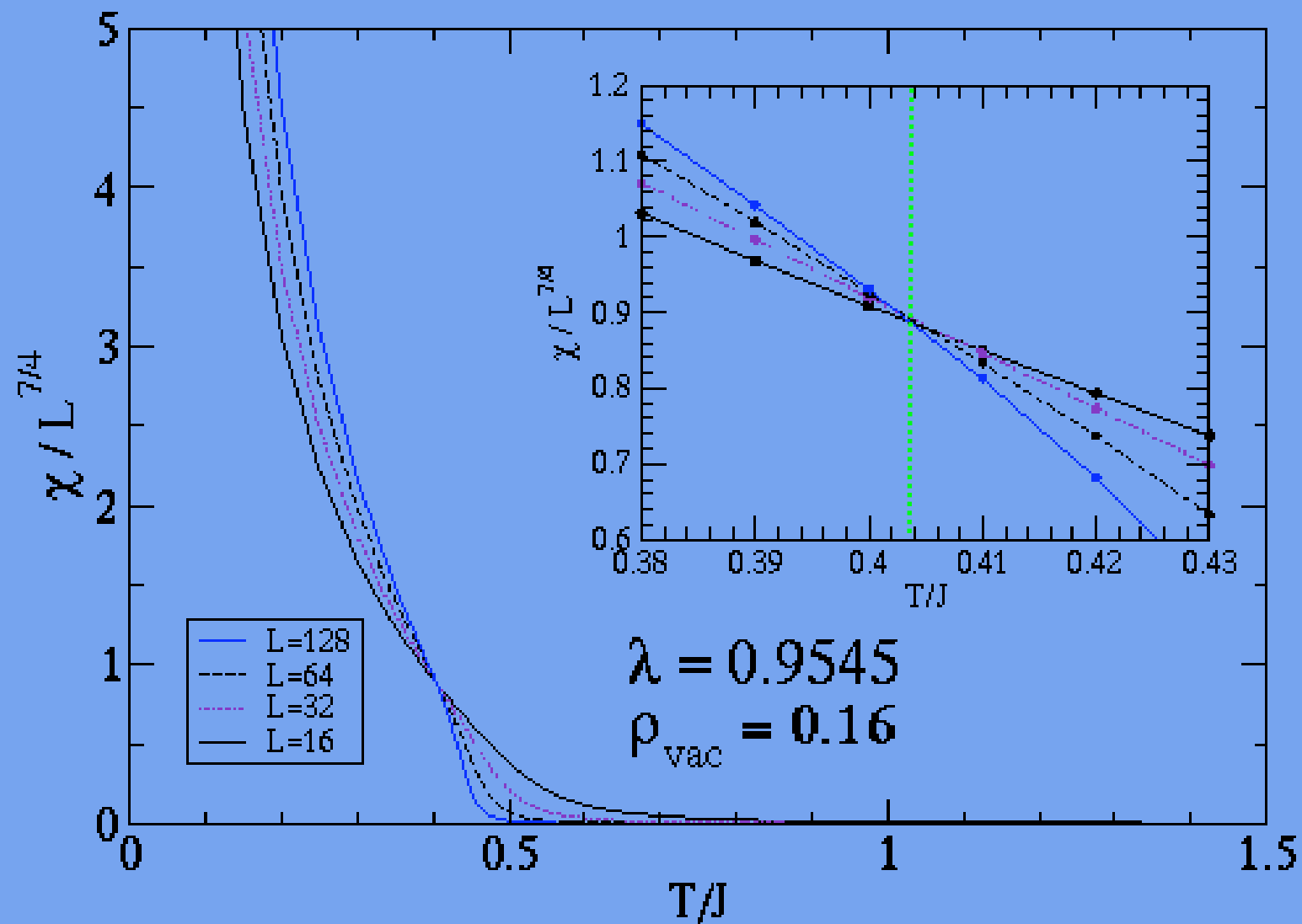
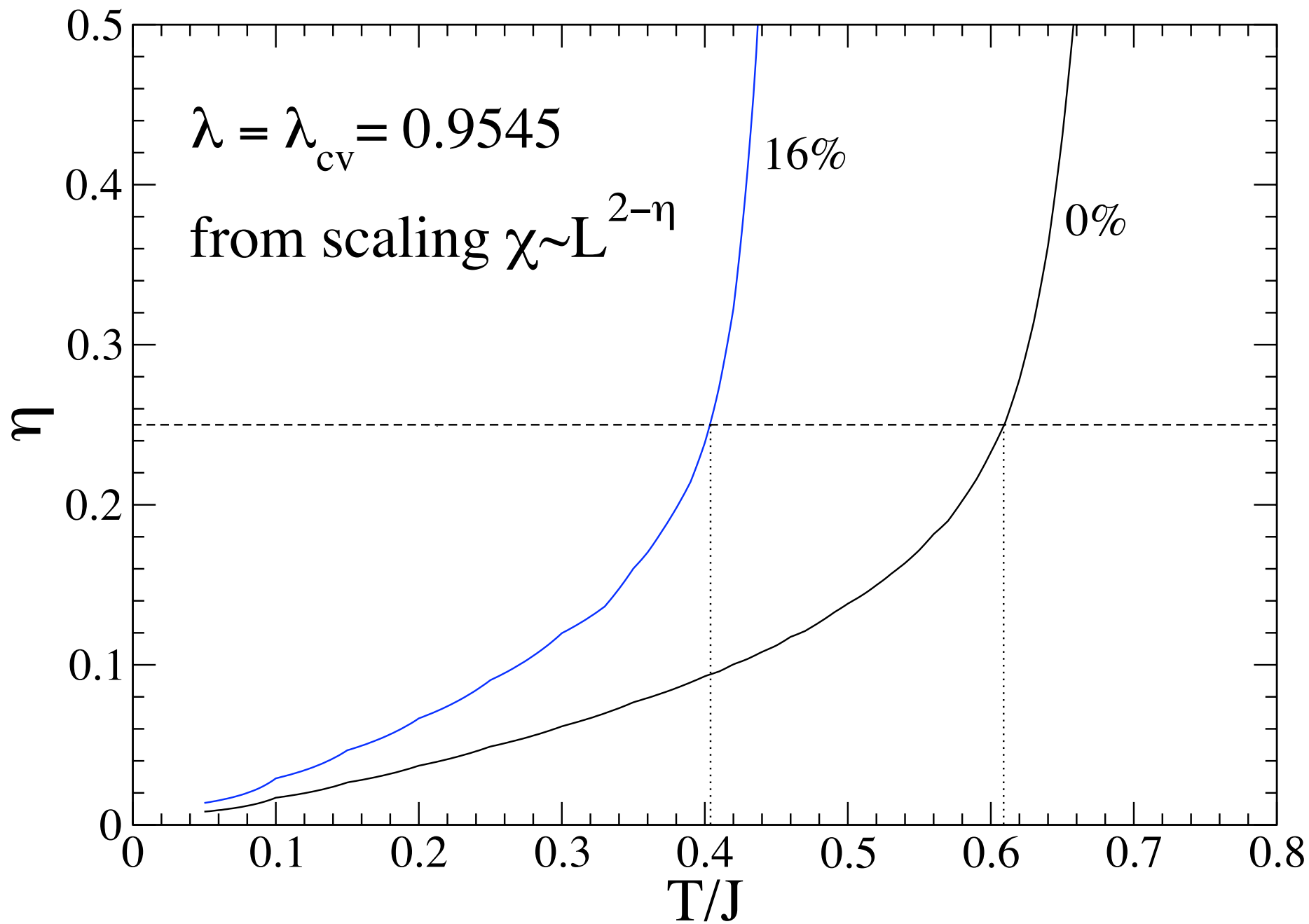
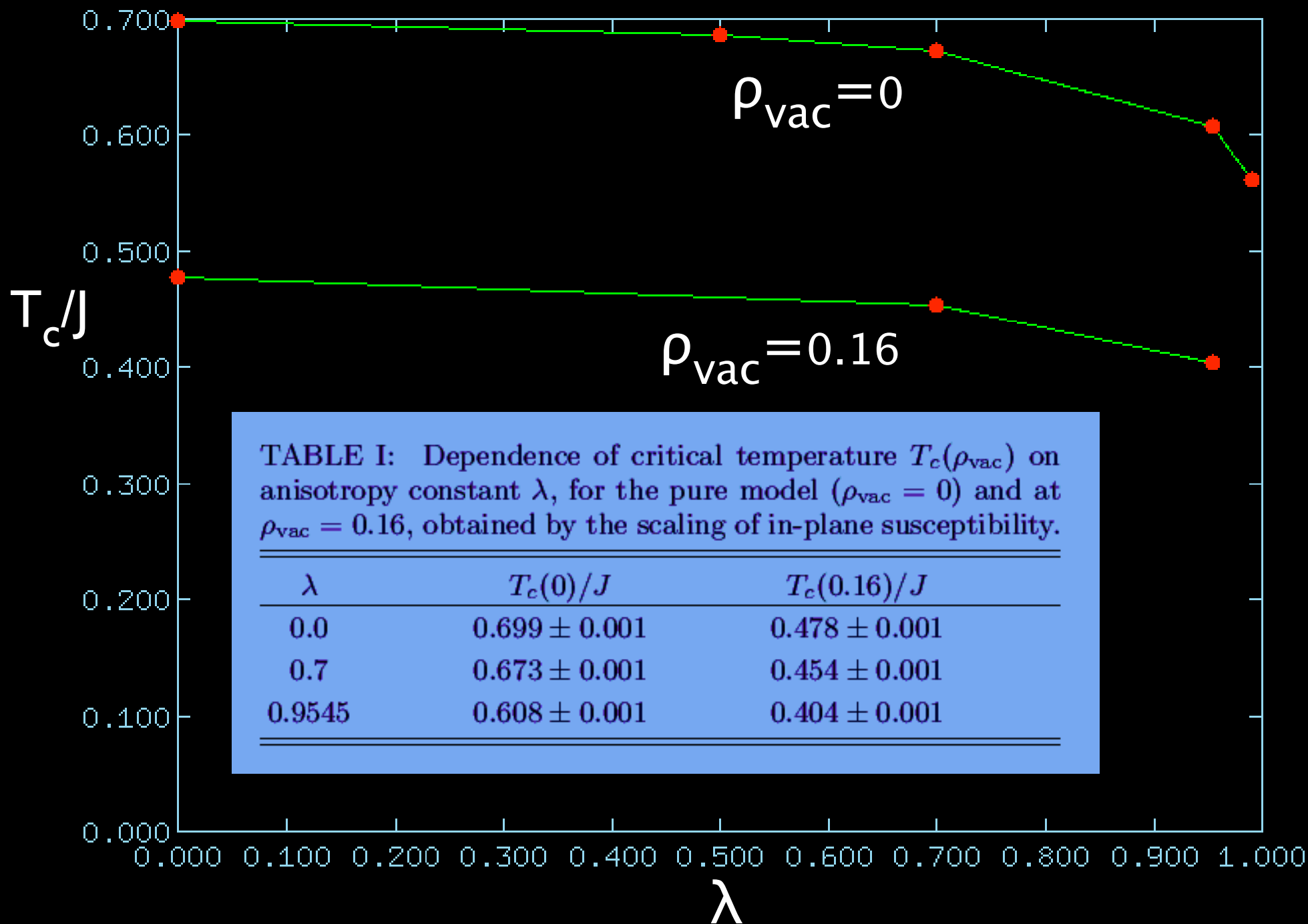
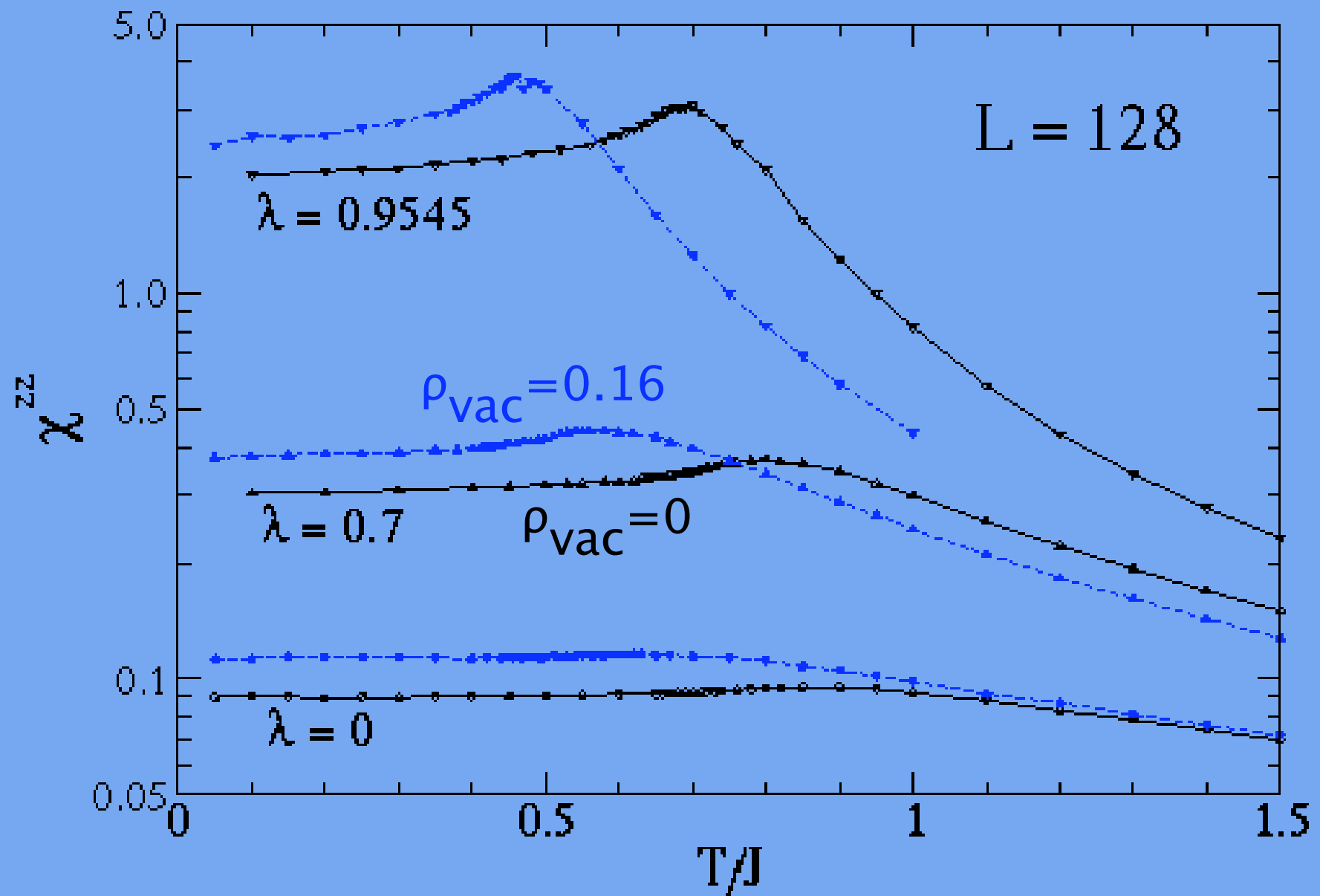


FIG. 8: Application of the finite-size scaling of in-plane susceptibility to estimate $T_c/J \approx 0.404$ (common crossing point of the data) at 16% vacancy density at the vortex-on-vacancy critical anisotropy.





susceptibilidade **fora** do plano fácil



Conclusões

- vórtices **são atraídos** pelas vacâncias.
- vórtices preferem formar nas vacâncias, de maior preferência, na **forma planar**.
- vórtices de **carga $q=\pm 2$** acontece ligados nas vacâncias.
- a presença de vacâncias **facilita** a transição de fase, igual ao modelo de rotor planar.

www.phys.ksu.edu/~wysin/

