Influence of nonmagnetic disorder on the Berezinskii-Kosterlitz-Thouless transition in planar-symmetry spin models

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2D easy-plane spin models with randomly placed vacancies

- either 2-component spins: planar rotator (PR)
- or 3-component spins: XY or easy-plane Heisenberg
- vacancy density $\rho_{vac} = 0$ to 0.50, square lattice
- Hamiltonian: $\sigma_i = 0$ (vacant) or 1 (occupied)

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \left(S_i^x S_j^x + S_i^y S_j^y \right), \tag{1}$$

Motivation for study:

- How is BKT vortex-pair unbinding transition affected by missing spins at random sites?
- MC studies of PR helicity modulus ϒ found (Leonel et al. 2003) $T_c \rightarrow 0$ at $\rho_{vac} \approx 0.3$
- MC studies of PR correlation function exponent η (Berche et al. 2003) $T_c \rightarrow 0$ at $\rho_{vac} \approx 0.41$,

  a number associated with percolation limit on a square lattice (59% of sites occupied).

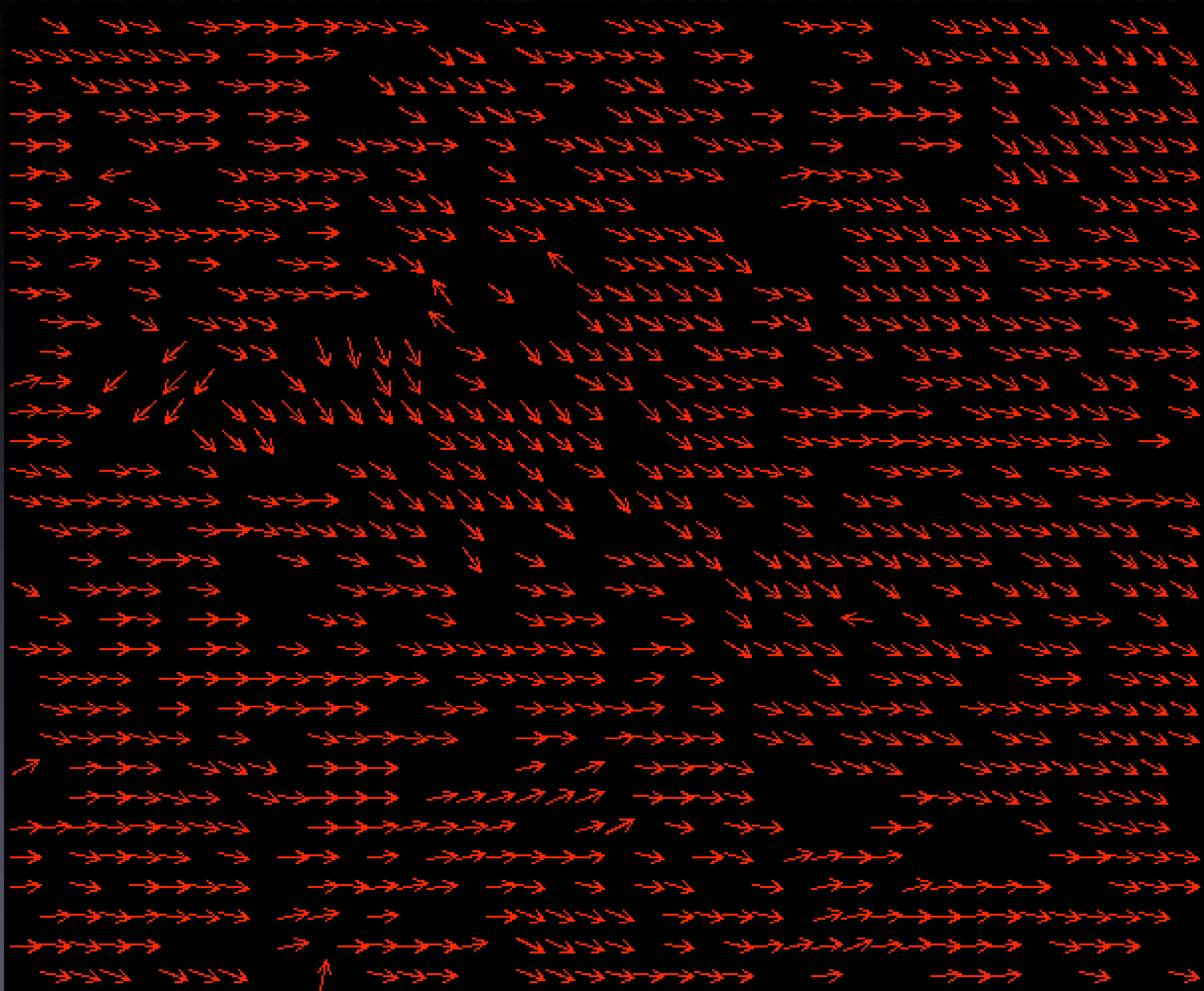
What questions are we interested in?

- What happens to vortices near spin vacancies?
- Different vacancy effects in PR and XY models?
- How does Tc fall with vacancy density?
- What vacancy density eliminates the BKT vortex unbinding transition?

PR

ρ_{vac} 0.33

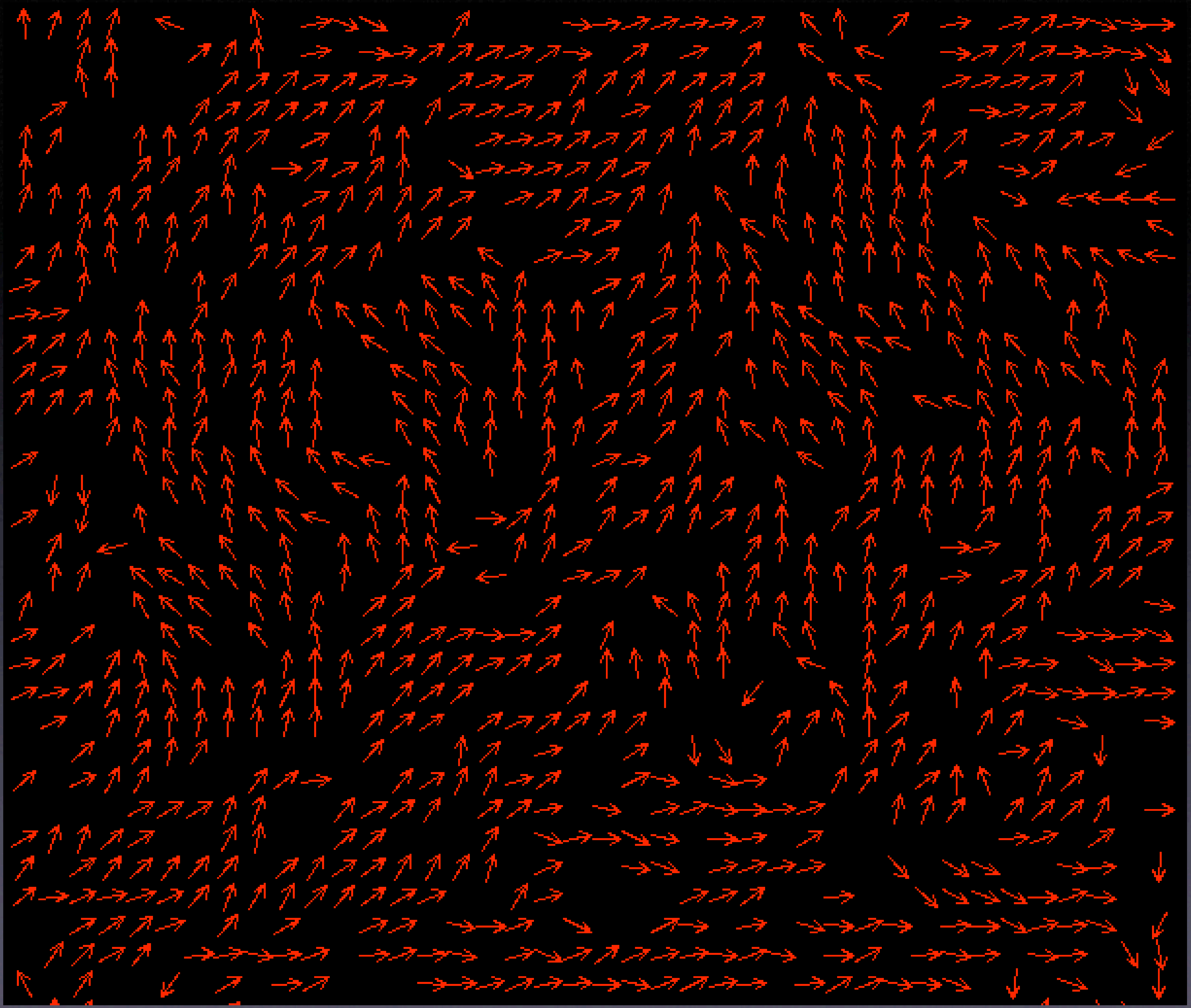
T/J 0.02



PR

ρ_{vac}
0.33

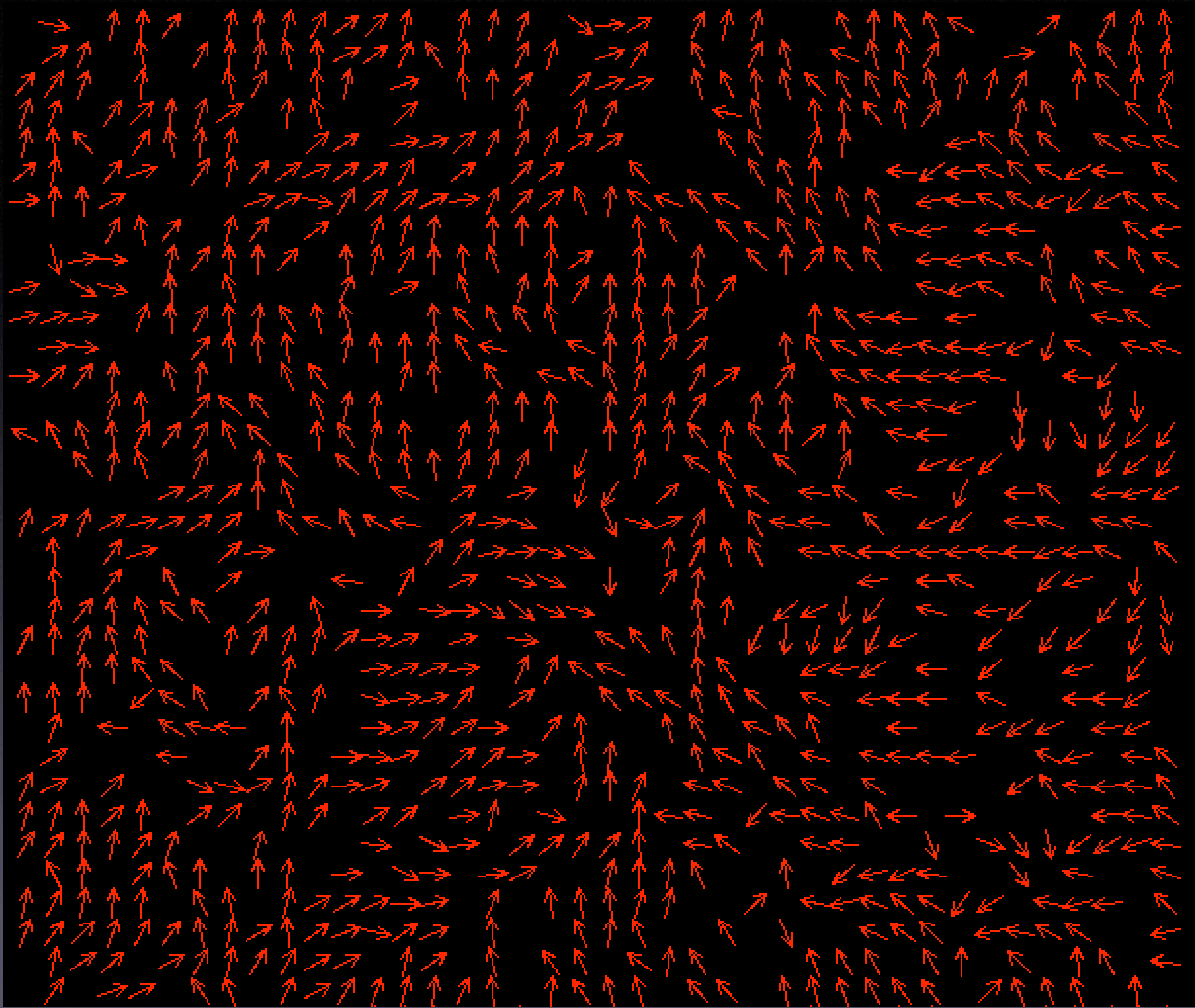
T/J
0.14



PR

ρ_{vac}
0.33

T/J
0.28



What quantities do we calculate?

- in-plane magnetization M and susceptibility χ
- Binder's fourth order cumulant U_L
- spin helicity modulus Υ
- use all of these to estimate BKT transition temperature Tc

$$\vec{M} = \sum_i \sigma_i \vec{S}_i. \tag{2}$$

Additionally, statistical fluctuations give the susceptibility components for temperature T,

$$\chi^{\alpha\alpha} = (\langle M_\alpha^2 \rangle - \langle M_\alpha \rangle^2)/(NT). \tag{3}$$

The number of spins in the system is $N = (1 - \rho_{\mathrm{vac}})L^2$. The average of χ^{xx} and χ^{yy} defines the in-plane susceptibility,

$$\chi = \frac{1}{2}(\chi^{xx} + \chi^{yy}). \tag{4}$$

A rough estimate of T_c can be obtained from the size-dependence of Binder's fourth order cumulant[23,24] U_L, defined by

$$U_L = 1 - \frac{\langle (M_x^2 + M_y^2)^2 \rangle}{2\langle M_x^2 + M_y^2 \rangle^2}. \tag{5}$$

Helicity

modulus

Another approach to determine T_c is based on the calculation of the helicity modulus per spin, $\Upsilon(T)$. It is a measure of the resistance to an infinitesimal spin twist Δ across the system along one coordinate, defined in terms of the dimensionless free energy, $f = F/(JS^2)$,

$$\Upsilon = \frac{1}{N}\frac{\partial^2 f}{\partial \Delta^2}. \tag{6}$$

Any general model Hamiltonian leads to the expression,

$$N\Upsilon = \left\langle \frac{\partial^2 H}{\partial \Delta^2} \right\rangle - \beta \left[\left\langle \left(\frac{\partial H}{\partial \Delta} \right)^2 \right\rangle - \left\langle \frac{\partial H}{\partial \Delta} \right\rangle^2 \right], \tag{7}$$

where $\beta = (k_B T)^{-1}$ is the inverse temperature. For ei-

$$G_s \equiv \frac{\partial H}{\partial \Delta} = \sum_{\langle i,j \rangle} \sigma_i \sigma_j \left(\hat{e}_{i,j} \cdot \hat{x} \right) \left(S_i^x S_j^y - S_i^y S_j^x \right), \tag{8a}$$

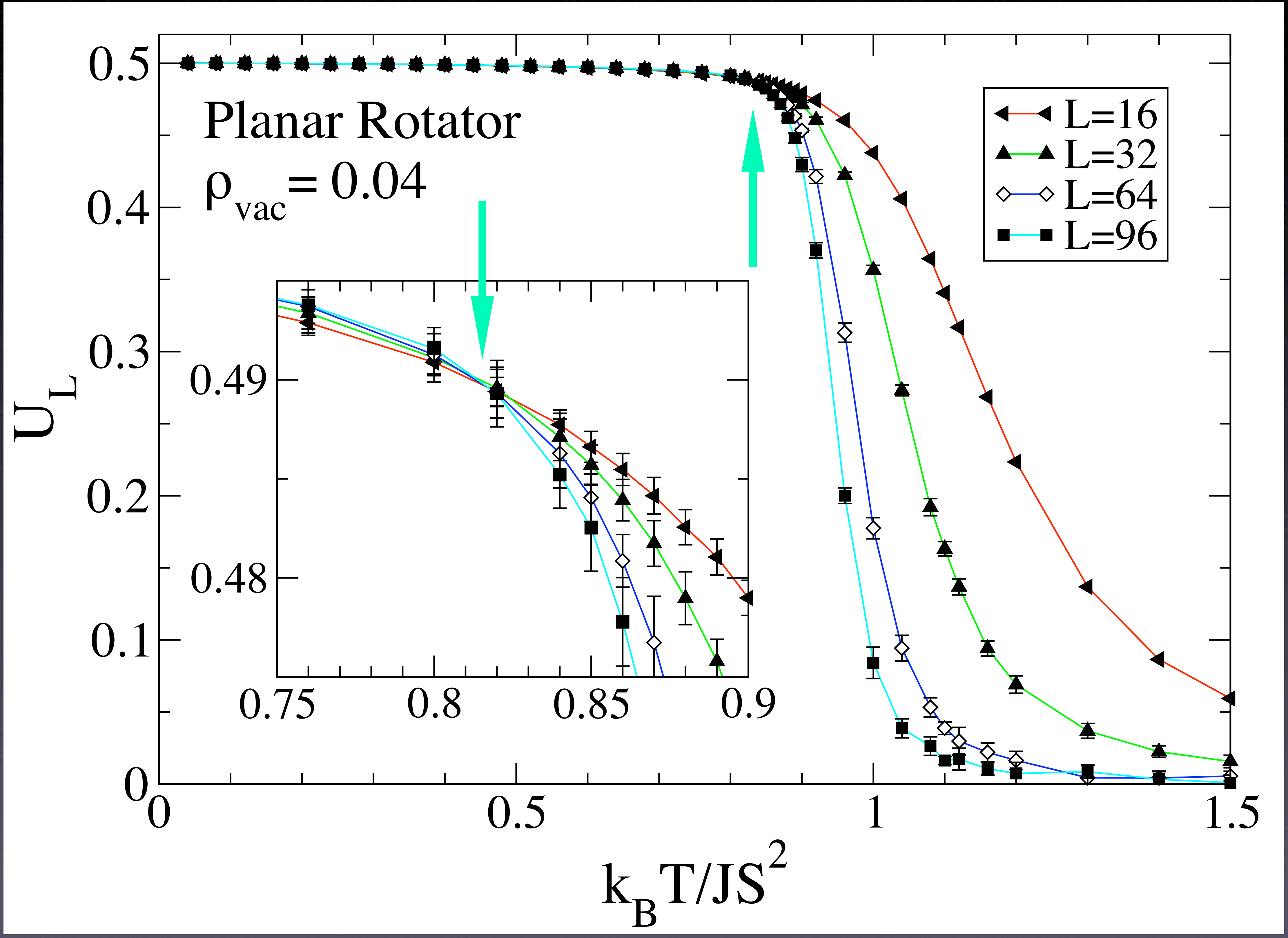
$$G_c \equiv \frac{\partial^2 H}{\partial \Delta^2} = \frac{1}{2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j \left(S_i^x S_j^x + S_i^y S_j^y \right), \tag{8b}$$

Hybrid Monte Carlo approach

- Wolff cluster (xy components only) + overrelaxation + Metropolis single spin flips.
- L x L systems, L = 16, 32, 64, 96, 160.
- averaging over 4 to 128 systems with different disorder for a given ρ_{vac}.
- averages of individual systems using 20,000 to 80,000 MC steps.

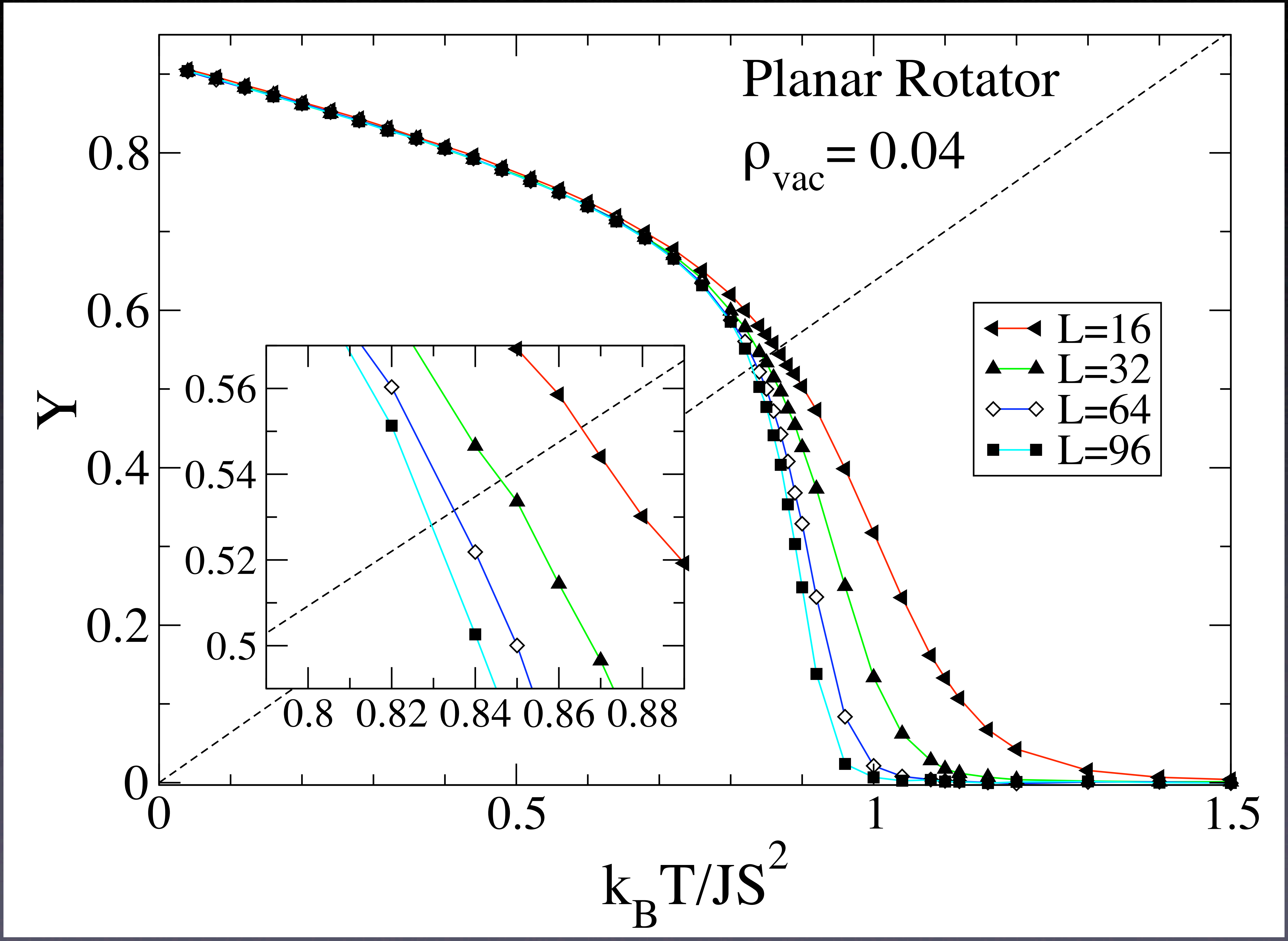
Tc from Binder's 4th cumulant, example.

common crossing point, → Tc/J≈0.815



Tc from helicity modulus, example.

from crossing with $\Upsilon = \frac{2}{\pi} k_B T.$ → Tc/J≈0.83

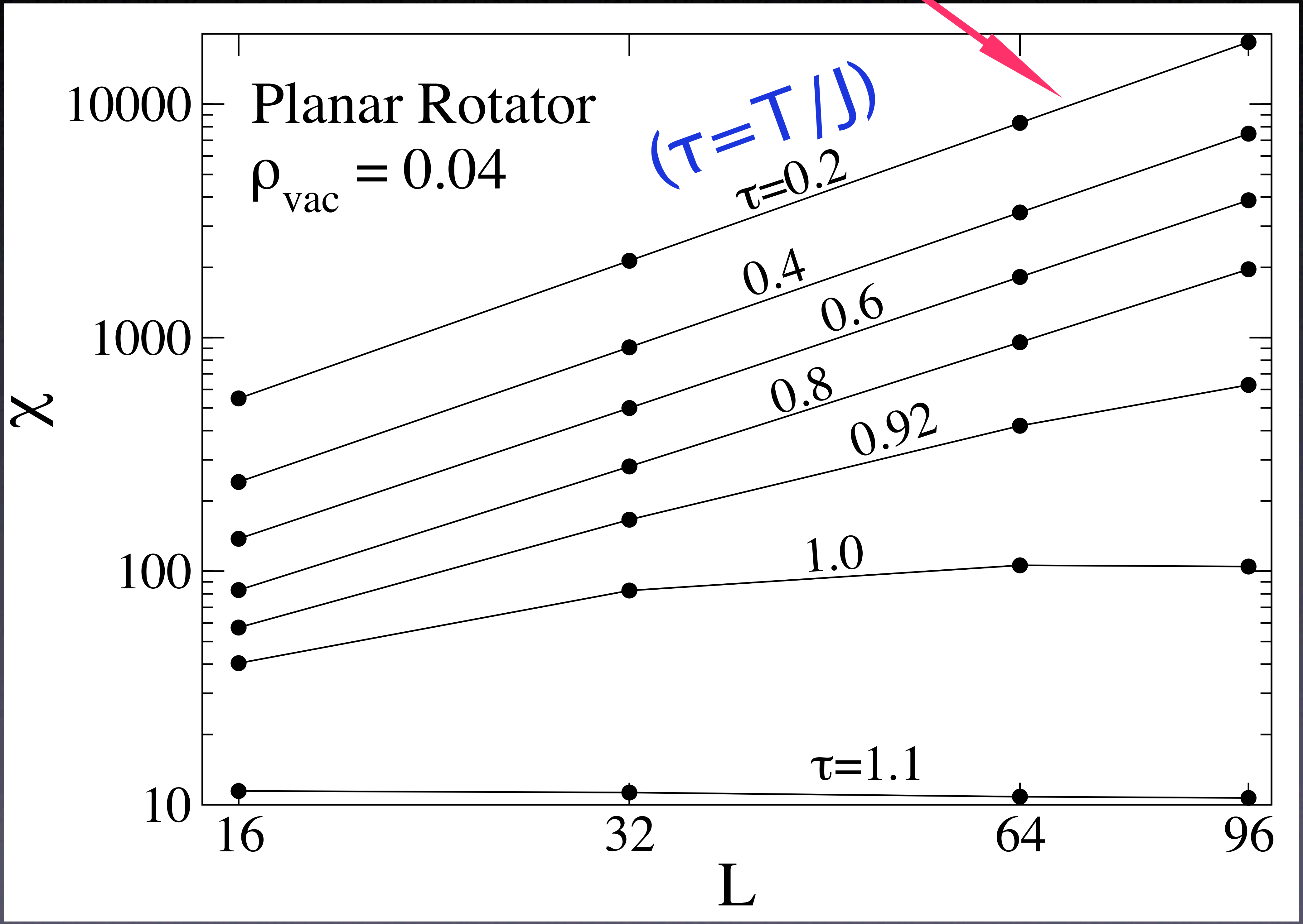


Using scaling of in-plane susceptibility

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

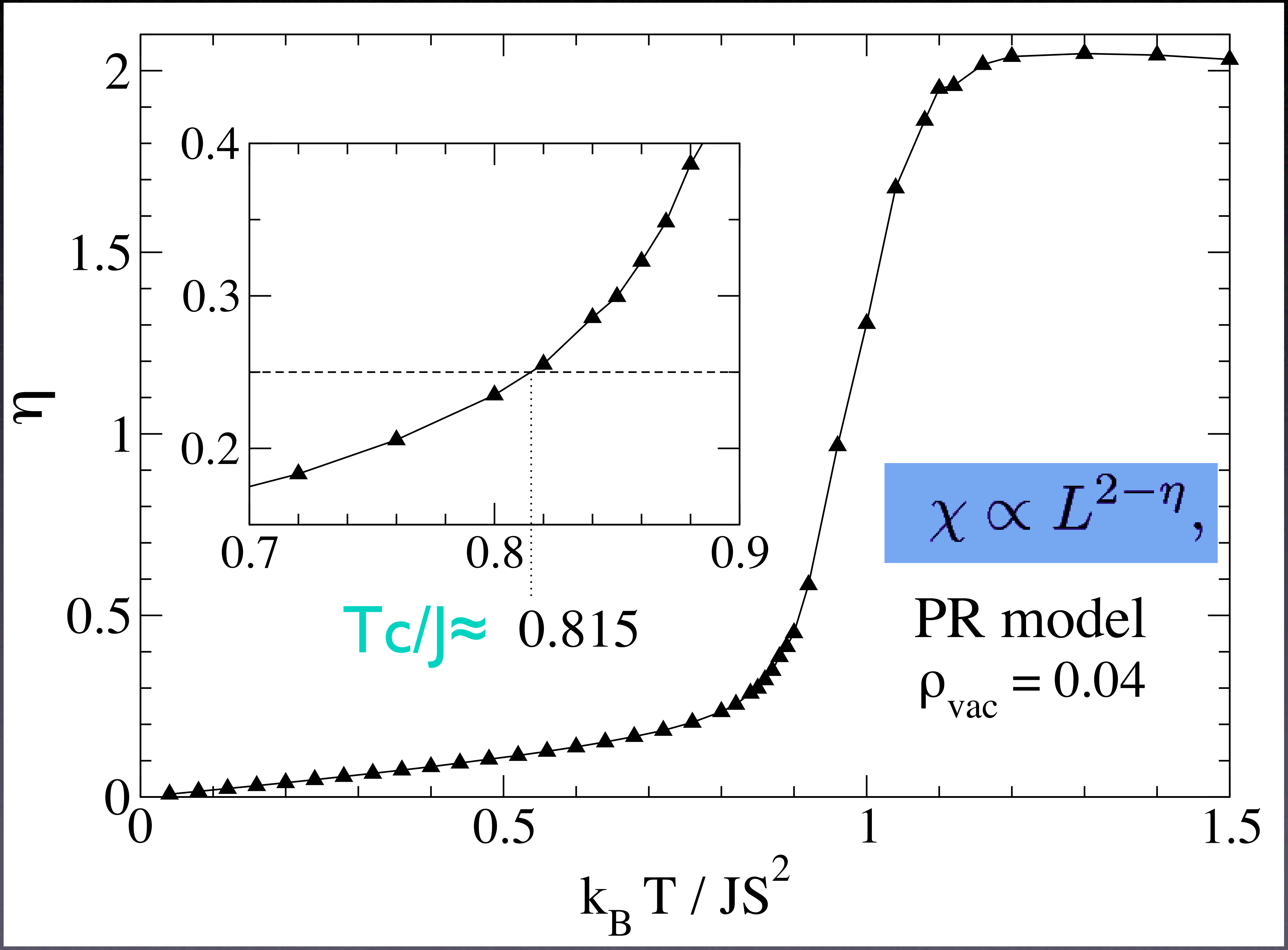
slope = 2-η

log-log scale

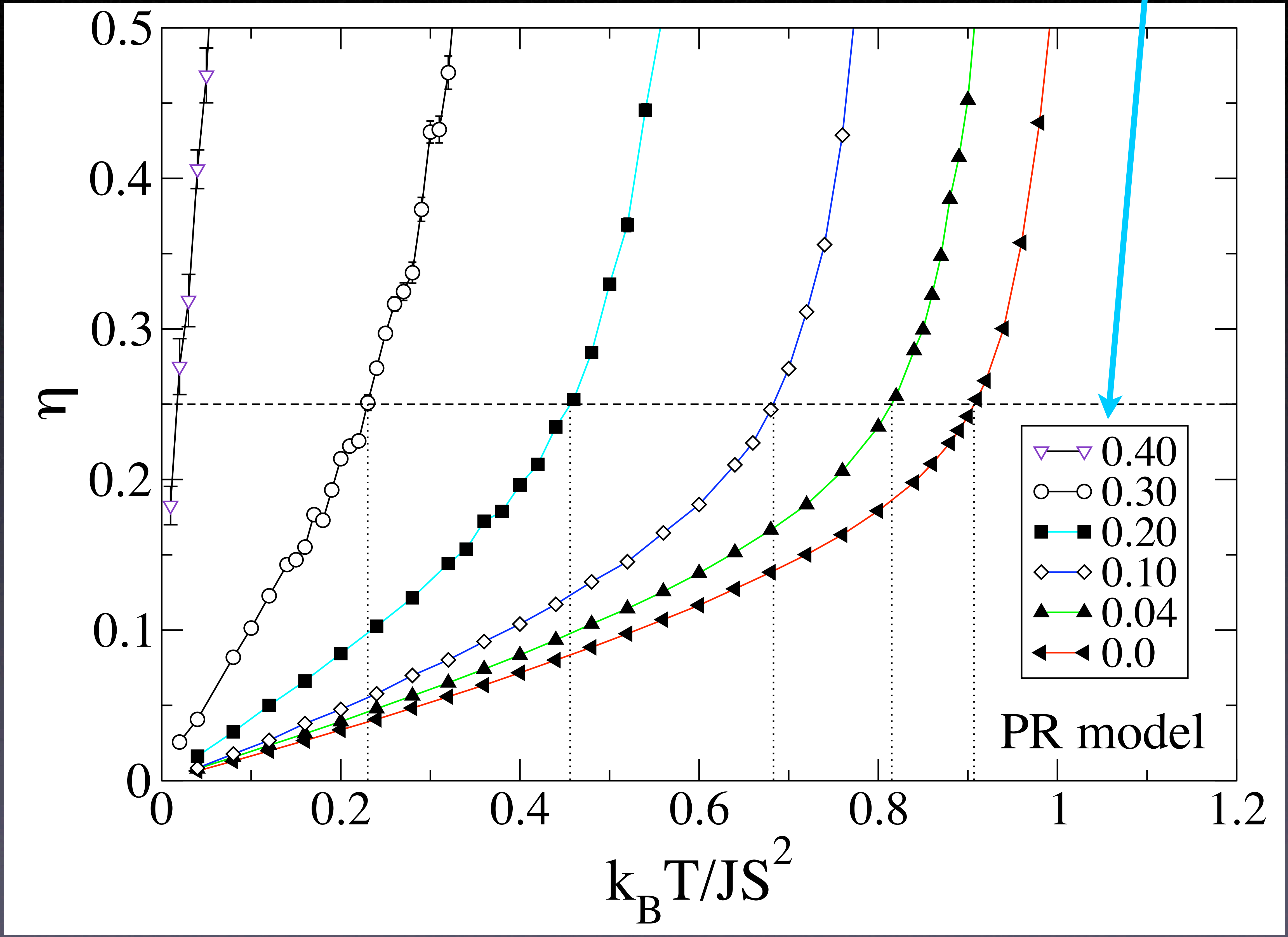


Tc from assumption of preserved symmetry

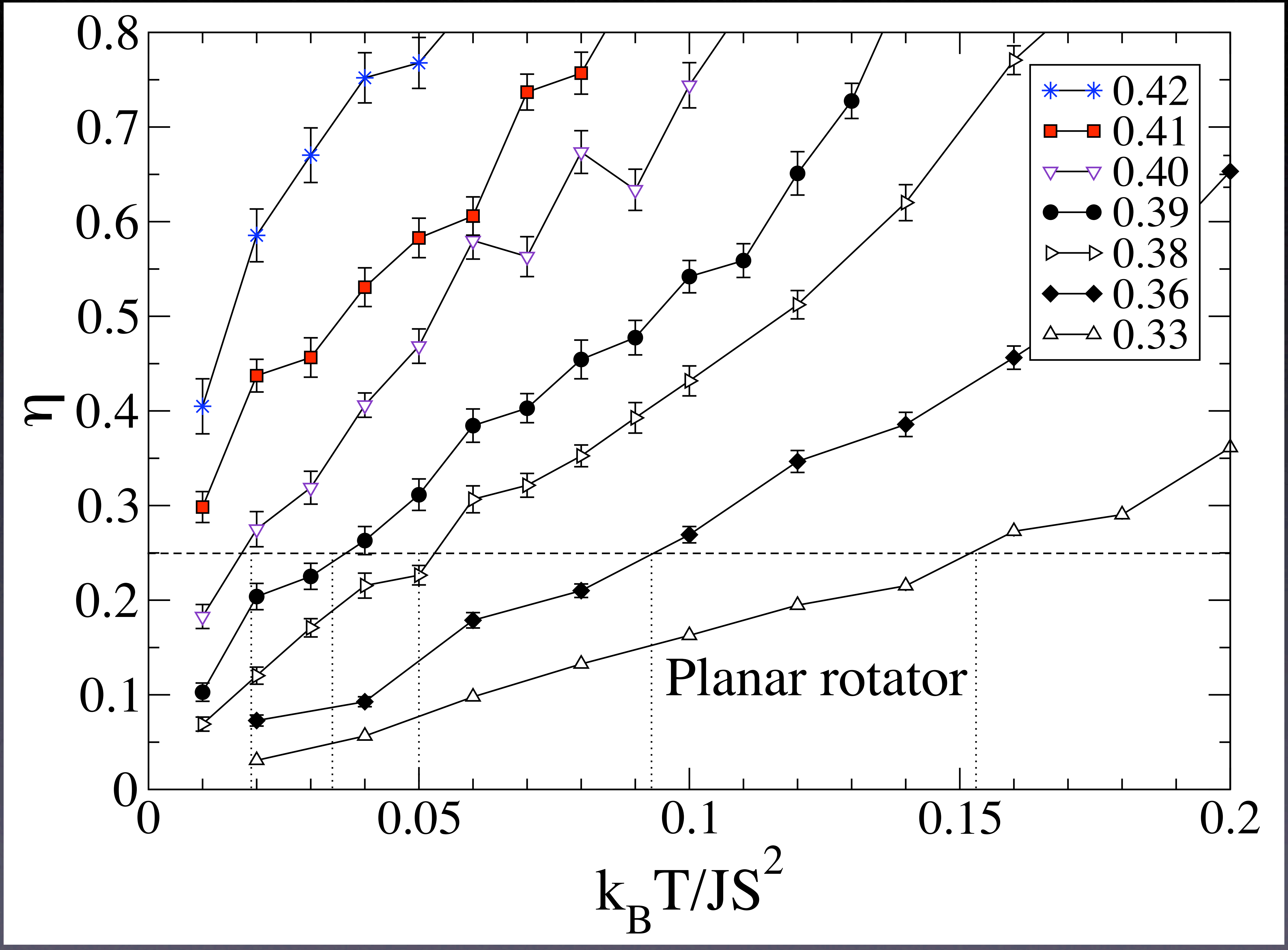
use correlation exponent: $\eta(T_c) = \frac{1}{4}.$



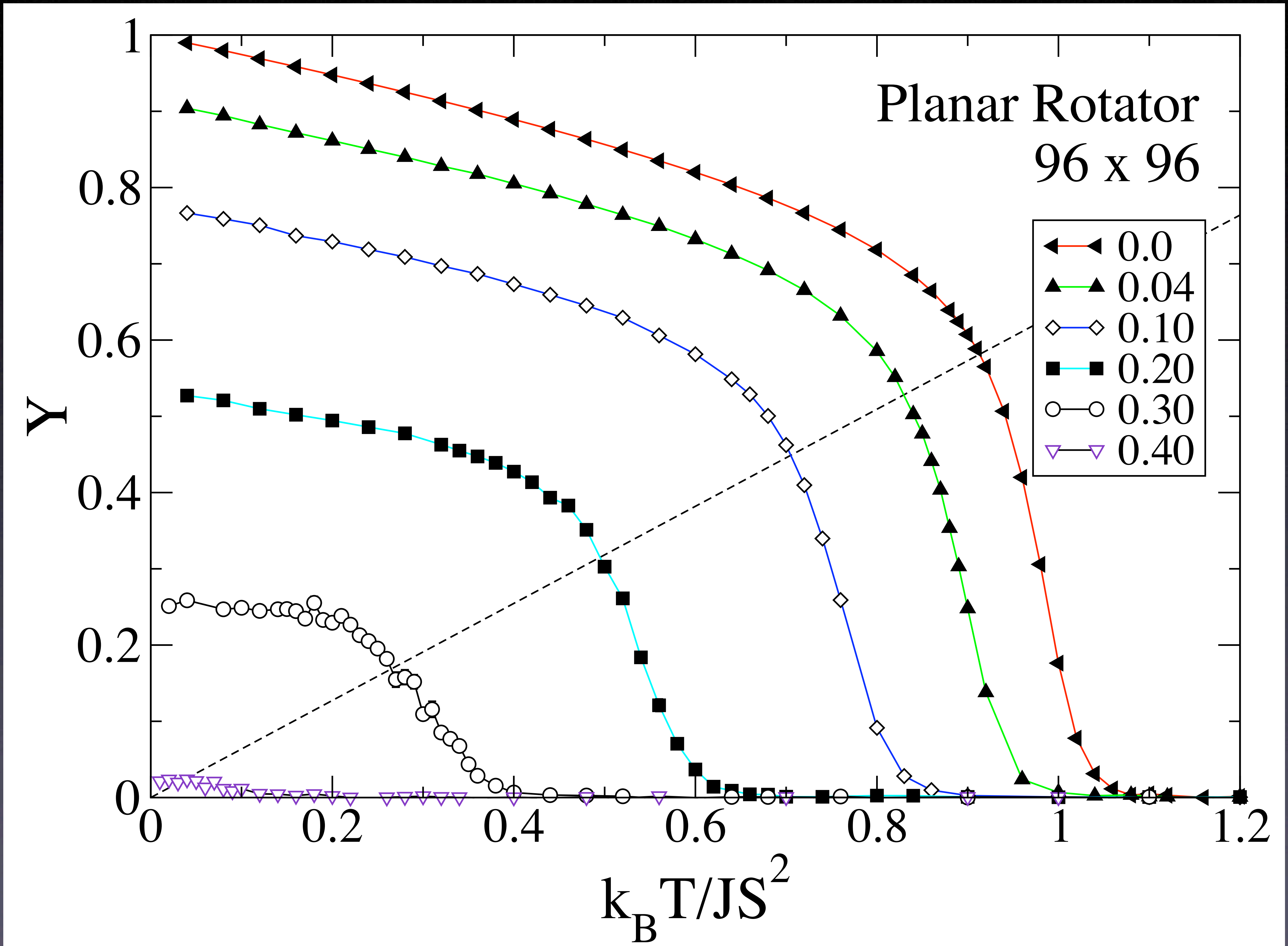
Planar rotator, trend with ρ_{vac}



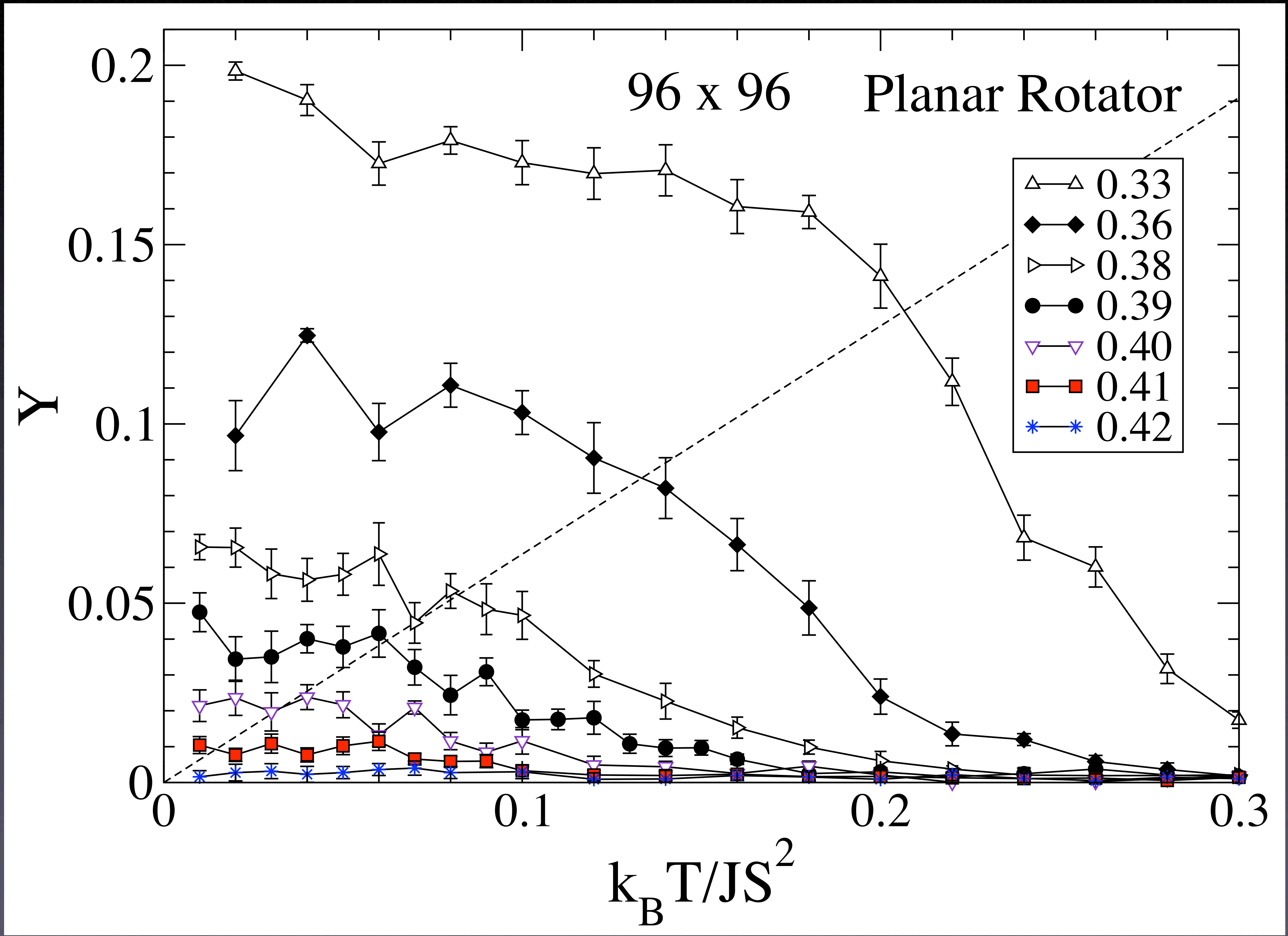
Planar rotator, trend with $\rho_{vac} \to \rho_c$



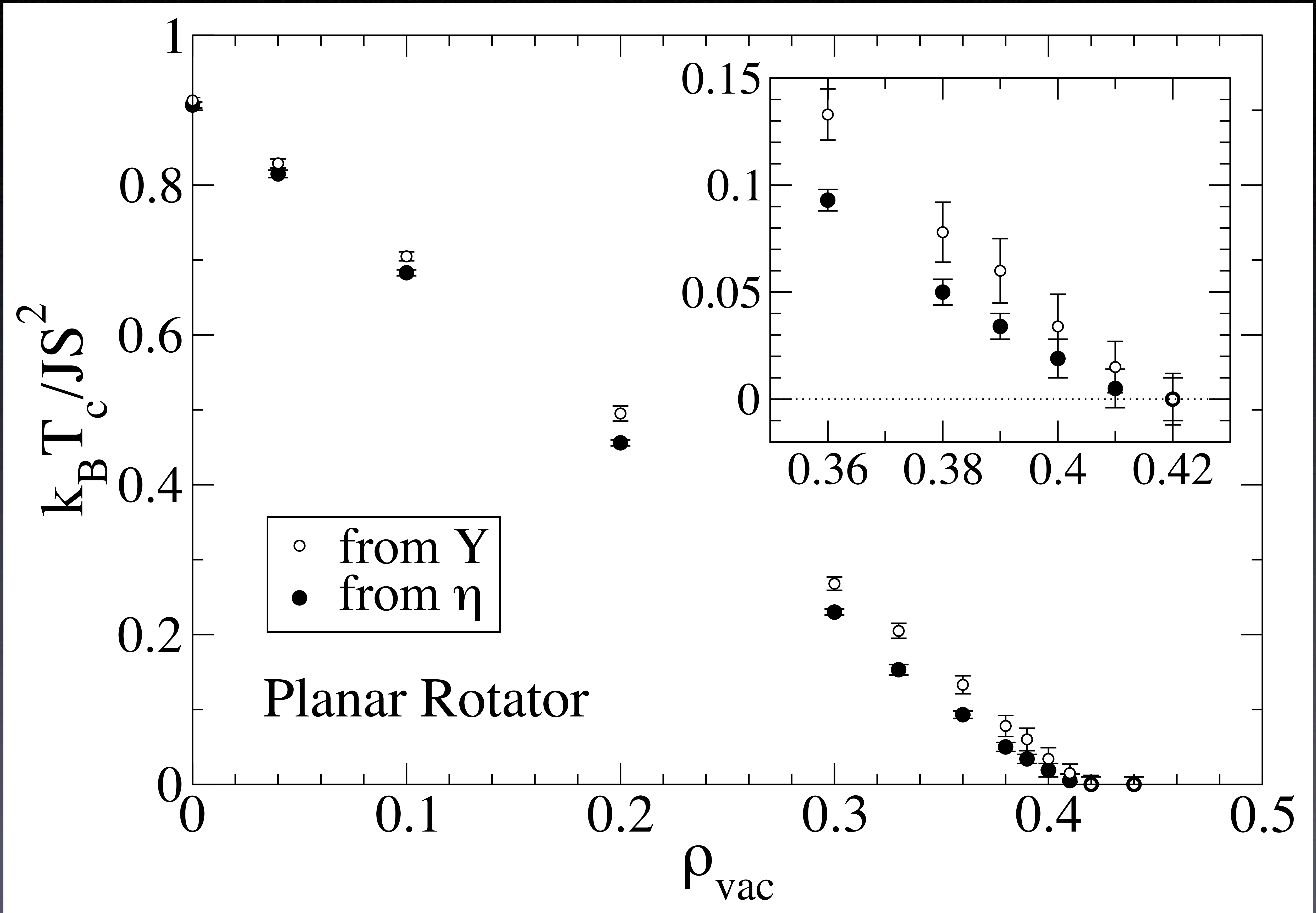
PR, helicity modulus, trend with ρ_{vac}



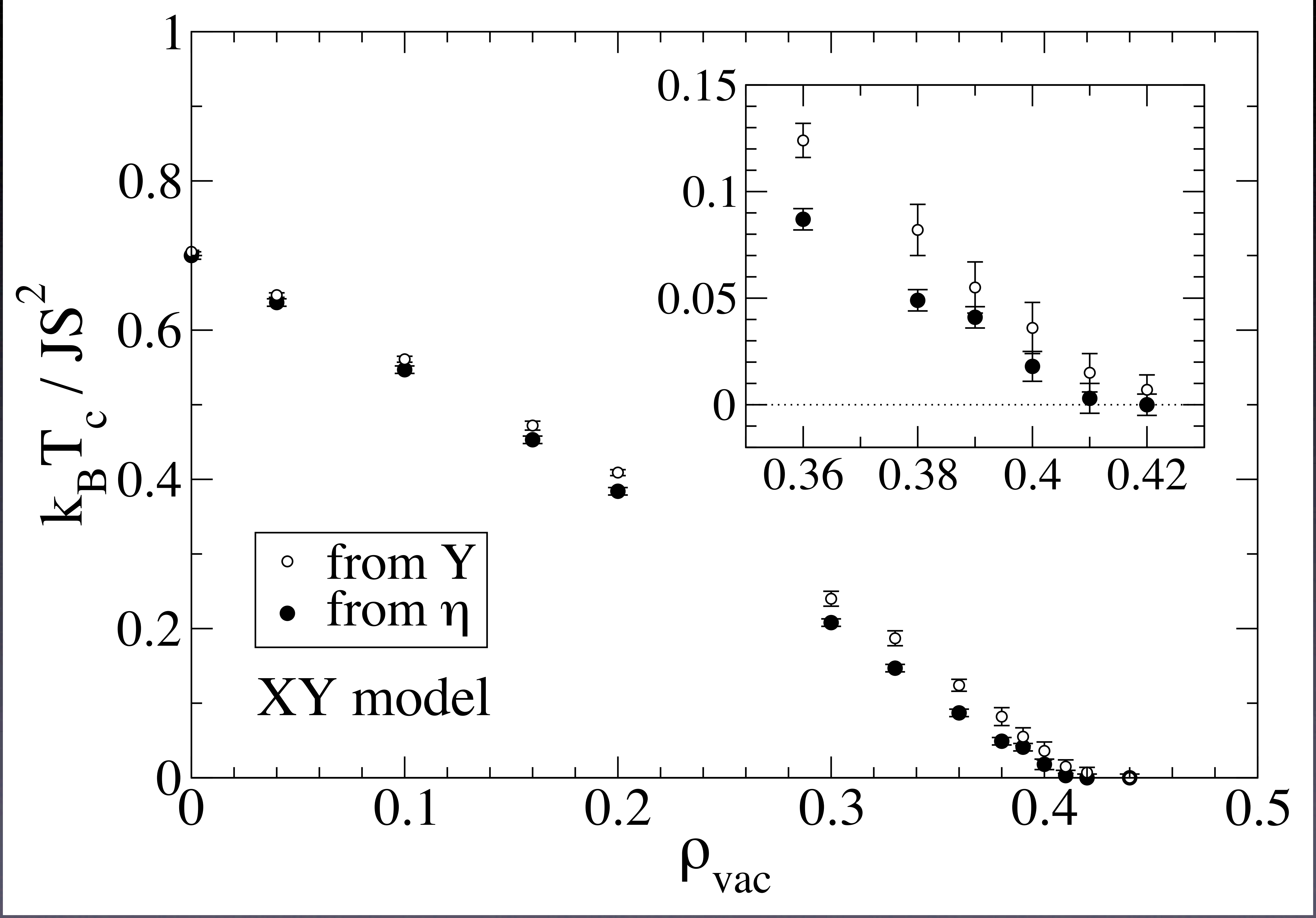
PR, helicity modulus, trend with $\rho_{vac} \rightarrow \rho_c$



Planar rotator, no transition for $\rho_{vac} > 0.41$



XY model, no transition for $\rho_{vac} > 0.41$



Conclusions

- Tc/J falls with increasing vacancy concentration.
- Tc/J driven to zero at the percolation limit, due to inadequate nearest neighbor couplings.
- At low ρ_{vac}, lower energy for vortex formation on vacancies compared to between vacancies.
- Can even generate vortices of double topological charge centered on vacancies!

more info: www.phys.ksu.edu/~wysin/