Are the critical exponents in an Ising fluid Fisher-renormalized?

Universität Linz
Theoretische Physik

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Abstract

We study the ferromagnetic order-disorder phase transition in Ising spin fluids with hard-core Yukawa exchange interaction truncated at various cut-off radii r_c. We have performed extensive Monte Carlo simulations in the canonical ensemble at a fixed density, employing the Wolff cluster algorithm for spin updates, and analyzed the data using the histogram reweighting technique and finite-size scaling (FSS) methods. Our system sizes range up to 10000 particles. We focus our interest on the dependence of critical quantities such as the Binder cumulant and various exponent ratios on the value of r_c, and on the question whether the Fisher-renormalized exponents expected for such systems can be observed in the simulations. It turns out that corrections to scaling decaying with a small exponent make it impossible to reach the asymptotic region with the restricted computational power available. Thus, we can only obtain effective exponents, with different (nonuniversal) values depending on the cut-off radius. A similar behavior is also found for the critical Binder cumulant. Nevertheless, a closer investigation of γ_{eff} as a function of temperature reveals a tendency towards a Fisher-renormalized asymptotic value.

Ising fluid - Model characteristics

- Interaction potential:

$$u(r_{ij}, s_i, s_j) = \begin{cases} \infty, & r_{ij} < \sigma \\ -J(r_{ij})\, s_i s_j, & \sigma < r_{ij} < r_c \\ 0, & r_{ij} > r_c \end{cases}$$

$$r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|, \qquad \mathbf{r}_i = (x_i, y_i, z_i), \qquad s_i = \pm 1$$

Yukawa exchange interaction $J(r) = \epsilon \frac{\sigma}{r} \exp[-\lambda(r-\sigma)]$

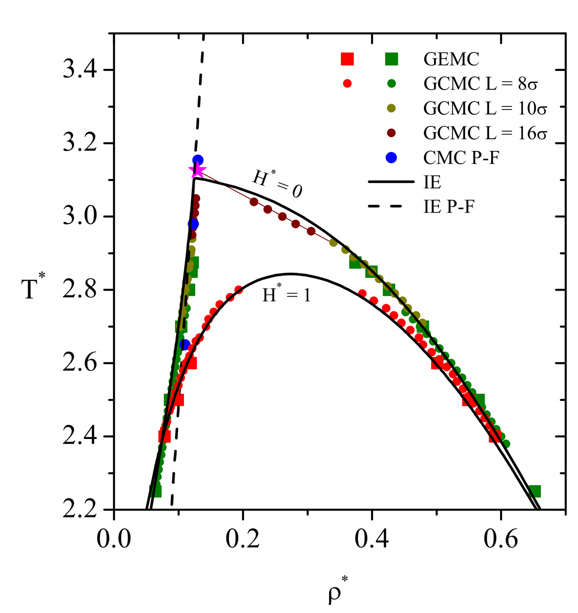
Cut-off radius r_c Screening parameter λ

- Potential energy:

$$E = \sum_{i<j}^{N} u(r_{ij}, s_i, s_j) - HM$$

$$M \equiv \sum_{i=1}^{N} s_i, \qquad H \ldots \text{ magnetic field}$$

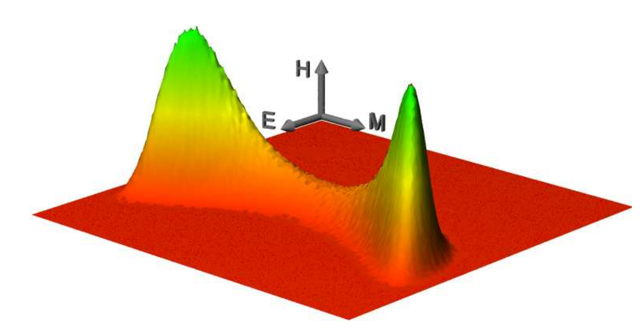
- Phase diagram:



- At $H = 0$ system shows 1st order gas-liquid + 2nd order para-ferromagnetic phase transitions

Monte Carlo simulations

- Canonical (NVT-) Ensemble with $\rho^* = 0.5$, PBC, $N = 108 \ldots 10000$
- Wolff cluster algorithm adapted for fluids
- Perform simulation near order-disorder phase transition temperature T_c
- Reweight histogram $H_T(M, E)$ to $H_{T'}(M, E)$ with $T' \in$ range around T_c
- Calculate thermodynamic quantities from H as functions of T: U, $\frac{\partial m}{\partial T}$, $\frac{\partial \ln m}{\partial T}$, χ, ...
  e.g. $\frac{\partial}{\partial K}\langle m^n\rangle = \langle m^n\rangle\langle E\rangle - \langle m^n E\rangle$, where $K = \epsilon/k_B T$, $m = M/N$

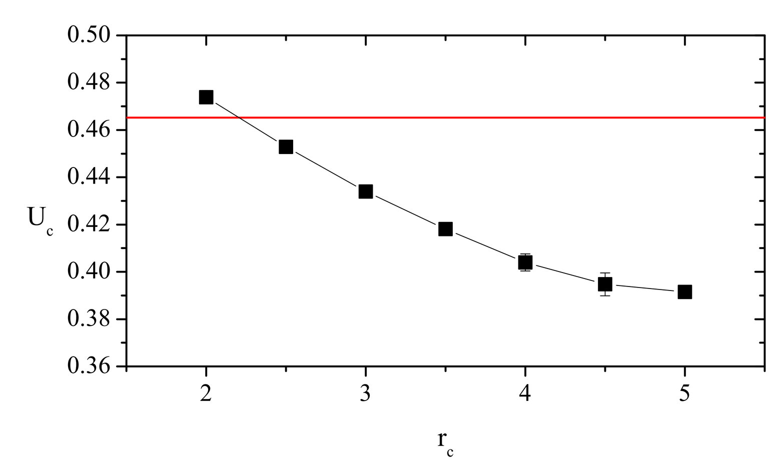


Critical Binder cumulant

- Binder cumulant U describes shape of distribution $P(m)$:

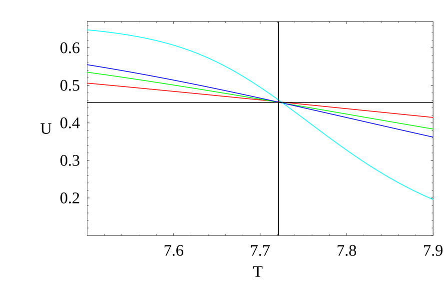
$$U_N(T) = 1 - \frac{\langle m^4\rangle_T}{3\langle m^2\rangle_T^2} \qquad \langle m^n\rangle_T = \int P_T(m) m^n dm$$

- U_N takes 'universal' value at T_c: $U_N(T_c) \equiv U_c \quad \forall N$
- Observe nonuniversal dependence of U_c on r_c

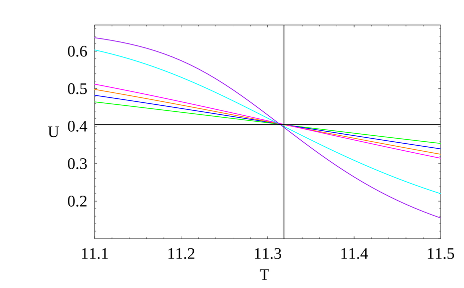


(red line ... 3D Ising lattice value)

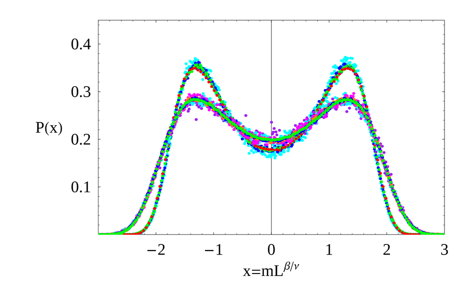
$r_c = 2.5$, $\lambda = 1$



$r_c = 4$, $\lambda = 1$



$P(mL^{\beta/\nu})$ at T_c for $r_c = 2.5$ and 4



(different colors correspond to different particle numbers N)

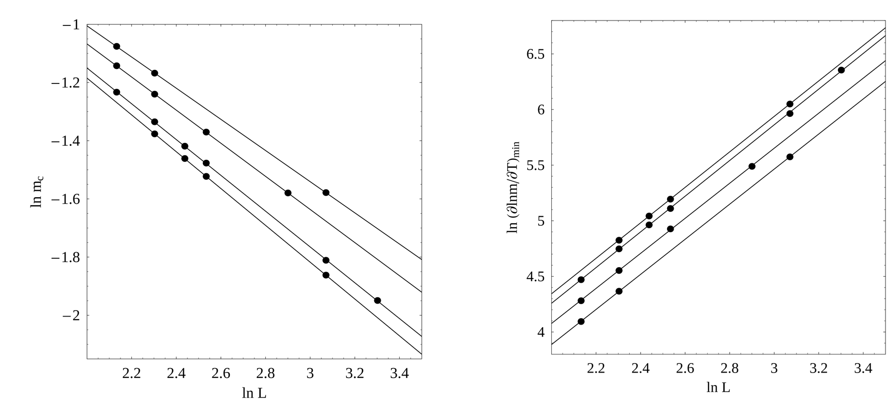
Finite-size scaling

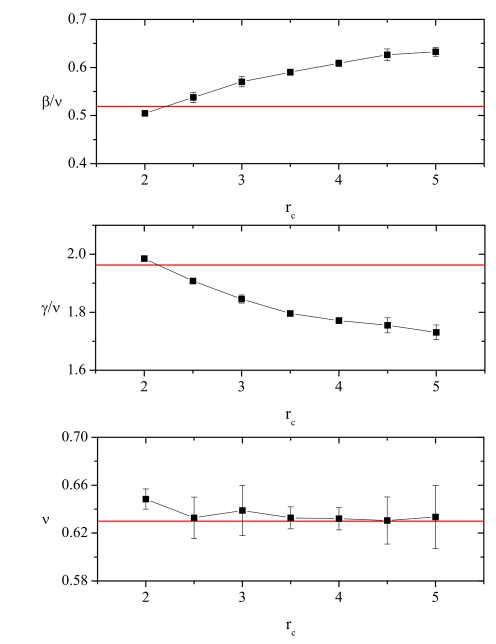
- Expect Fisher-renormalization of critical exponents due to constraint on ρ and $\alpha_{\text{Ising}} > 0$
- FSS relations:

$$\chi_{\max} \propto L^{\gamma/\nu} \qquad m_c \propto L^{-\beta/\nu}$$

$$\left(\frac{\partial \ln\langle|m|\rangle}{\partial T}\right)_{\min} \propto L^{1/\nu} \qquad \left(\frac{\partial \ln\langle m^2\rangle}{\partial T}\right)_{\min} \propto L^{1/\nu} \qquad \left(\frac{\partial U}{\partial T}\right)_{\min} \propto L^{1/\nu}$$

- Comparison with 3D Ising lattice values (red lines) at $\lambda = 1$:





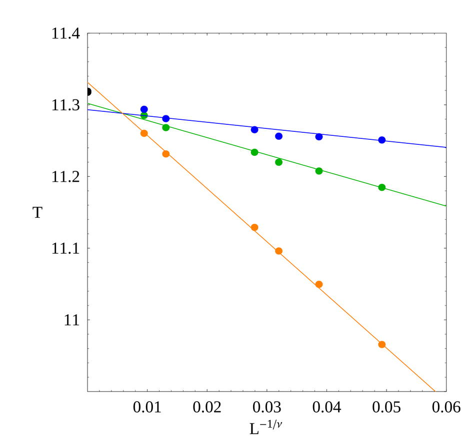
- Behavior cannot be explained by Fisher-renormalization alone!

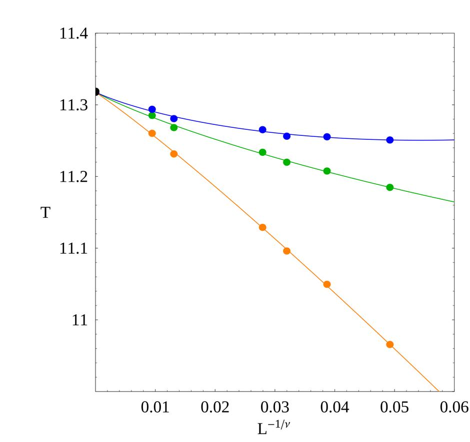
Shifting technique - Corrections to Scaling (CtS)

- T_c shift in finite system: $T_{\text{peak}}(L) - T_c(\infty) \propto L^{-\frac{1}{\nu}}$, therefore

$$T_{\text{peak}}(L) = T_c(\infty) + AL^{-\frac{1}{\nu}}$$

$$T_{\text{peak}}(L) = T_c(\infty) + AL^{-\frac{1}{\nu}}(1 + BL^{-\omega}) \quad \text{with CtS}$$





$r_c = 4$, $\lambda = 1$

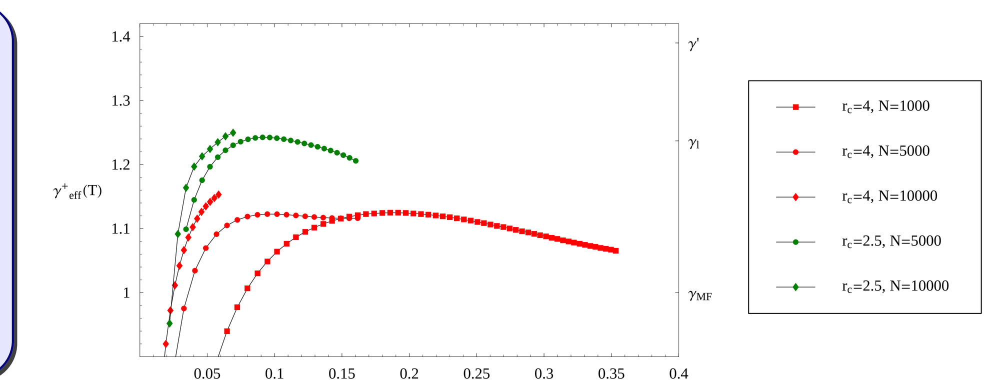
- $(\partial \ln\langle m^2\rangle/\partial T)_{\min}$
- $(\partial \ln\langle|m|\rangle/\partial T)_{\min}$
- $\chi_{\max}$
- $T_c = 11.3189(76)$ from cumulant crossing

- Corrections due to constraint (Fisher corrections to scaling) are present
- Smallest correction exponent $\omega \approx 0.3 \Rightarrow$ correction term only negligible for $\mathbf{N} \gtrsim \mathbf{30000}$!
- Cannot reach asymptotics in our study $\Rightarrow$ observe only effective exponents!
- Simulation of bulk behavior away from $T_c \Rightarrow$ estimation of asymptotic exponents:

$$\gamma^+_{\text{eff}}(T) = -\frac{\partial \ln \chi}{\partial \ln|t|} \qquad t > 0$$

$$t = 1 - T_c/T$$

$$\chi = V^{-1}\left(\langle M^2\rangle - \langle|M|\rangle^2\right)$$



Conclusion: We cannot reach asymptotics, but see a tendency of $\gamma_{\text{eff}}(T)$ towards the Fisher-renormalized value $\gamma' > \gamma_I$ (lattice value) for $r_c = 2.5$