Critical behavior in the grand and the canonical ensemble

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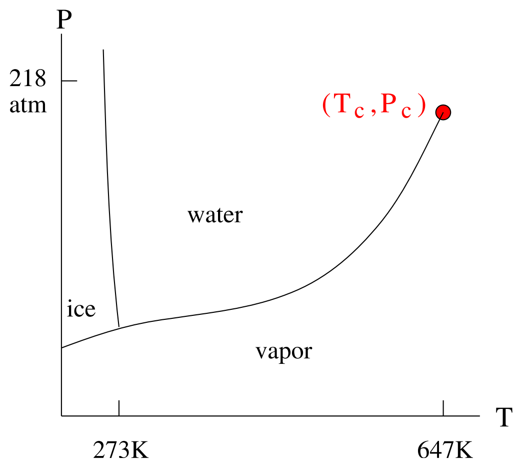
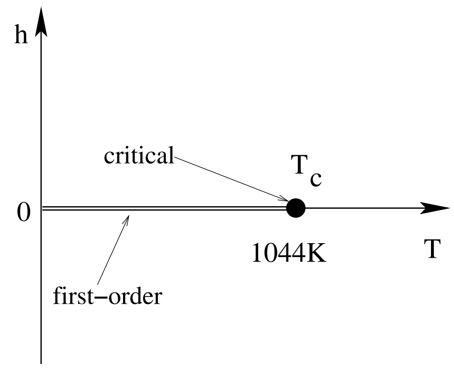
The Netherlands

– General introduction to the modern theory of critical phenomena
– Scaling behavior of critical systems with a fixed number of vacancies or magnetic spins

Introductions

- *Examples*





The liquid-gas critical point of H_2O: $T_c = 647K$, $p_c = 218$ atm.

The ferromagnetic point of Fe: $h_c = 0$, $T_c = 1044K$.

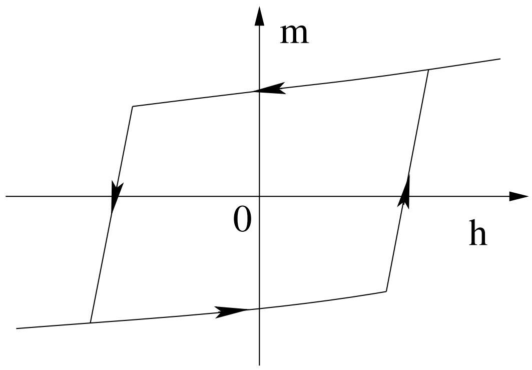
- *Theoretical Treatments*
  - Write out Hamiltonian $\mathcal{H}$
  - Calculate partition function $Z = \sum e^{-\mathcal{H}/k_b T}$

    or free energy $F = -\ln Z$
  - Derive quantities of interest

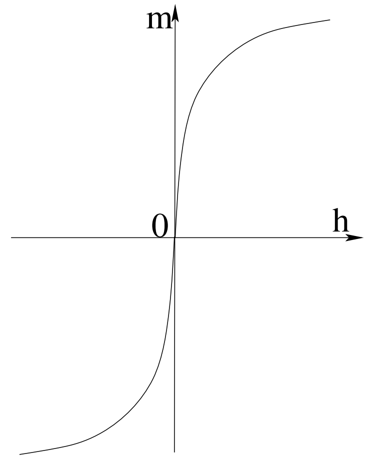
    First derivative: ρ_{H_2O}, m

    Second derivative: C, χ

⋆ nth-order transition: nth derivative is singular, but $(n-1)$th derivative is analytic.



First-order

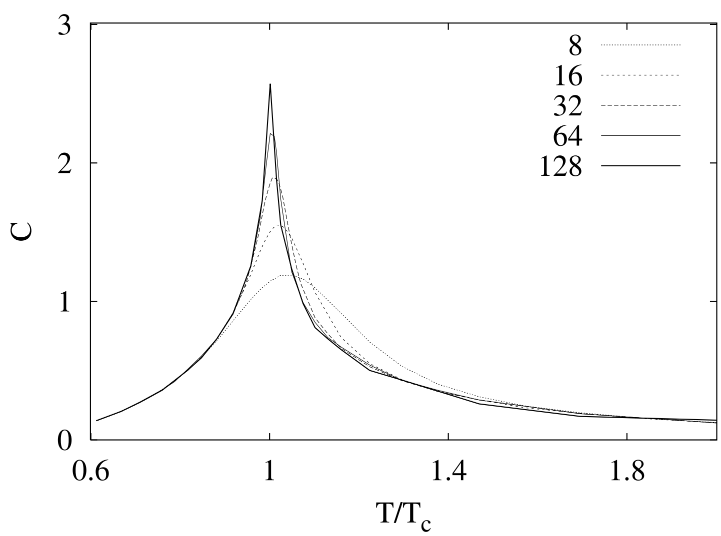


Second-order

- *Critical phenomena*

Specific-heat : $C \propto |T - T_c|^{-\alpha}$
Susceptibility : $\chi \propto |T - T_c|^{-\gamma}$
Magnetization: $m \propto |T - T_c|^{\beta}$

At T_c, correlation: $g(r) \propto r^{-2X}$



Specific heat C of the critical Ising model.

⋆ Universality: critical exponents, $\alpha, \gamma, \cdots$, take same values in different systems.

- *Theoretical models*

  (1) Ising model with vacancies:

  $\mathcal{H}/k_{\mathrm{B}}T = -K\sum s_i s_j - \mu \sum s_k^2 \, (s = 0, \pm 1)$

  $K-$ interaction strengths; $\mu-$ chemical potential

  (2) lattice gas:

  $\mathcal{H}/k_{\mathrm{B}}T = K\sum \delta_{\sigma_i,\sigma_j}(1-\delta_{\sigma_i,0}) - \mu\delta_{\sigma_i,1} \, (\sigma_i = 1, 0)$

  (3) dilute q-state Potts model

  $\mathcal{H}/k_{\mathrm{B}}T = K\sum \delta_{\sigma_i,\sigma_j}(1-\delta_{\sigma_i,0}) + \mu\delta_{\sigma_i,0} \, (\sigma_i = 0, 1, \cdots, q)$

- *Fractal geometry at T_c*

Scale invariance: clusters of all possible sizes occur

$\Downarrow$

Renormalization group technique

$\Downarrow$

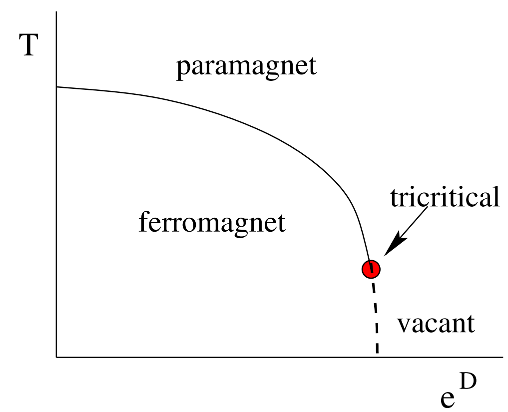
Various fixed points are for various universalities

Grand and Canonical ensembles

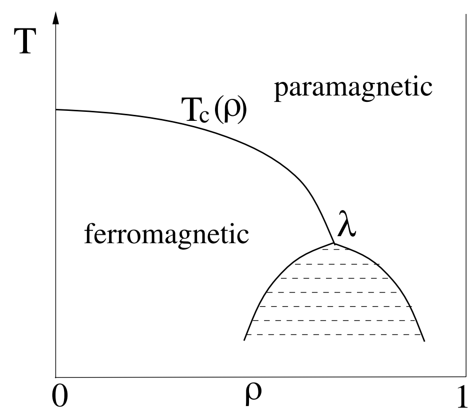
Grand (T, μ): particle number $N\rho$ fluctuates.

Canonical (T, ρ): ρ is conserved

- ***Phase diagrams***



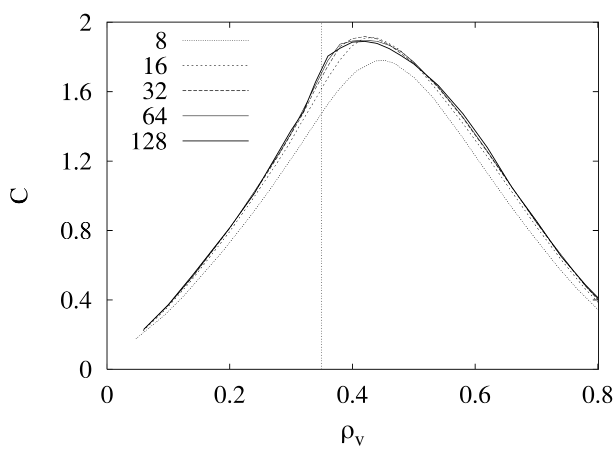
(T, μ)



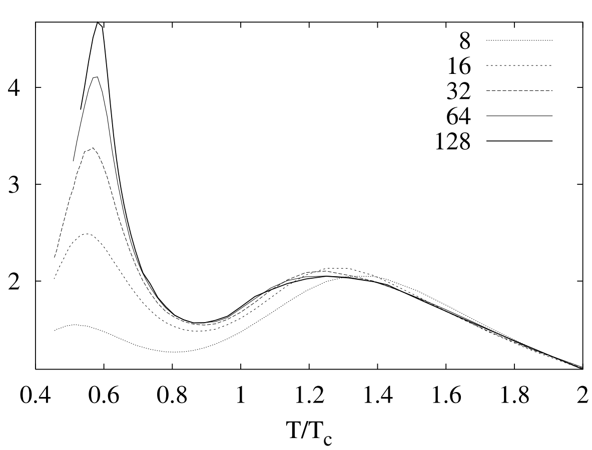
(T, ρ_v)

Question: *Is there any difference in critical phenomena in different ensembles?*

- ***Simulation***



$T = T_c$



$\rho_v = \rho_{vc}$

- *Experiment*

	Experiments	Models
Ferro- and antiferromagnets Binary fluids	< 0	0.11
He_3 and He_4 mixture	-0.9	$1/2$
Explanation	*CONVERGENT* (K, ρ_v)	(K, D)

Exponent α of specific heat $C \propto t^{-\alpha}$

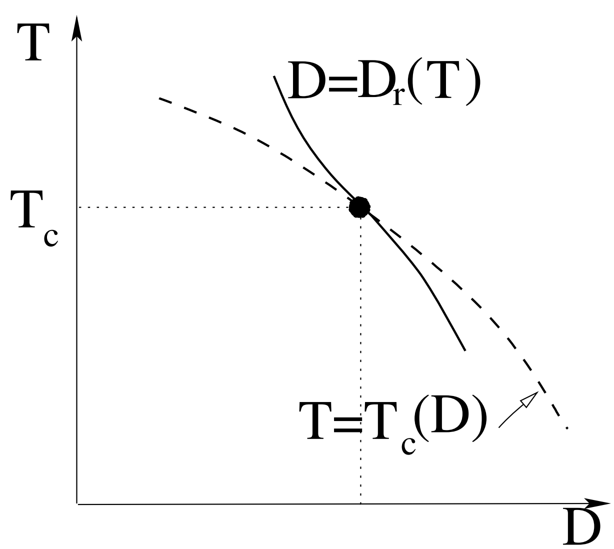
Analytical calculations

I Mean field calculations for tricritical Ising model

Vacancy density ρ_v fixed at tricriticality:

$\Rightarrow$ *mean-field critical* Ising-like.

II Fisher's renormalization



Constraint $\Rightarrow$ Path of constrained systems is *singular* near the critical point

Singularity of C arises from both *singular* and *analytical* parts of free energy

Results: $\alpha > 0 \Rightarrow \alpha' = -\alpha/(1-\alpha)$;

$\alpha = 0 \Rightarrow C' = 1/\ln|T - T_c|$.

! C is *convergent*

Finite-size interpretation:

Free energy: $\boxed{f(t,l) = l^{-d} f_s(t l^{y_t})}$ (unconstrained)

$\Rightarrow \boxed{f'(t,l) = l^{-d} f'_s(t l^{d-y_t})}$ (constrained)

At criticality: $C \propto L^{2y_t - d} \Rightarrow C' \propto L^{d-2y_t}$

III Generalization of Fisher's renormalization

Including *subleading* thermal field $\Rightarrow$

$$\boxed{f'(t_1, t_2, l) = l^{-d} f'_s(t_1 l^{d-y_{t1}}, t_2 L^{y_{t2}})}$$

! Leading behavior of C depends on relative magnitude of $d - y_{t1}$ and y_{t2}.

! Renormalization for magnetic constraint is similar to the above formula.

IV General understanding

Equivalence of F:

$$F^{(\mathrm{g})}(T,\mu,L) = F^{(\mathrm{c})}(T, \rho^{(g)}(T,\mu,L), L) \quad (L \to \infty)$$

Nonequivalence of $E \equiv \partial F/\partial T$:

$$E^{(\mathrm{g})}(T,\mu,L) = E^{(\mathrm{c})}(T, \rho^{(g)}(T,\mu,L), L) + \frac{\partial F}{\partial \rho}\frac{\partial \rho}{\partial T}$$

Numerical Investigation

! *ONLY* geometric cluster algorithm can *EFFICIENTLY* simulate large constrained systems.

I Quantity sampled

(a) Specific heat $C \propto L^{Y_c}$:

$Y_c = 2y_{t1} - 2 \Rightarrow$ $\boxed{Y_c' = 2 - 2y_{t1}}$ (thermal)

or $\boxed{Y_c' = 2y_{t2} - 2}$

Susceptibility $\chi \propto L^{Y_\chi}$:

$Y_\chi = 2y_{h1} - 2 \Rightarrow$ $\boxed{Y_\chi' = 2y_{h2} - 2}$ (magnetic)

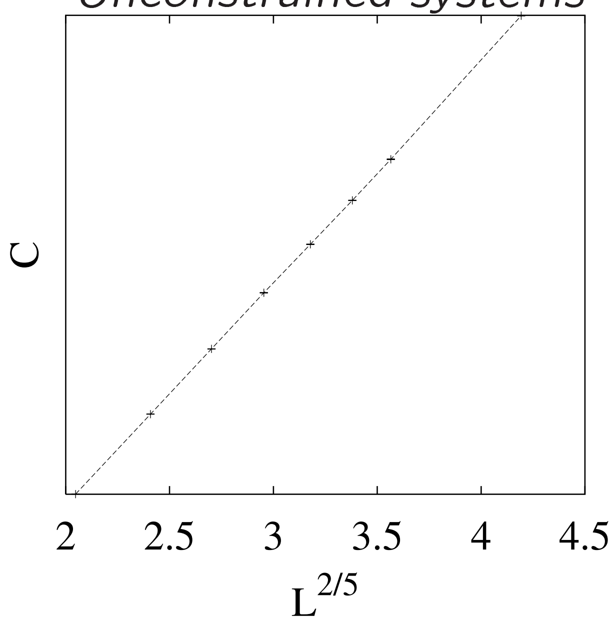
(b) Long-distance correlation functions g_e and g_m

No modification is expected

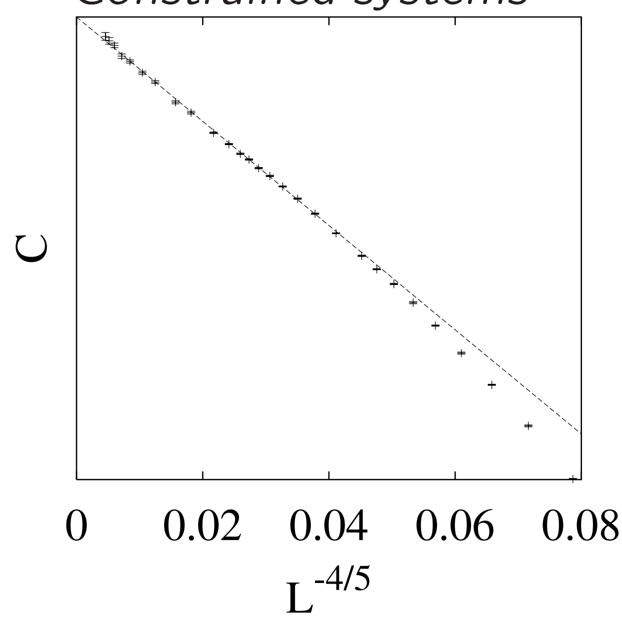
(b) Others, e.g., Binder-ratio, structure factors of $C \cdots$

II Thermal constraint (*2D* $q = 3$ *Potts model*)

Unconstrained systems



Constrained systems



CONVERGENT

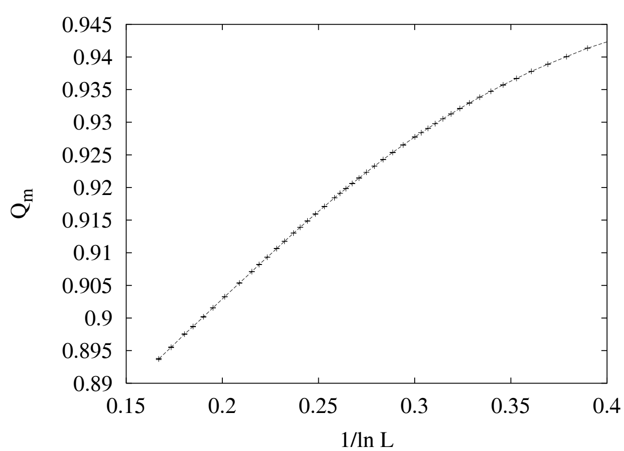
⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆

Y_c *of* $C \propto L^{Y_c}$

Model	Theory	Numerical	Mean-field
crit. 2D Ising	$1/\ln L$	$1/\ln^2 L$	
hard-hexagon	$-2/5$	$-0.796(5)$	
crit. 2D $q=3$	$-2/5$	$-0.802(4)$	
crit. 3D Ising	$-0.174(2)$	$-0.35(2)$	
2D anti Ising	$1/\ln L$	$1/\ln L$	
crit. 2D $q=4$	-1	$-1.50(6)$	
tricr. 2D Ising	$-2/5$	$-0.398(4)$	
tricr. 2D $q=3$	$-6/7$	$-0.840(8)$	
tricr. 3D Ising	-1	$-0.987(8)$	$\ln L$

! Long-range correlations are *NOT* affected.

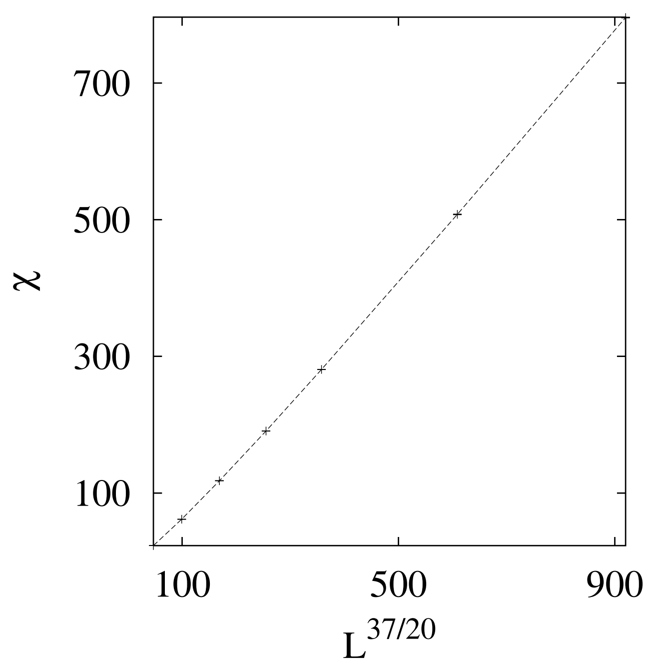
! *NEW* finite-size corrections are induced.

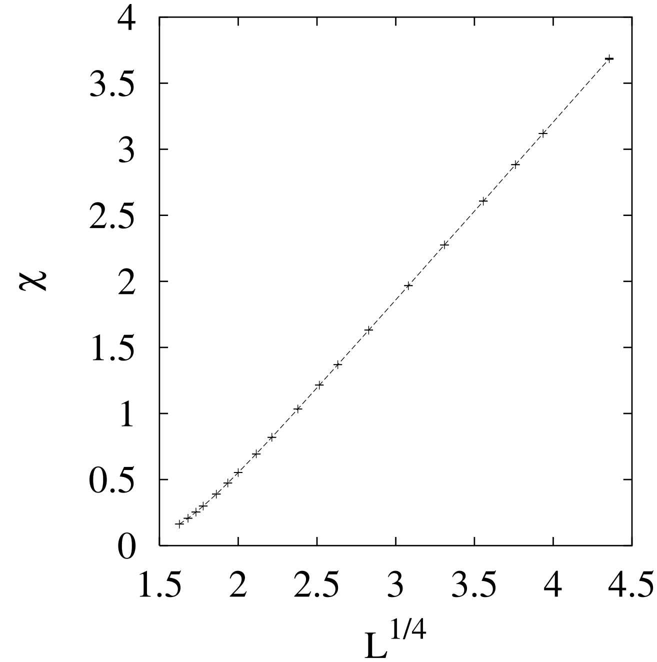


Binder ratio for critical 2D Ising model

III Magnetic constraint (*2D tricritical Ising model*)

Unconstrained systems   *Constrained systems*





! χ can be *divergent* under constraint.

! *WE ASSUME*

$$X_{h2} = 2 - y_{h2} = \frac{(g+2)(10-g)}{8g}$$

g – coupling constant for Coulomb gas particles.

⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆ ⋆

Y_χ *of* $\chi \propto L^{Y_\chi}$

Model	Theory y_{h2}	Theory Y_χ	Numerical Y_χ
crit. 2D Ising	13/24	−11/12	−1.01(2)
crit. 2D $q = 3$	2/3	−2/3	−0.77(4)
crit. 2D $q = 4$	7/8	−1/4	−0.224(8)
tricr. 2D $q = 3$	12/21	2/21	0.126(2)
tricr. 2D Ising	9/8	1/4	0.253(2)

CONCLUSIONS

- Geometric algorithm enables *EFFICIENT* simulations of constrained systems

- Constrained *critical* phenomena are *NOT* completely understood

- Constrained *tricritical* 3D Ising systems are *NOT* explained mean-field calculations.

- Fisher's renormalization is generalized.

- An approach is provided to numerically observe subleading scaling fields.