Universal scaling and the essential singularity at the abrupt Ising transition

Jaron Kent-Dobias James Sethna

Cornell University

16 March 2017

Outline

- Renormalization and the Ising model

Outline

- Renormalization and the Ising model
- Metastability and complex free energy

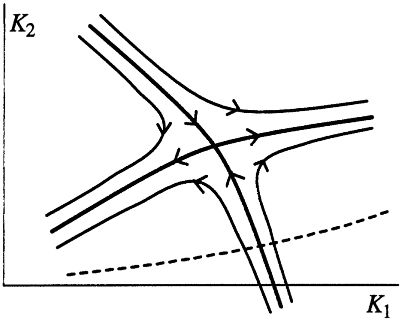
Outline

- Renormalization and the Ising model
- Metastability and complex free energy
- Analytic constraints on the stable free energy

Outline

- Renormalization and the Ising model
- Metastability and complex free energy
- Analytic constraints on the stable free energy
- Closed-form results for the 2D Ising susceptibility

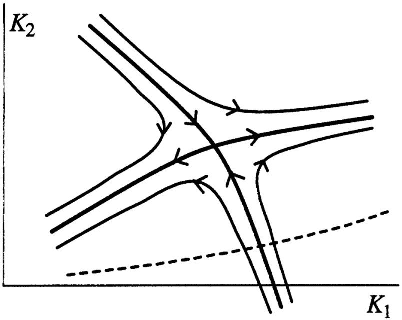
Renormalization and the Ising Model



From *Scaling and Renormalization in Statistical Physics* by John Cardy

RG analytically maps system space onto itself.

Renormalization and the Ising Model

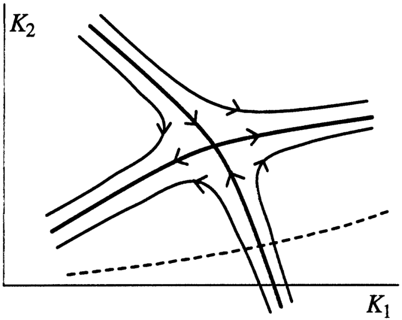


From *Scaling and Renormalization in Statistical Physics* by John Cardy

RG analytically maps system space onto itself.

Fixed points correspond to phases, criticality.

Renormalization and the Ising Model



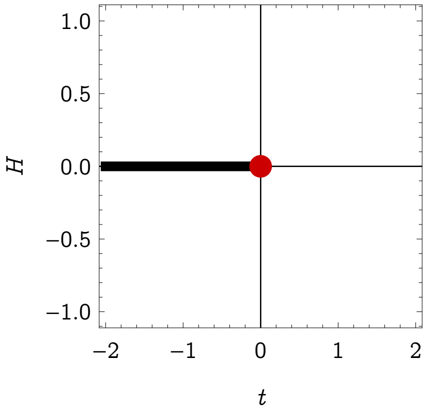
From *Scaling and Renormalization in Statistical Physics* by John Cardy

RG analytically maps system space onto itself.

Fixed points correspond to phases, criticality.

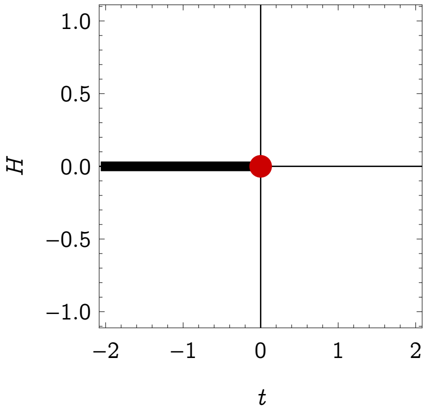
Nonanalytic behavior is preserved by RG.

Renormalization and the Ising Model



Ising critical point has power laws, logarithms in thermodynamic variables.

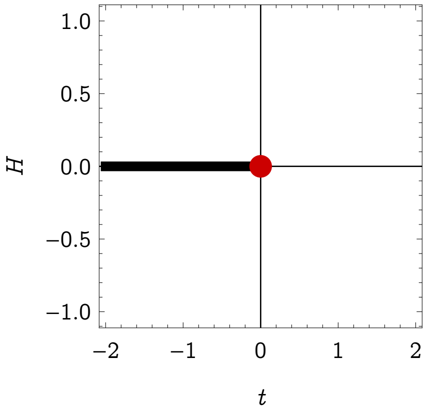
Renormalization and the Ising Model



Ising critical point has power laws, logarithms in thermodynamic variables.

Connected to line of abrupt transitions.

Renormalization and the Ising Model

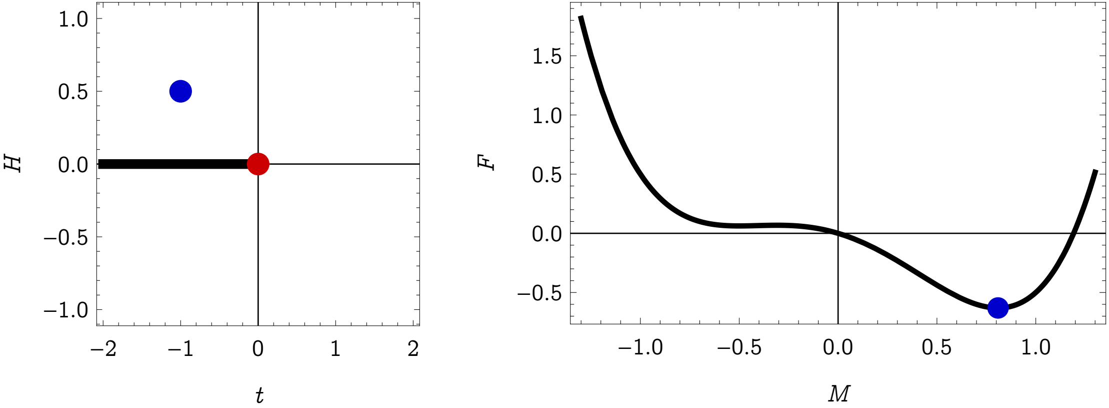


Ising critical point has power laws, logarithms in thermodynamic variables.

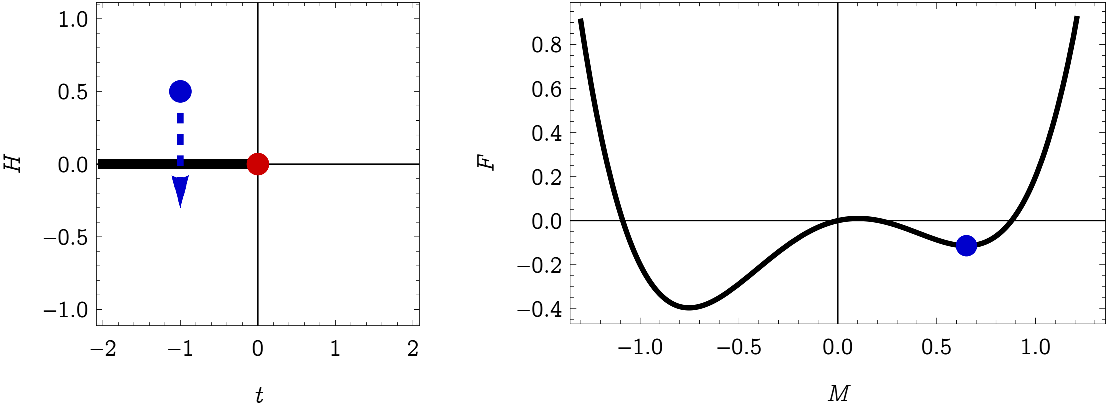
Connected to line of abrupt transitions.

We've identified nonanalytic behavior along the abrupt transition line.

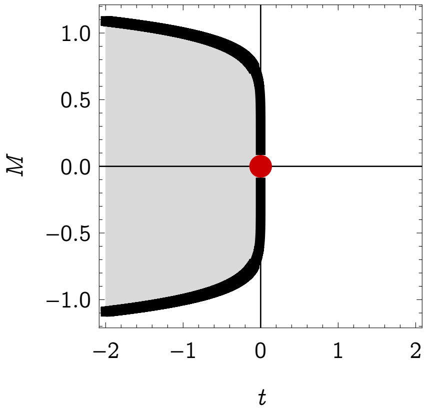
Metastability & Complex Free Energy



Metastability & Complex Free Energy

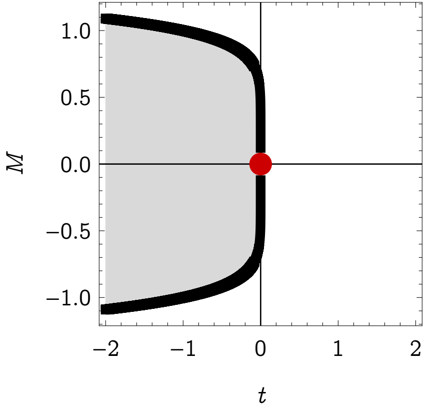


Metastability & Complex Free Energy



Thermodynamics can be continued into metastable phase.

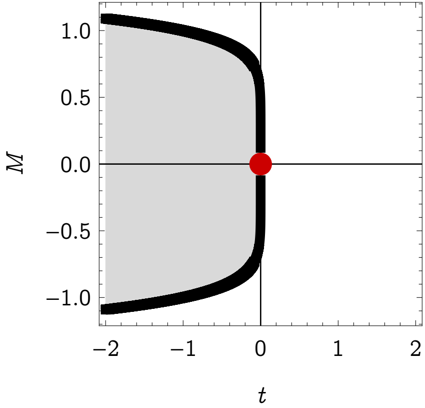
Metastability & Complex Free Energy



Thermodynamics can be continued into metastable phase.

Decay rate related to imaginary free energy, $\Gamma \propto \frac{1}{kT}\,\mathrm{Im}\,F$ (Langer 1969).

Metastability & Complex Free Energy



Thermodynamics can be continued into metastable phase.

Decay rate related to imaginary free energy, $\Gamma \propto \frac{1}{kT}\,\mathrm{Im}\,F$ (Langer 1969).

Ising metastable decay somewhat well studied (Günther 1980, Houghton 1980)

Metastability & Complex Free Energy

Decay of metastable phase occurs when domain of critical size forms.

Metastability & Complex Free Energy

Decay of metastable phase occurs when domain of critical size forms.

Domain of N spins entering the stable phase causes a free energy change

$$\Delta F = \Sigma N^{\sigma} - MHN$$

with $1 - \frac{1}{d} \leq \sigma < 1$.

Metastability & Complex Free Energy

Decay of metastable phase occurs when domain of critical size forms.

Domain of N spins entering the stable phase causes a free energy change

$$\Delta F = \Sigma N^\sigma - MHN$$

with $1 - \frac{1}{d} \leq \sigma < 1$.

Metastable phase is stable to domains smaller than

$$N_{\text{crit}} = \left(\frac{MH}{\sigma\Sigma}\right)^{-1/(\sigma-1)}$$

but larger will grow to occupy the entire system, decay to stable phase.

Metastability & Complex Free Energy

Formation of critical domain has energy cost

$$\Delta F_{\text{crit}} = \Delta F\Big|_{N=N_{\text{crit}}} \sim \left(\frac{\Sigma}{(MH)^{\sigma}}\right)^{1/(1-\sigma)}$$

Metastability & Complex Free Energy

Formation of critical domain has energy cost

$$\Delta F_{\text{crit}} = \Delta F\Big|_{N=N_{\text{crit}}} \sim \left(\frac{\Sigma}{(MH)^{\sigma}}\right)^{1/(1-\sigma)}$$

Probability of such a domain forming is

$$P_{\text{crit}} \sim e^{-\beta \Delta F_{\text{crit}}}$$

Metastability & Complex Free Energy

Formation of critical domain has energy cost

$$\Delta F_{\text{crit}} = \Delta F\Big|_{N=N_{\text{crit}}} \sim \left(\frac{\Sigma}{(MH)^{\sigma}}\right)^{1/(1-\sigma)}$$

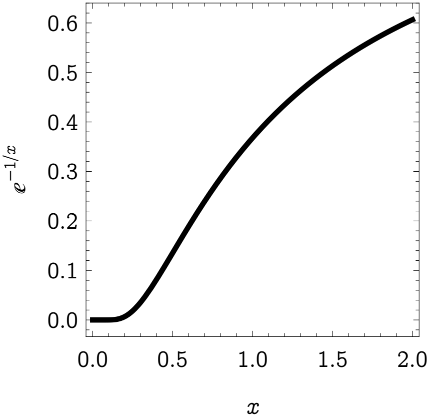
Probability of such a domain forming is

$$P_{\text{crit}} \sim e^{-\beta \Delta F_{\text{crit}}}$$

Imaginary free energy is therefore

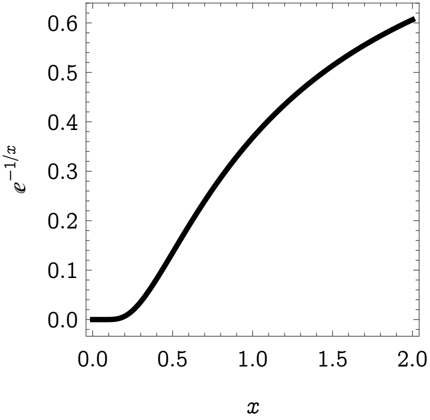
$$\operatorname{Im} F \sim \Gamma \sim P_{\text{crit}} \sim e^{-\beta \Delta F_{\text{crit}}} = e^{-\beta(\Sigma/(MH)^{\sigma})^{1/(1-\sigma)}}$$

Metastability & Complex Free Energy



Im F has an essential singularity of the form $e^{-1/H^{\sigma/(1-\sigma)}}$.

Metastability & Complex Free Energy

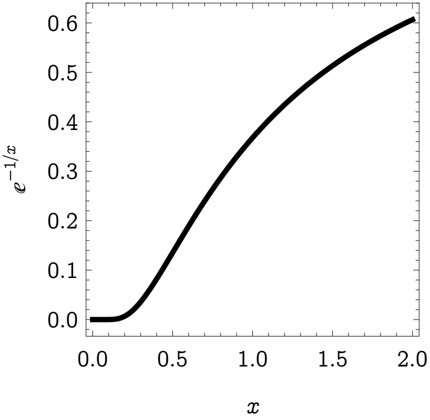


Im F has an essential singularity of the form $e^{-1/H^{\sigma/(1-\sigma)}}$.

Near critical point, $\sigma = 1 - \frac{1}{d}$, and

$$\text{Im}\, F \sim e^{-1/H^{d-1}}$$

Metastability & Complex Free Energy



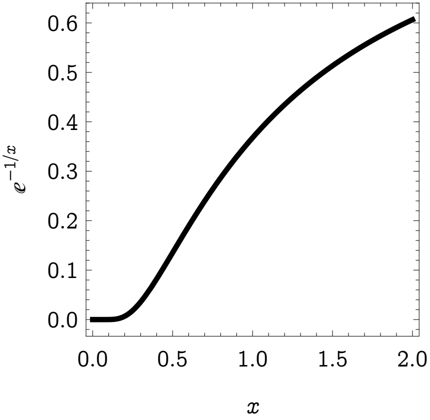
Im F has an essential singularity of the form $e^{-1/H^{\sigma/(1-\sigma)}}$.

Near critical point, $\sigma = 1 - \frac{1}{d}$, and

$$\text{Im}\, F \sim e^{-1/H^{d-1}}$$

Nonanalytic behavior is universal!

Metastability & Complex Free Energy



Im F has an essential singularity of the form $e^{-1/H^{\sigma/(1-\sigma)}}$.

Near critical point, $\sigma = 1 - \frac{1}{d}$, and

$$\text{Im } F \sim e^{-1/H^{d-1}}$$

Nonanalytic behavior is universal!

Can directly observe by measuring metastable decay rate, but what else?

Analytic Constraints on the Stable Free Energy

The Metastable Ising Model

Near the Ising critical point, $\sigma = 1 - \frac{1}{d}$ and

$$M = t^{\beta}\mathcal{M}(h/t^{\beta\delta}) \qquad \Sigma = t^{\mu}\mathcal{S}(h/t^{\beta\delta})$$

with $\mathcal{M}(0)$ and $\mathcal{S}(0)$ nonzero and finite.

The Metastable Ising Model

Near the Ising critical point, $\sigma = 1 - \frac{1}{d}$ and

$$M = t^{\beta}\mathcal{M}(h/t^{\beta\delta}) \qquad \Sigma = t^{\mu}\mathcal{S}(h/t^{\beta\delta})$$

with $\mathcal{M}(0)$ and $\mathcal{S}(0)$ nonzero and finite.

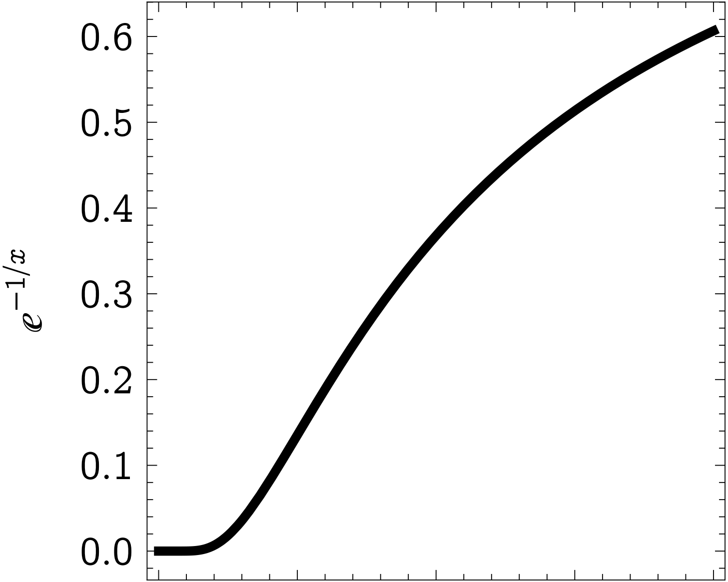
Therefore,

$$\Delta F_{\text{crit}} \sim \Sigma\left(\frac{MH}{\Sigma}\right)^{-(d-1)} = X^{-(d-1)}\mathcal{F}(X)$$

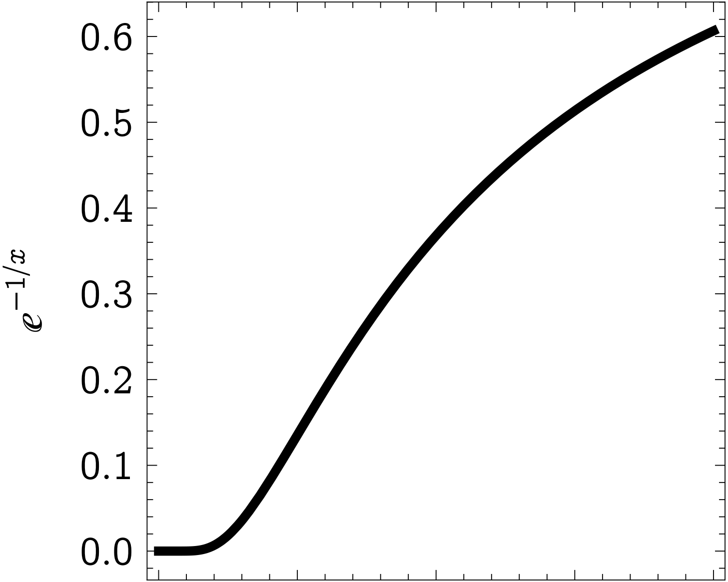
for $X = h/t^{\beta\delta}$, and

$$\operatorname{Im} F = t^{2-\alpha}\mathcal{I}(X)e^{-\beta/X^{(d-1)}}$$

The Essential Singularity



The Essential Singularity



The Essential Singularity

Analytic properties of the partition function imply that

$$F(X) = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\operatorname{Im} F(X')}{X' - X} \, \mathrm{d}X'$$

The Essential Singularity

Analytic properties of the partition function imply that

$$F(X) = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\operatorname{Im} F(X')}{X' - X} \, \mathrm{d}X'$$

Only predictive for high moments of F, or

$$f_n = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\operatorname{Im} F(X')}{X'^{n+1}} \, \mathrm{d}X'$$

for $F = \sum f_n X^n$.

The Essential Singularity

Results from field theory indicate that $\mathcal{I}(X) \propto X + \mathcal{O}(X^2)$ for $d = 2$, so that

$$\operatorname{Im} F = t^{2-\alpha}\left(AX + \mathcal{O}(X^2)\right) e^{-\beta/X^{(d-1)}}$$

The Essential Singularity

Results from field theory indicate that $\mathcal{I}(X) \propto X + \mathcal{O}(X^2)$ for $d = 2$, so that

$$\mathrm{Im}\, F = t^{2-\alpha}\left(AX + \mathcal{O}(X^2)\right) e^{-\beta/X^{(d-1)}}$$

The resulting moments for $n > 1$ are

$$f_n = At^{2-\alpha}\frac{\Gamma(n-1)}{\pi(-B)^{n-1}}$$

The Essential Singularity

Results from field theory indicate that $\mathcal{I}(X) \propto X + \mathcal{O}(X^2)$ for $d = 2$, so that

$$\operatorname{Im} F = t^{2-\alpha}\left(AX + \mathcal{O}(X^2)\right) e^{-\beta/X^{(d-1)}}$$

The resulting moments for $n > 1$ are

$$f_n = At^{2-\alpha} \frac{\Gamma(n-1)}{\pi(-B)^{n-1}}$$

Not a convergent series—the real part of F for $H > 0$ is also nonanalytic!

The Essential Singularity

In two dimensions, the Cauchy integral does not converge, normalize with λ,

$$F(X \mid \lambda) = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\operatorname{Im} F(X')}{X' - X} \frac{1}{1 + (\lambda X')^2} \, \mathrm{d}X'$$

The Essential Singularity

In two dimensions, the Cauchy integral does not converge, normalize with λ,

$$F(X \mid \lambda) = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\operatorname{Im} F(X')}{X' - X} \frac{1}{1 + (\lambda X')^2} \, \mathrm{d}X'$$

Exact result has form

$$F(X \mid \lambda) = \frac{A}{\pi} \frac{1}{1 + (\lambda X)^2} \Big[X e^{B/X} \operatorname{Ei}(-B/X) + \frac{1}{\lambda} \operatorname{Im}\big(e^{-i\lambda B}(i + \lambda X)(\pi + i \operatorname{Ei}(i\lambda B))\big) \Big]$$

The Essential Singularity

In two dimensions, the Cauchy integral does not converge, normalize with λ,

$$F(X \mid \lambda) = \frac{1}{\pi} \int_{-\infty}^{0} \frac{\operatorname{Im} F(X')}{X' - X} \frac{1}{1 + (\lambda X')^2} \, \mathrm{d}X'$$

Exact result has form

$$F(X \mid \lambda) = \frac{A}{\pi} \frac{1}{1 + (\lambda X)^2} \Big[X e^{B/X} \operatorname{Ei}(-B/X) + \frac{1}{\lambda} \operatorname{Im}\big(e^{-i\lambda B}(i + \lambda X)(\pi + i \operatorname{Ei}(i\lambda B))\big) \Big]$$

The Cauchy integral is only predictive for high moments.

The Essential Singularity

What about the susceptibility $\chi = \frac{\partial^2 F}{\partial h^2}$?

The Essential Singularity

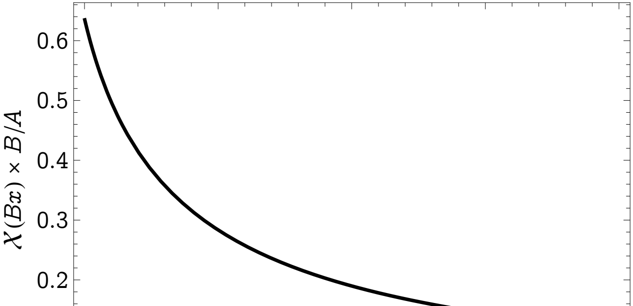
What about the susceptibility $\chi = \frac{\partial^2 F}{\partial h^2}$?

Has a well-defined limit as $\lambda \to 0$, simple functional form:

$$\chi = t^{-\gamma} \mathcal{X}(h/t^{\beta\delta})$$

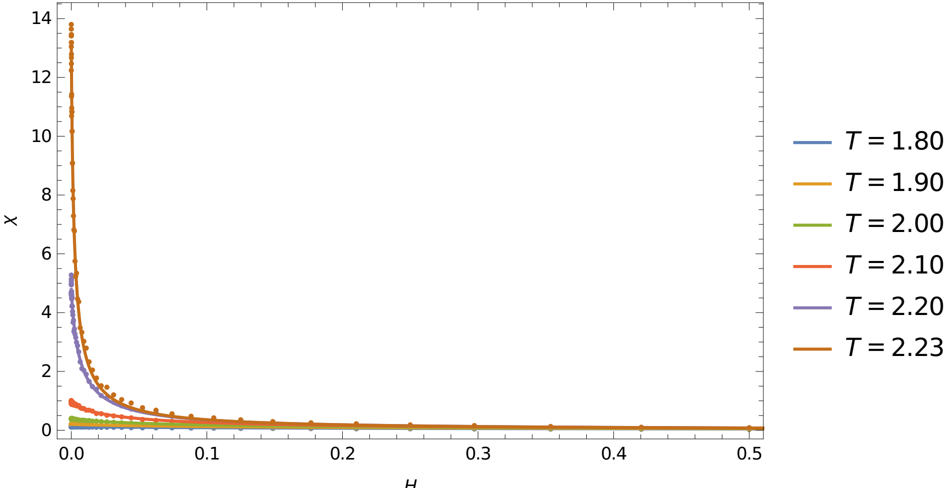
where the scaling function is

$$\mathcal{X}(X) = \frac{A}{\pi X^3}\left[(B - X)X + B^2 e^{B/X}\,\mathrm{Ei}(-B/X)\right]$$



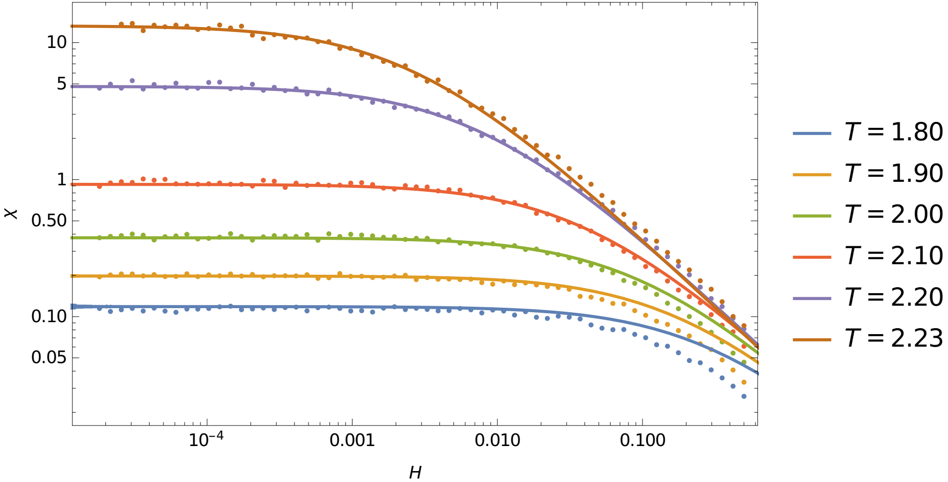
The Essential Singularity

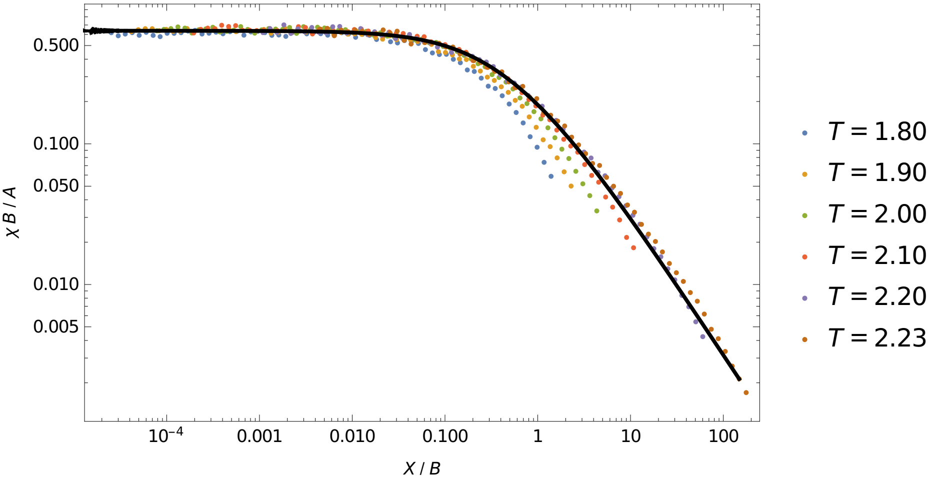
Two parameter fit to simulations yields $A = -0.0939(8)$, $B = 5.45(6)$, close agreement in limit of small t and H!



The Essential Singularity

Two parameter fit to simulations yields $A = -0.0939(8)$, $B = 5.45(6)$, close agreement in limit of small t and H!





0.500
0.100
0.050
0.010
0.005
10^{-4}
0.001
0.010
0.100
1
10
100
χ B / A
X / B
T = 1.80
T = 1.90
T = 2.00
T = 2.10
T = 2.20
T = 2.23

What's Next

We have an explicit form for a new component of the universal scaling forms near the Ising abrupt transition.

What's Next

We have an explicit form for a new component of the universal scaling forms near the Ising abrupt transition.

Hope to form a parametric scaling variables that include this, correct leading analytic corrections to scaling, and (maybe?) extend smoothly through the metastable region.

What’s Next

We have an explicit form for a new component of the universal scaling forms near the Ising abrupt transition.

Hope to form a parametric scaling variables that include this, correct leading analytic corrections to scaling, and (maybe?) extend smoothly through the metastable region.

Remain on the lookout for other universal properties to incorporate.

Questions?