The density of states method applied to the Ising model with an *imaginary* magnetic field

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Ising model ?

Ising model in external field: $Z = \sum_{\{\sigma\}} \exp(+\beta \sum_{<ij>} \sigma_i \sigma_j) \exp(h \sum_i \sigma_i)$

What happens for an ***imaginary*** external field $h = ih_I$??

- sign problem: weight factor $\exp(ih_I M)$, where $M \equiv \sum_i \sigma_i$
- Z may vanish $\longrightarrow$ new thermodynamic singularities

Combination of:
- sign problem benchmark
- interesting critical phenomena
- hardly studied numerically

(Seung-Yeon Kim)

$$Z = \sum_{\{\sigma\}} \exp(+\beta \sum_{<ij>} \sigma_i \sigma_j) \ \exp(h \sum_i \sigma_i)$$

$$Z \propto \text{Polynomial}(x \equiv \exp(\beta), y \equiv \exp(h))$$

- $Z = 0$ in complex-x plane: *Fisher zeroes*
- $Z = 0$ in complex-y plane: *Lee-Yang zeroes*

Lee & Yang (1952):

- Lee-Yang zeroes on the unit circle, ie. h pure imaginary (or 0)

- above T_c, zeroes accumulate along "*edge singularity*" $h_I^c(T)$

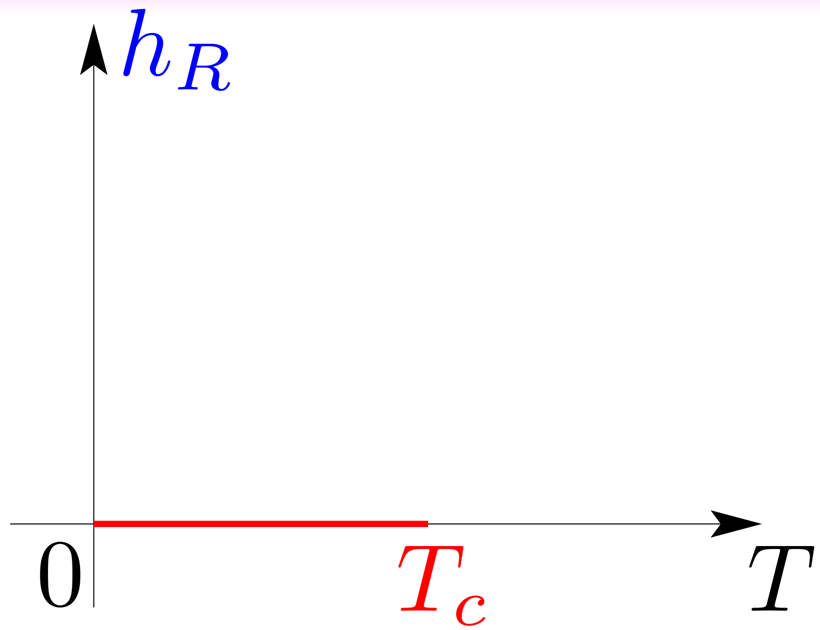
Fisher (1978):

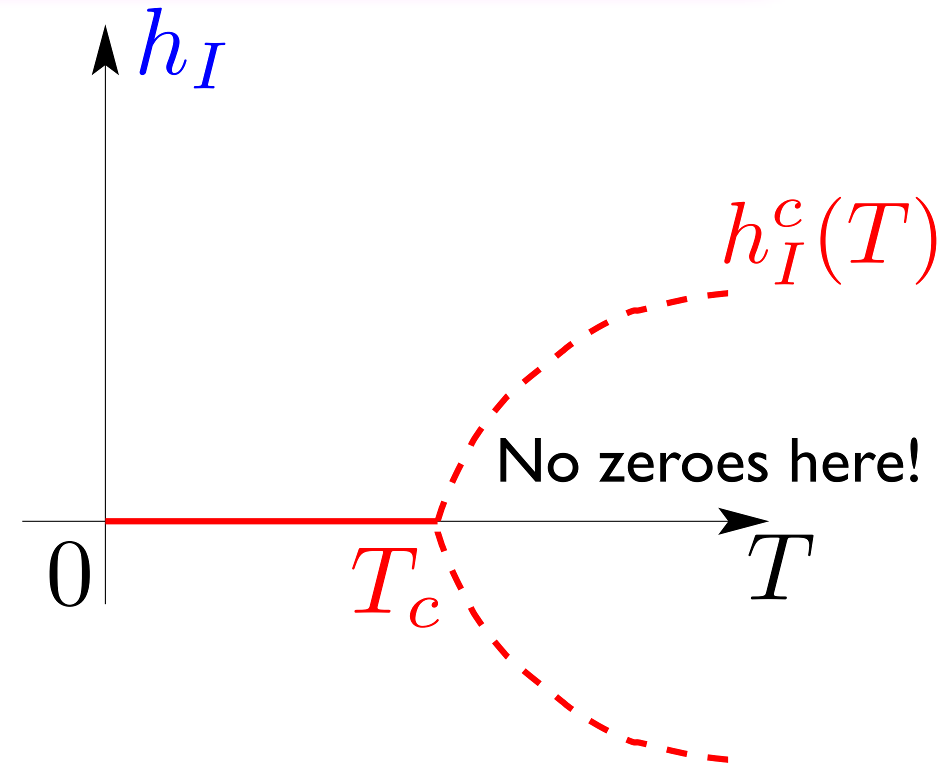
Edge singularity can be viewed as 2nd-order phase transition (interaction $i\phi^3$)

Ising phase diagram: similarity with QCD

Ising:

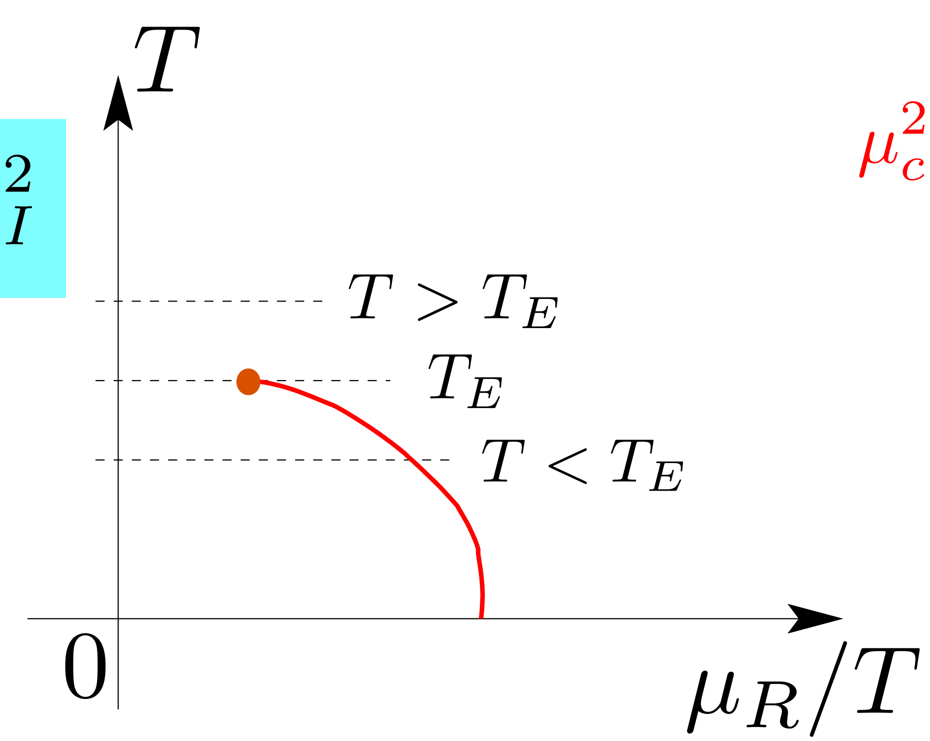
$$h = h_R + i h_I$$

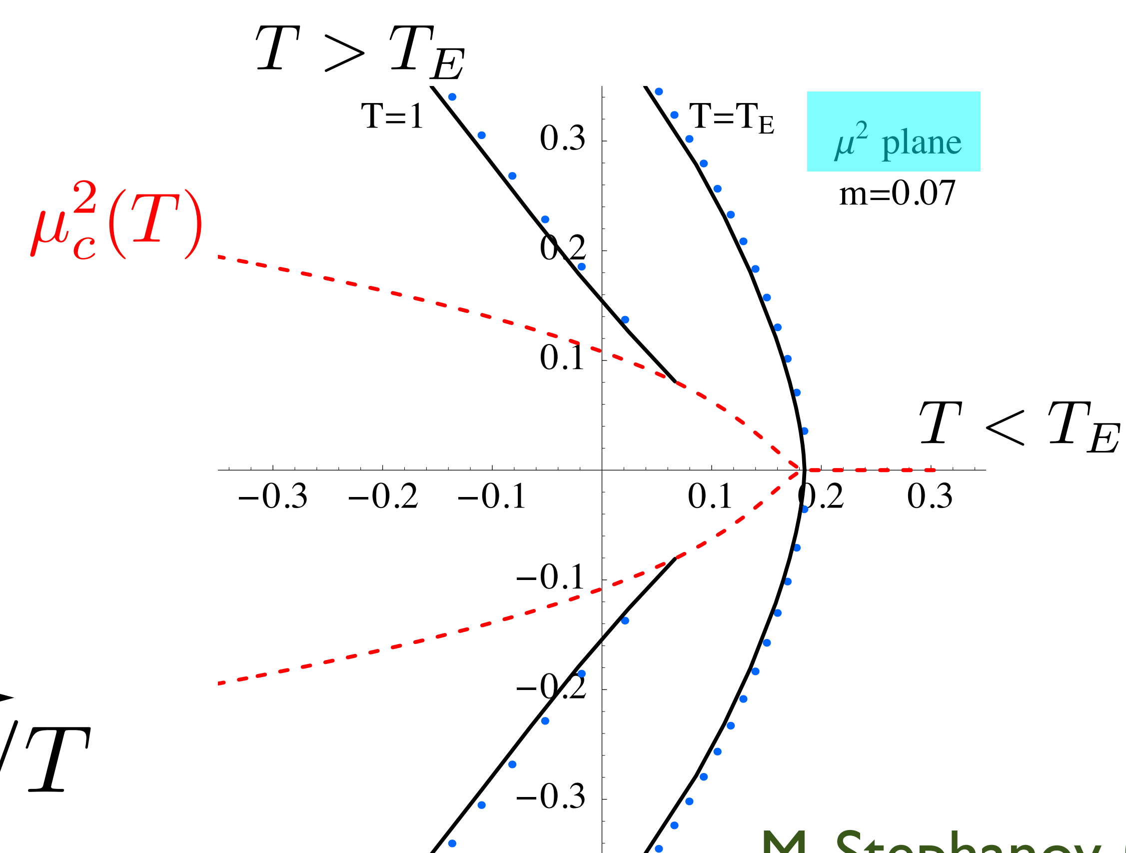




QCD:

$$\mu^2 = \mu_R^2 + i\mu_I^2$$

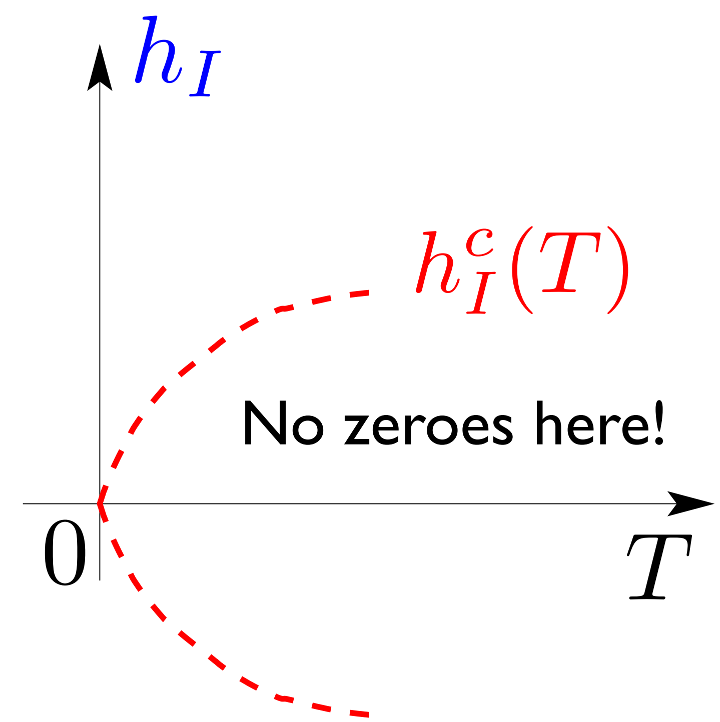




M. Stephanov, 0603014

Ising model in $d = 1, 2, 3$

- $d = 1$ always disordered: $T_c = 0$
  - Analytically solvable
  - Severe sign pb (Z vanishes!)



Good benchmark pb

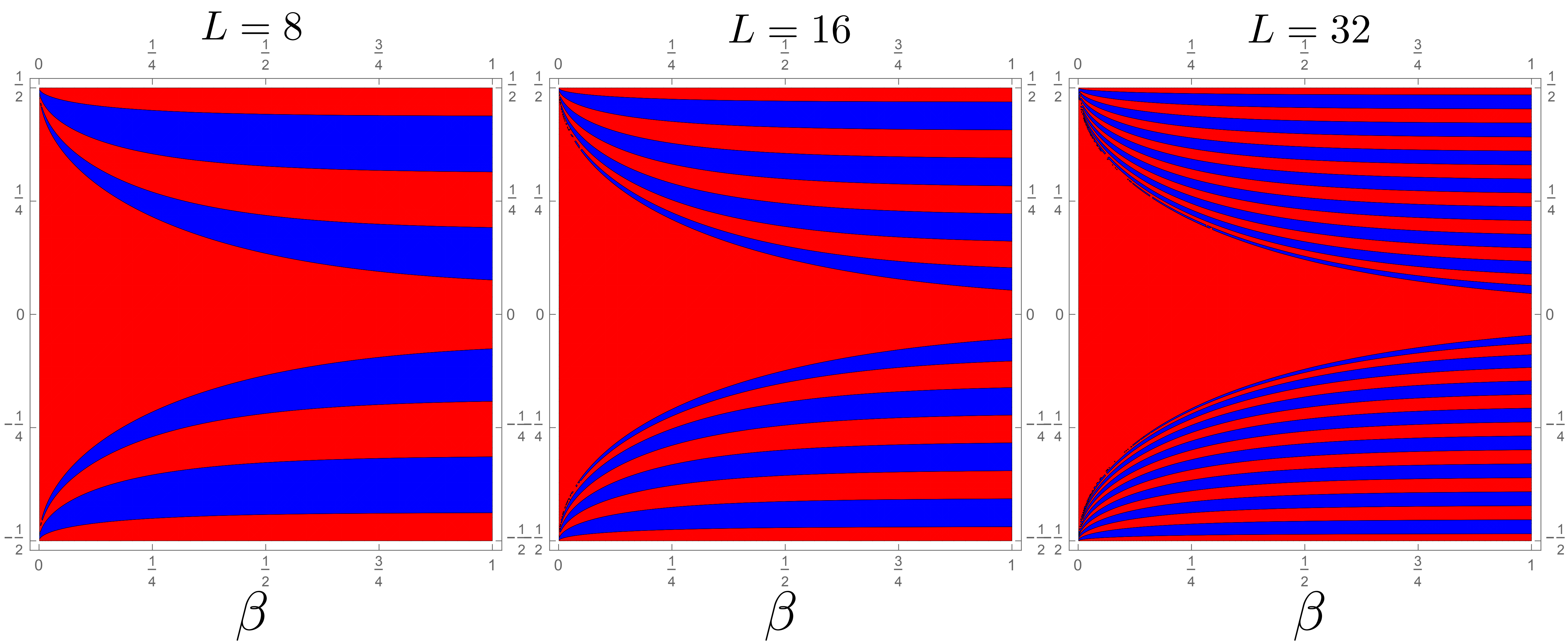
- $d = 2$:
  - Critical exponents known (CFT) -- different for $T \gtrless T_c$
  - Almost no numerical work (Seung-Yeon Kim, 1998-2006)

- $d = 3$: just starting (M. Stephanov et al, 1605.06039)

Solving the Ising model in $d = 1$: $Z = \sum_{\{\sigma\}} e^{+\beta \sum_{\langle ij \rangle} \sigma_i \sigma_j} \; e^{i h_I \sum_i \sigma_i}$

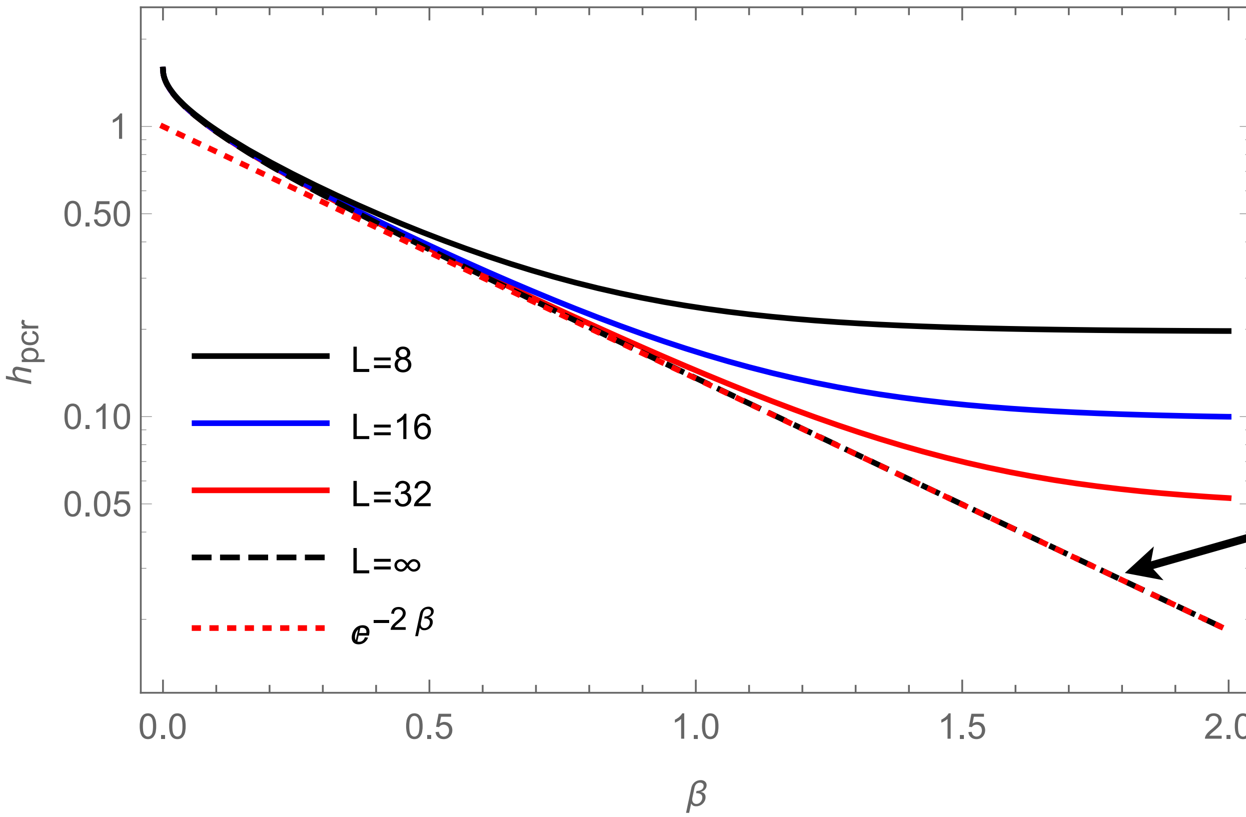
Diagonalize transfer matrix: $T = \begin{pmatrix} e^{+\beta + i h_I} & e^{-\beta} \\ e^{-\beta} & e^{+\beta - i h_I} \end{pmatrix}$

$$Z = \lambda_1^L + \lambda_2^L$$

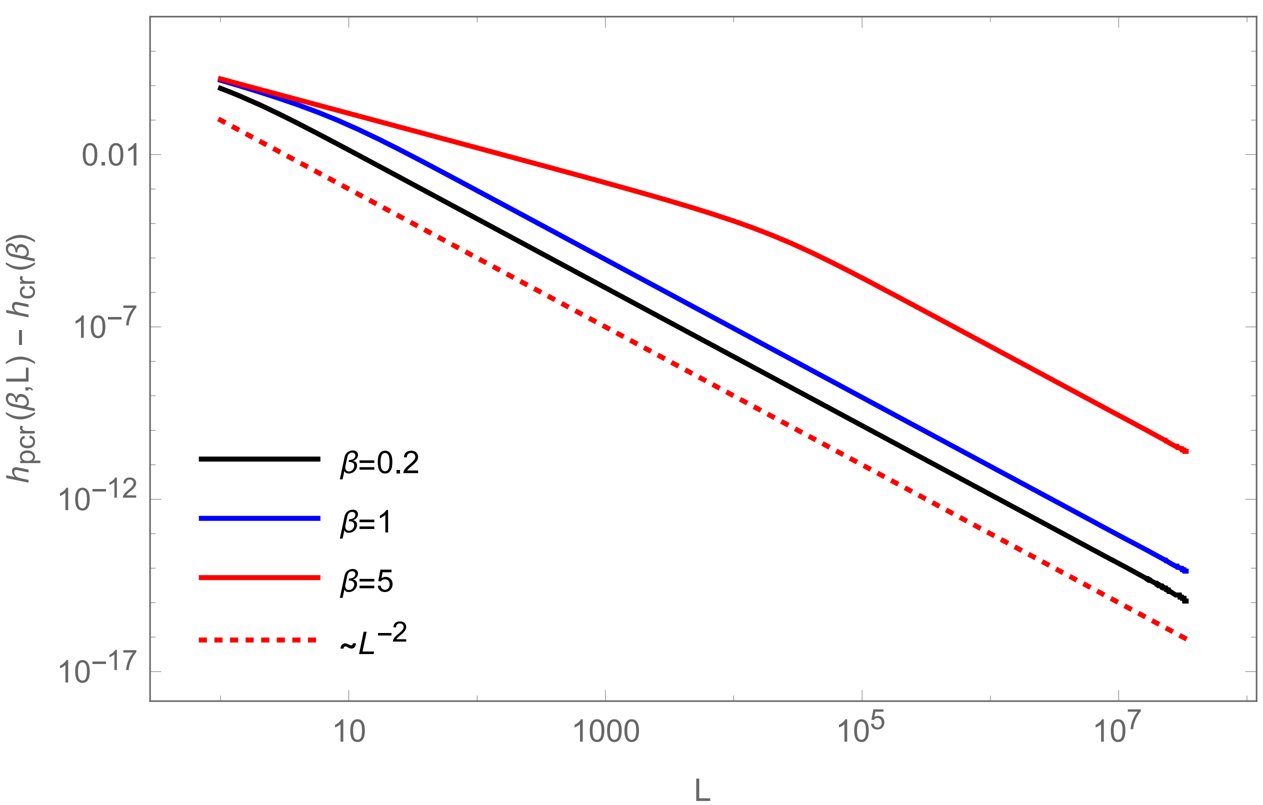


$Z(\beta, h_I/\pi)$ positive (red), negative (blue)

Finite-size effects



For $L = \infty, \quad h_{\text{crit}} \sim \exp(-2\beta)$

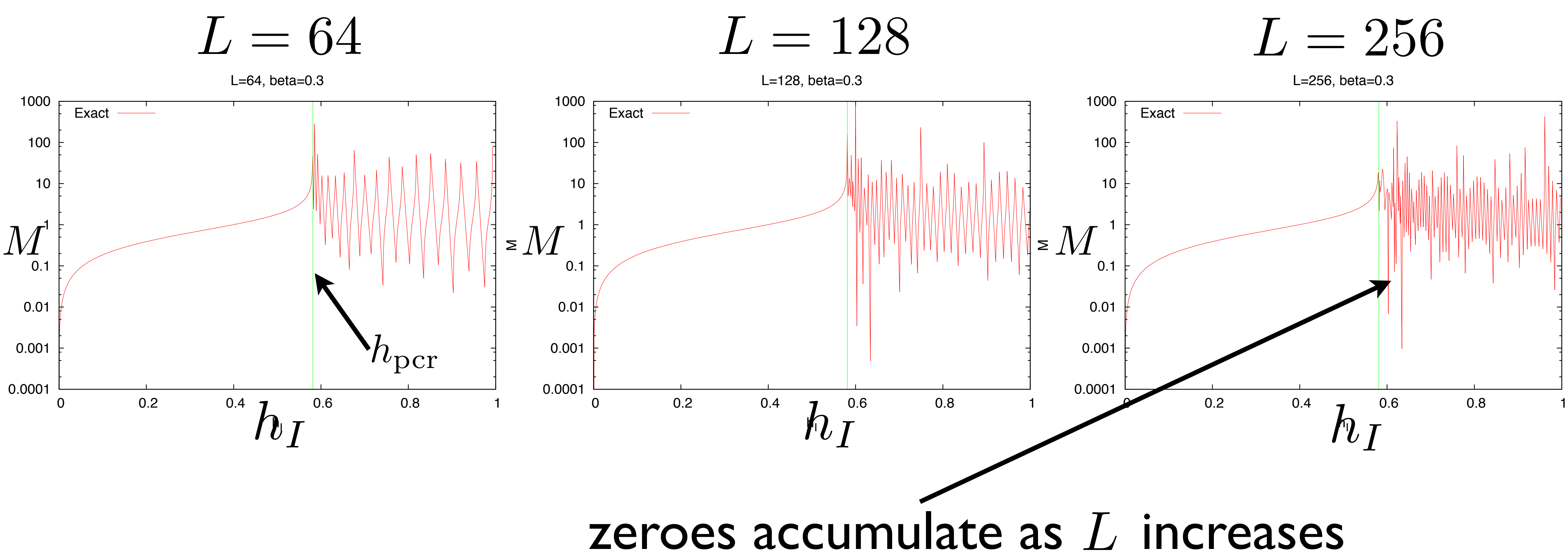


$$h_{\text{pcr}}(L) - h_{\text{crit}} \propto L^{-2}$$

Magnetization

$M(\beta, h_I) \equiv \langle \sigma \rangle_{\beta, h_I}$ - is *imaginary*

- *diverges* when $h_I \to h_{\rm pcr}(\beta)$ since $Z \to 0$



Monte-Carlo: density of states

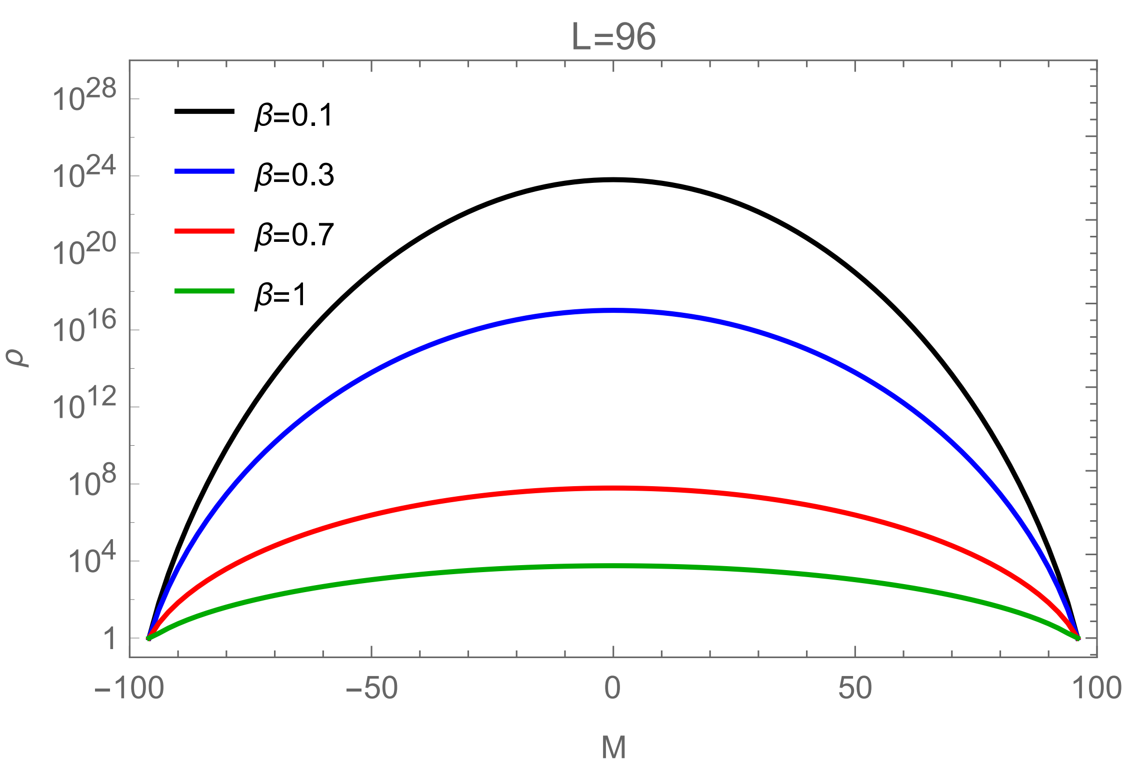
"stratified sampling",
Hammersley & Handscomb, 1964

QCD: Gocksch, 1988

$$Z = \sum_{\{\sigma\}} e^{+\beta \sum_{\langle ij \rangle} \sigma_i \sigma_j} \; e^{i h_I \sum_i \sigma_i} = \sum_{M=-V}^{+V} \left[\sum_{\{\sigma\}} \delta(M - \sum_i \sigma_i) \; e^{+\beta \sum_{\langle ij \rangle} \sigma_i \sigma_j} \right] e^{i h_I M}$$

$$= \sum_{M=-V}^{+V} \rho(\mathbf{M}) \; e^{i h_I M}$$

- Sample $\rho(M)/\rho(M-2), M = 2, 4, .., L$ by independent MC



- Relative accuracy on $\rho(M)$

  $\sim$ *independent of* M

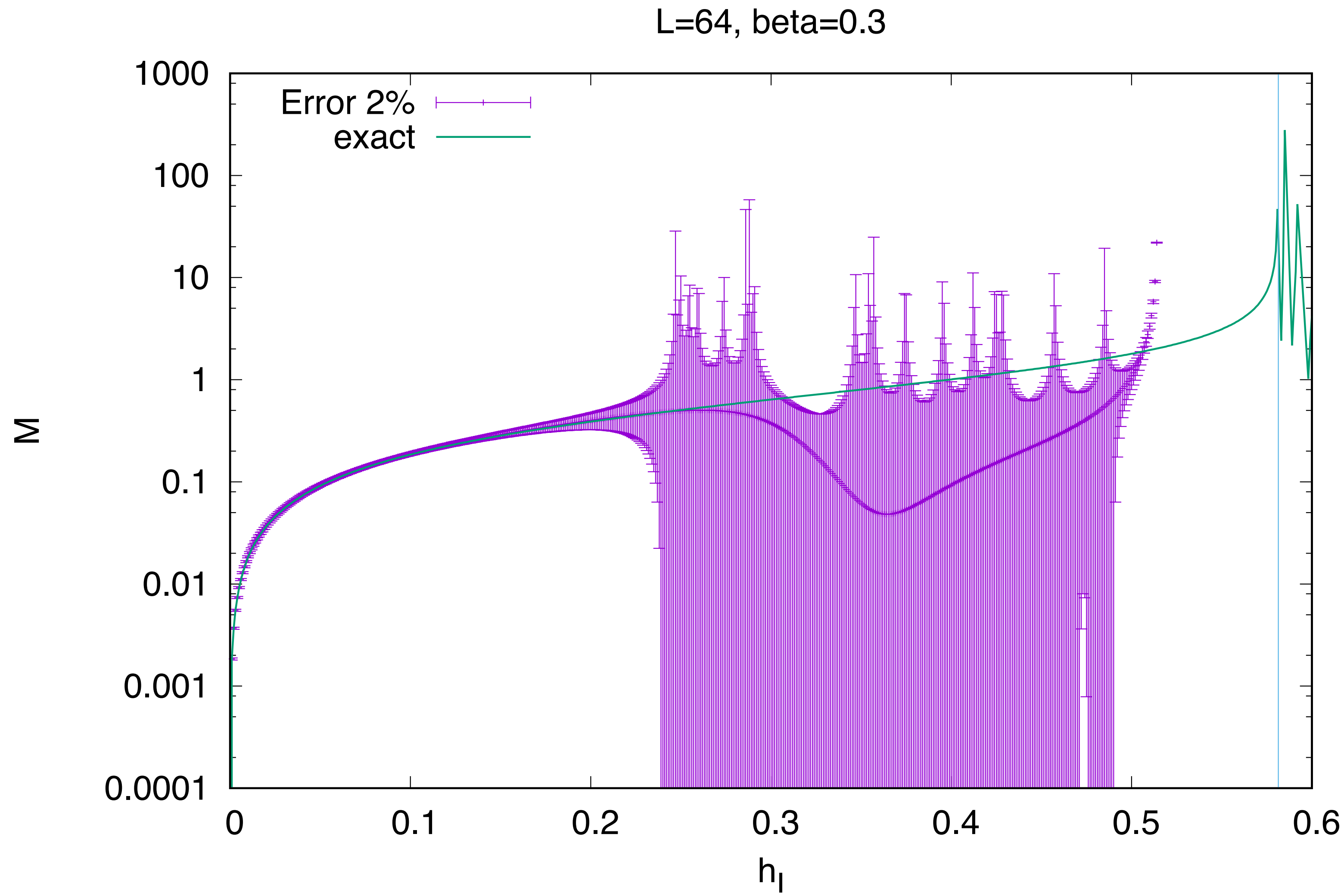
  $\rightarrow$ "Exponential error suppression"

  "Overlap pb" solved

- $\rho(M = \pm L) = 1 \rightarrow Z$ normalized

- *Fourier transform* $\rho(M)$ to obtain $Z(h_I) \Rightarrow$ **Sign Problem!**

How difficult is it to measure the magnetization $M(h_I)$?



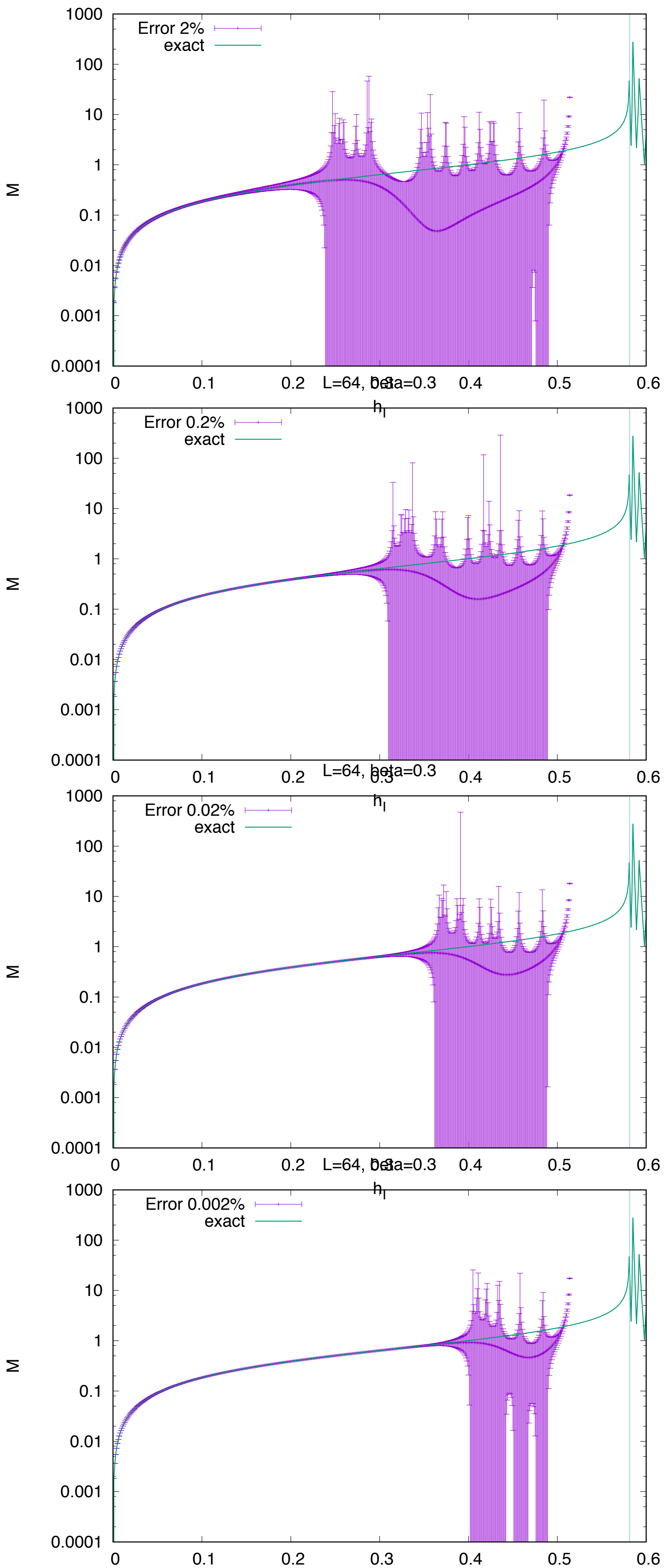
- Computer effort required to increase accessible range of h_I ?

  (fixed volume)

- Computer effort required to increase accessible volume ?

  (fixed h_I)

$M(h_I)$: $\beta = 0.3, L = 64$



Work

1

10^2

10^4

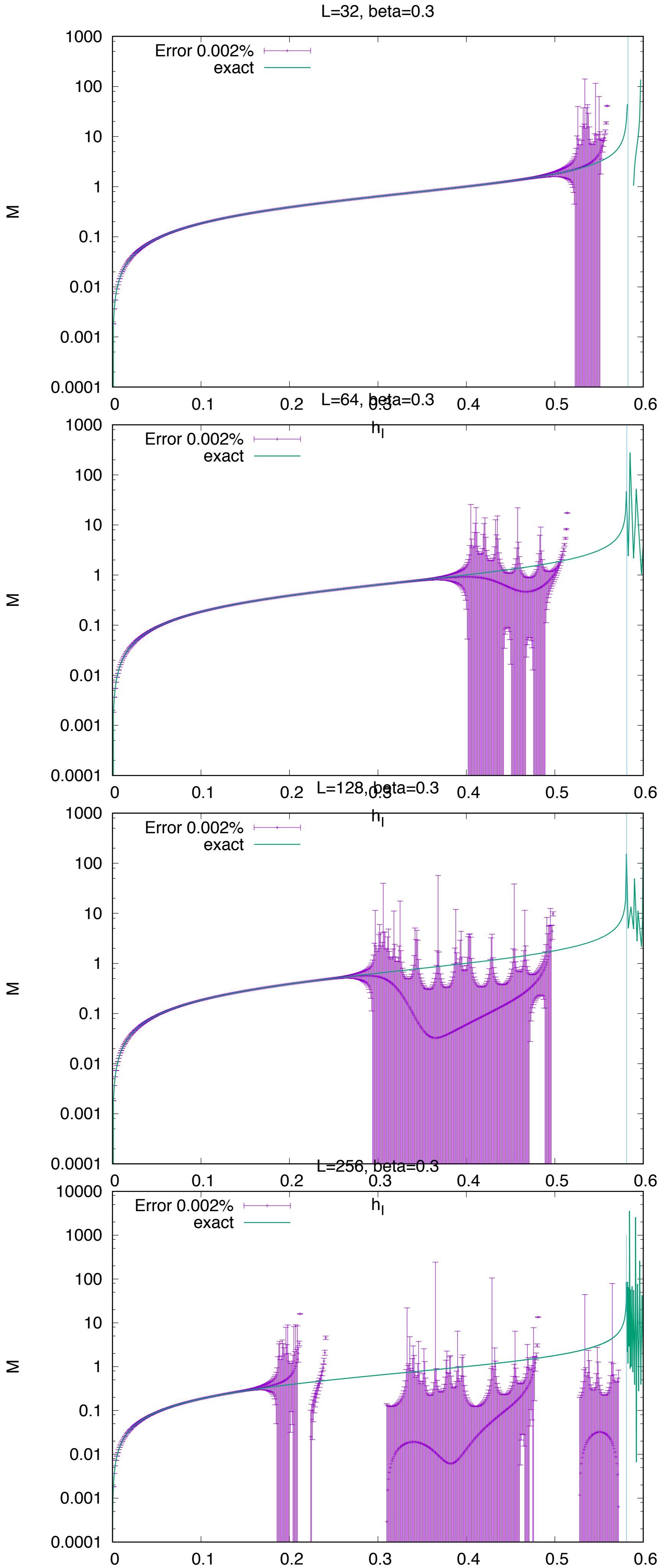
10^6

Increasing the statistics

Each factor of 100 in stats enlarges the range of h_I by a ~ constant amount

Exponential complexity

$\sim \exp(h_I)$



$L = 32$

$L = 64$

$L = 128$

$L = 256$

All at same temperature,
same statistics

$$M(h_I)\text{: } \beta = 0.3,\ \frac{\delta\rho}{\rho} = 0.002\%$$

Increasing the volume

Each factor of 2 in volume shrinks the range of h_I by a ~ constant amount

Exponential complexity

$$\sim \exp(\text{Volume})$$

Trying to overcome exponential complexity: idea 1

- Use different ("dual") variables: $Z = \sum_{\{\sigma\}} \exp(+\beta \sum_{<ij>} \sigma_i \sigma_j) \; \exp(h \sum_i \sigma_i)$

$$\exp(\beta \sigma_i \sigma_j) = \cosh\beta \sum_{k=0,1} (\tanh\beta \; \sigma_i \sigma_j)^k \qquad \exp(i h_I \sigma_i) = \cos(h_I) \sum_{m=0,1} (\mathbf{i} \tan(h_I) \sigma_i)^m$$

monomers: $m=0,1$

$$Z = (\cosh\beta)^{Vd} (\cos h_I)^V \sum_{\{k,m\}} (\tanh\beta)^{\sum k} (\mathbf{i} \tan h_I)^{\sum m}$$

Constraint: $m_x + \sum_\mu (k_{x,+\hat{\mu}} + k_{x-\hat{\mu},\hat{\mu}}) = 0 \mod 2 \; \forall x$

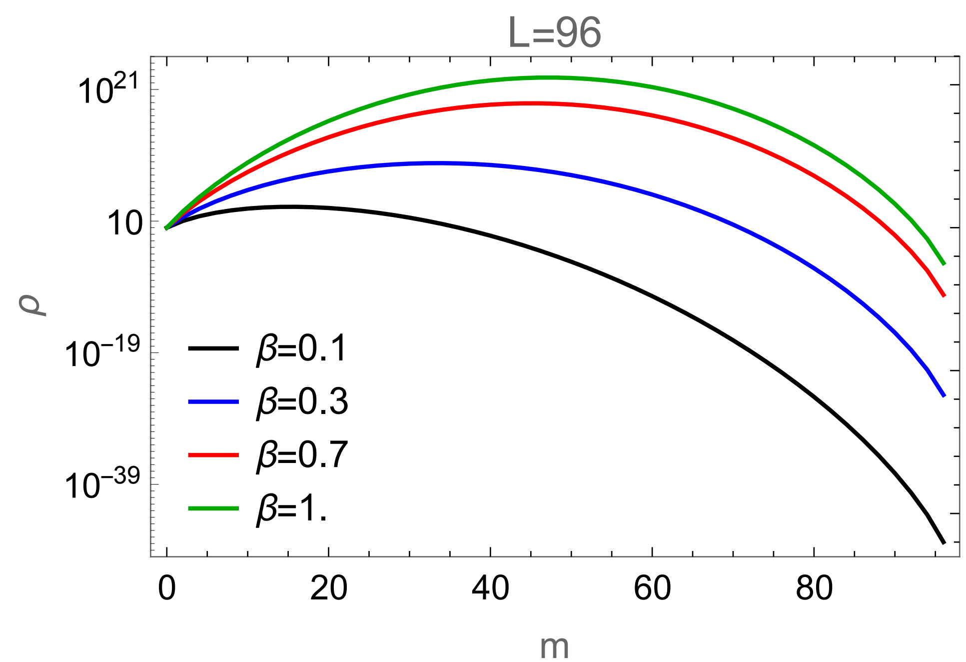
$$Z \sim \sum_{m=0}^{V} \left[\sum_{\{k\}} \delta(m - \sum_i m_i) \; (\tanh\beta)^{\sum k} \right] (\mathbf{i} \tan h_I)^m$$

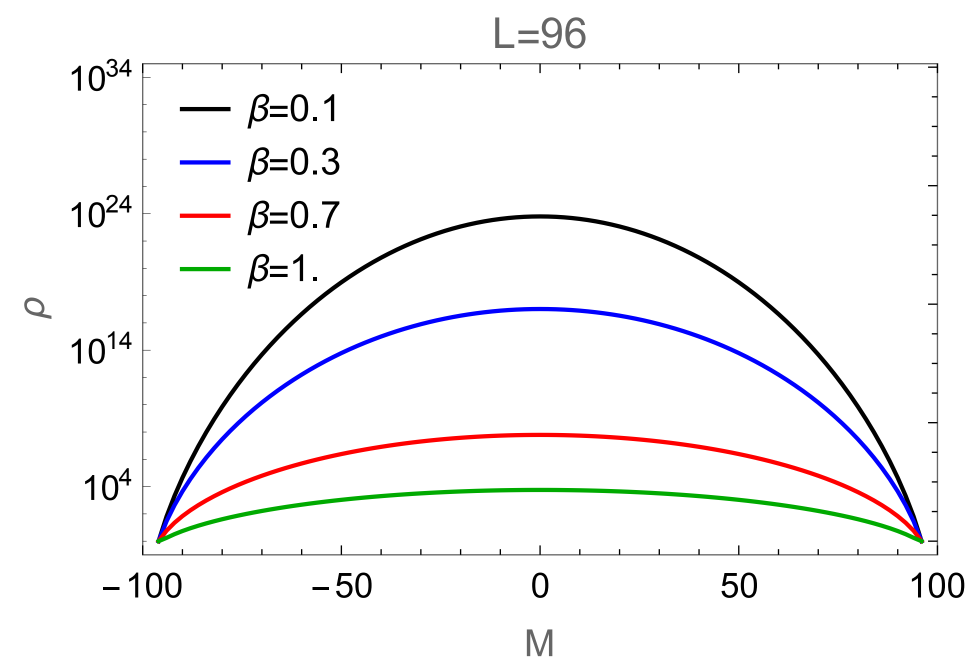
$$= \sum_{m=0}^{V} \rho(\mathbf{m}) \; (\mathbf{i} \tan h_I)^m$$

Sample *monomer sectors* with worm + Wang-Landau algorithm

Dual variables: $Z = \sum_{m=0}^{V} \rho(\mathbf{m})\ (\mathbf{i} \tan h_I)^m$

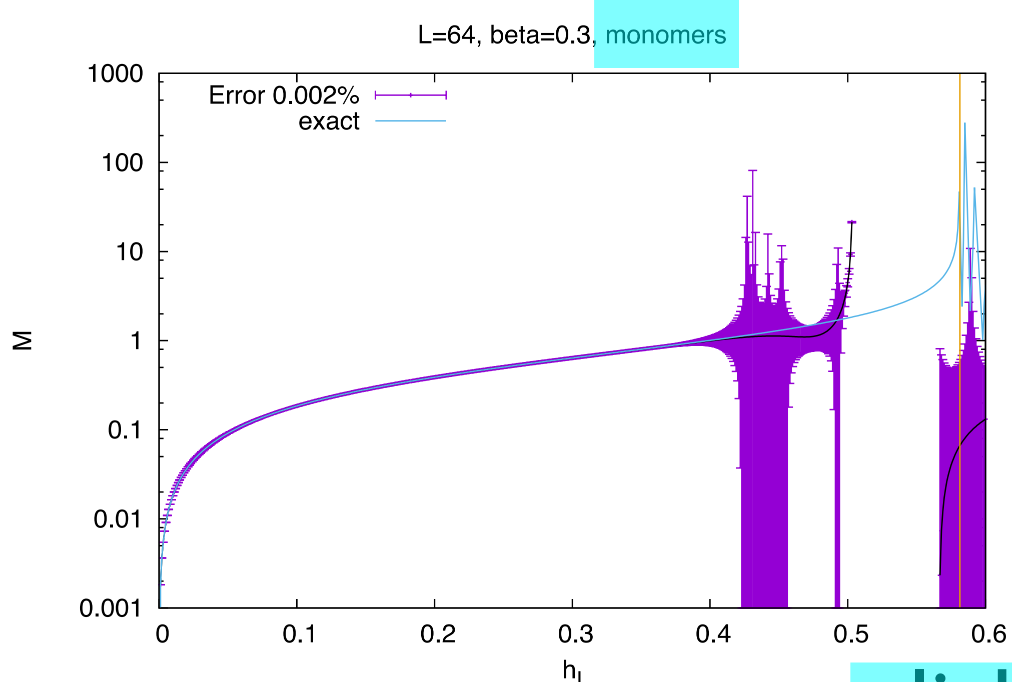
- Compare density of states: monomer or magnetization sectors



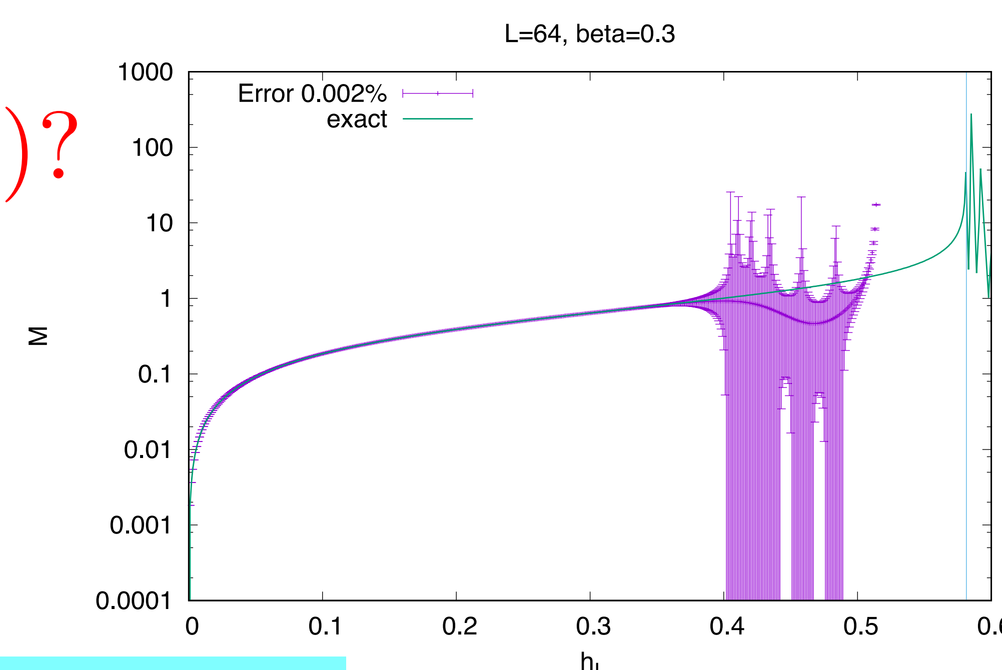


monomers: multiply by $(\mathbf{i} \tan h_I)^m$

magnetization: multiply by $\cos(h_I M)$



$M(h_I)$?



slight improvement

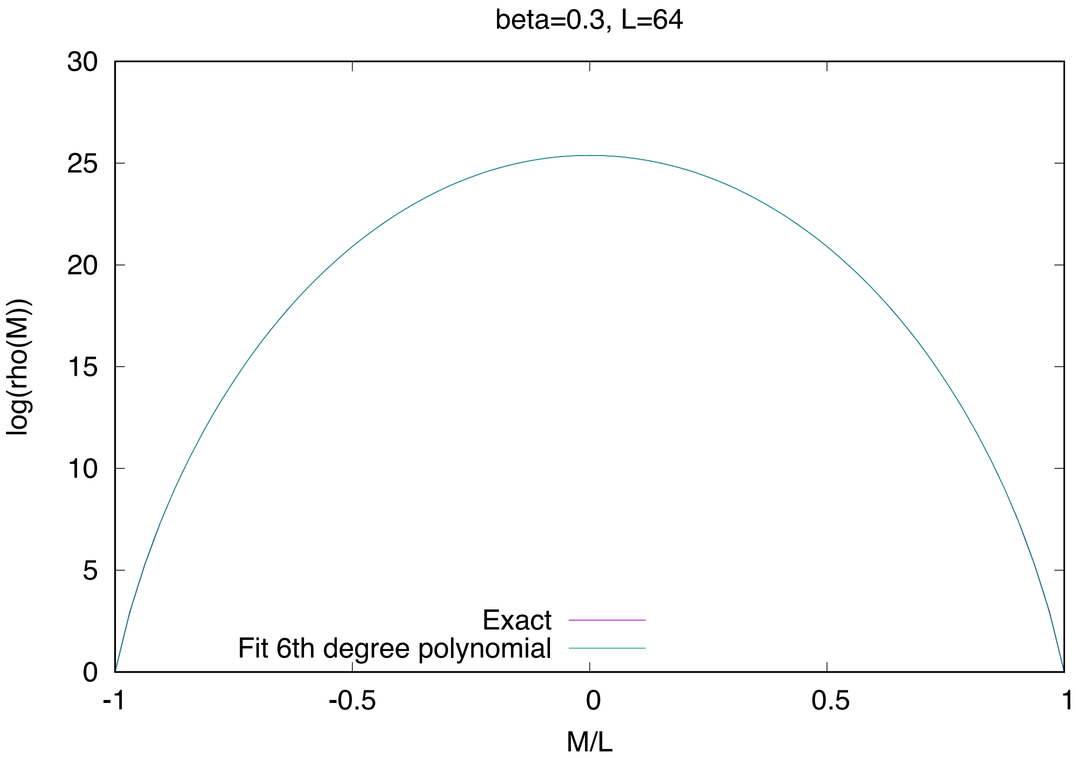
Trying to overcome exponential complexity: idea II

- Smoothen Monte-Carlo data to decrease statistical noise:

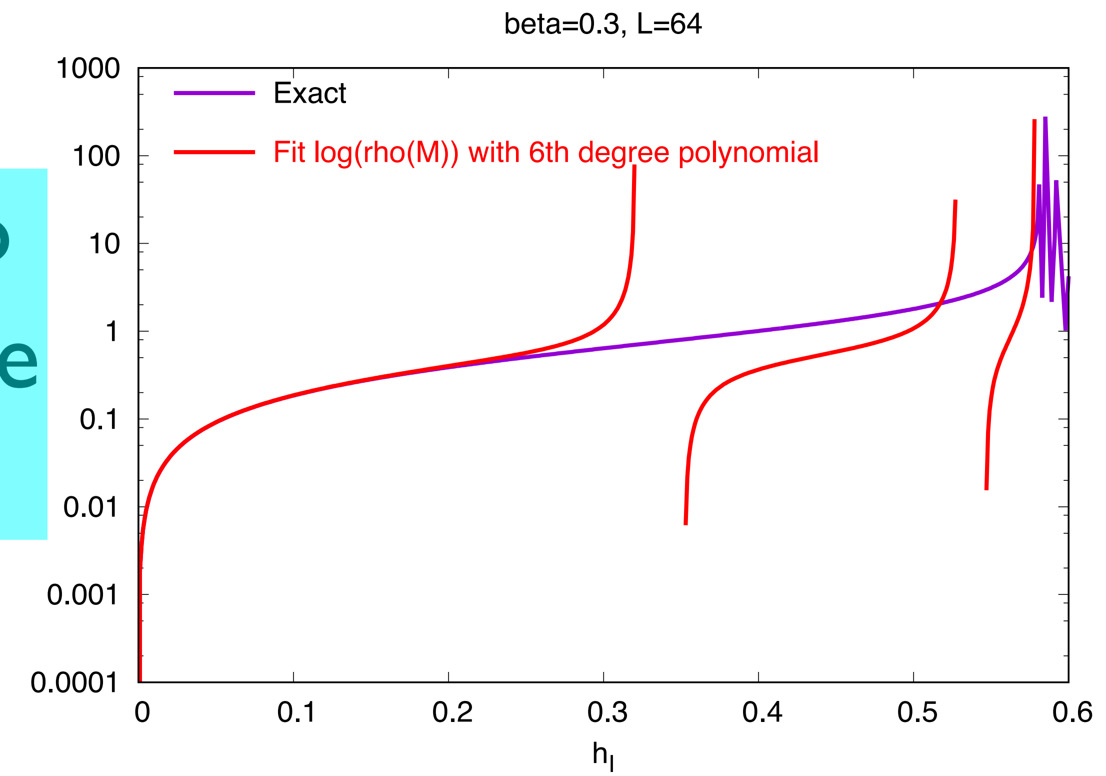
Fit $\log(\rho(M))$ or $\rho(M)/\rho(M-2)$ with *clever* ansatz

cf. "compressed sensing"

A) Fit $\log(\rho(M))$ with 6th degree polynomial

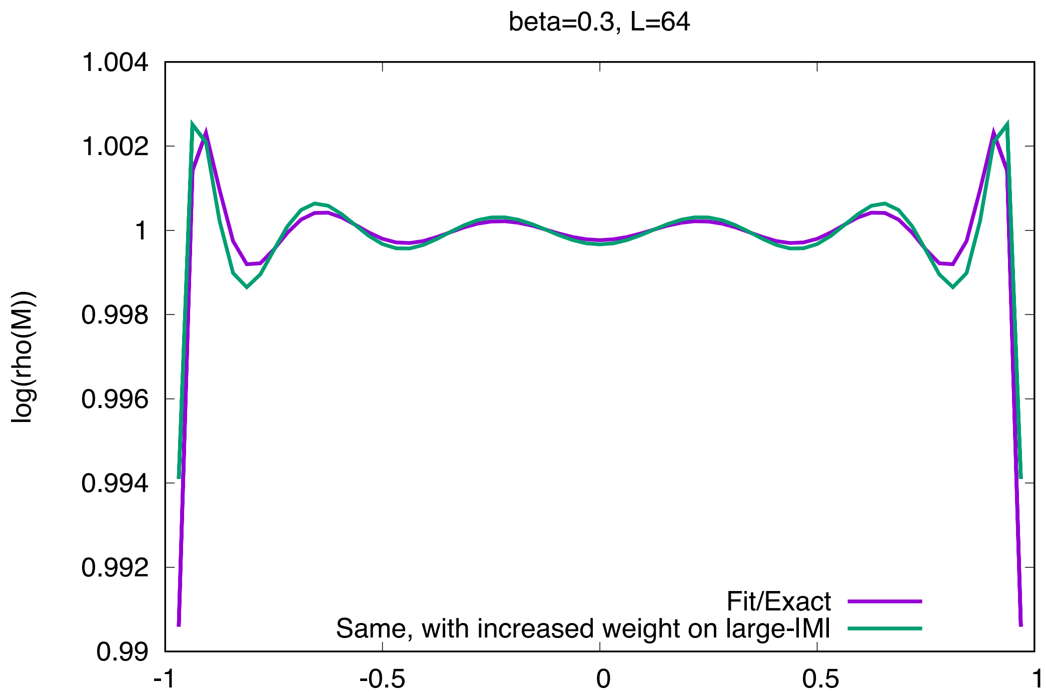


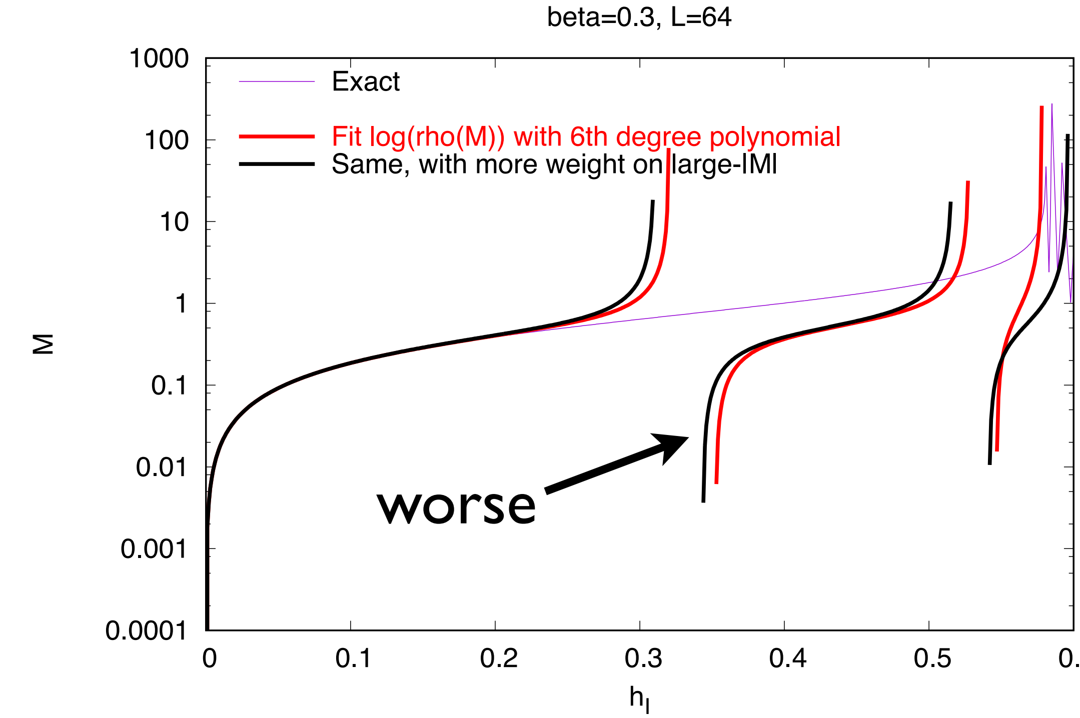
perfect fit to the naked eye *but*



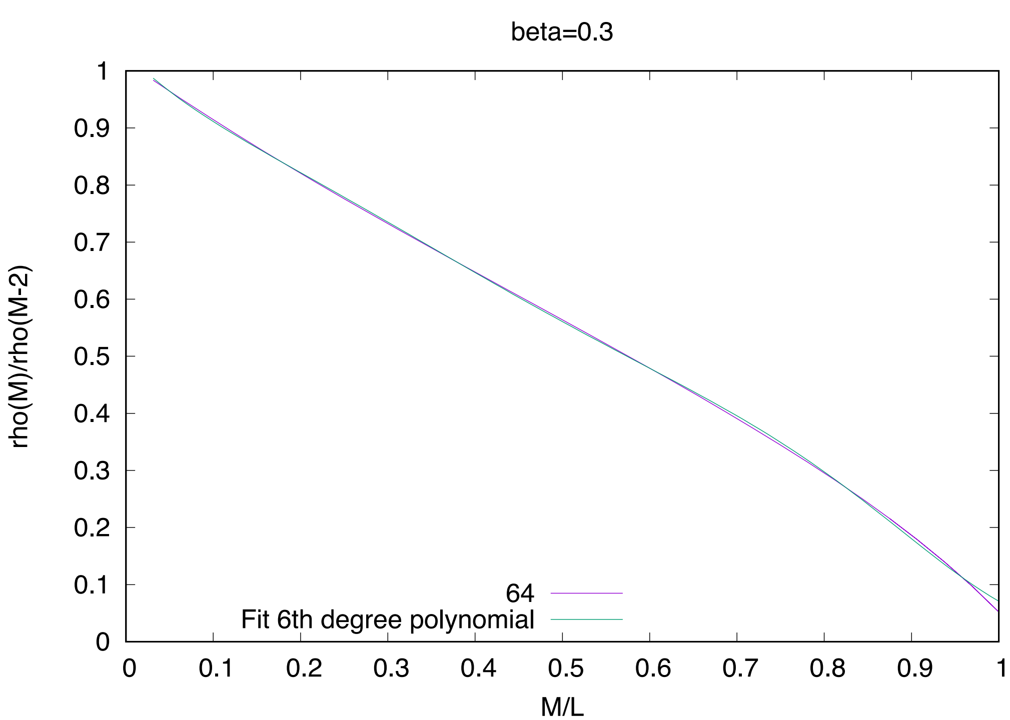
Trying to overcome exponential complexity: idea II

- Origin of systematic error: extreme magnetization sectors?





B) Fit $\rho(M)/\rho(M-2)$ with 6th degree polynomial



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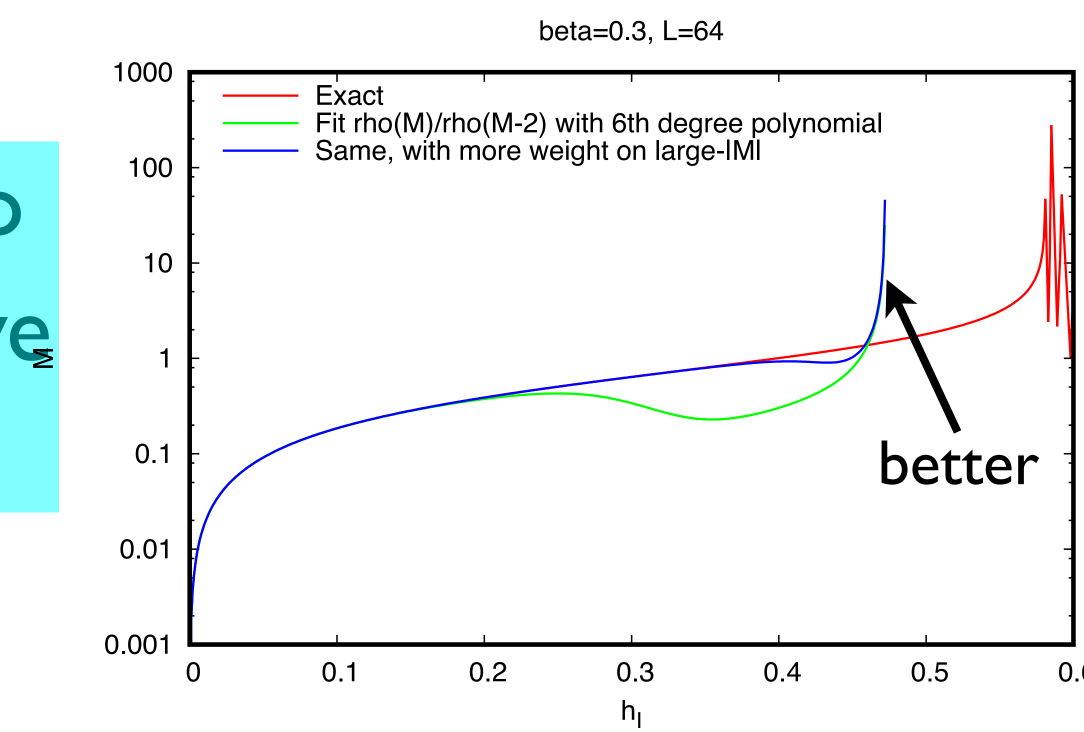

Conclusions

- Ising model with imaginary h: interesting, severe sign pb
- Density-of-states method (Gocksch 1988 for $\mu \neq 0$ QCD):

  - gives "exponential error suppression", i.e.

    near-constant relative accuracy $\delta\rho/\rho$, even for rare states

  - does not address exponential complexity issue, i.e.

    CPU effort $\propto \exp(\#\mathrm{d.o.f.})$

- *Fitting* the density of states introduces a bias
- Crux of the problem: $M(h_I) \longleftrightarrow \rho(M)$ by Fourier transf.

  Same as in QCD: $Z_{\mathbf{C}}(Q) \longleftrightarrow Z_{\mathbf{GC}}(\mu = i\mu_I)$