Tricriticality in the triangular Blume-Capel ferromagnet

D. Mataragkas, *A. Vasilopoulos*, N. G. Fytas, Dong-Hee Kim

https://arxiv.org/abs/2411.11689

University of Essex

광주과학기술원 GIST Gwangju Institute of Science and Technology

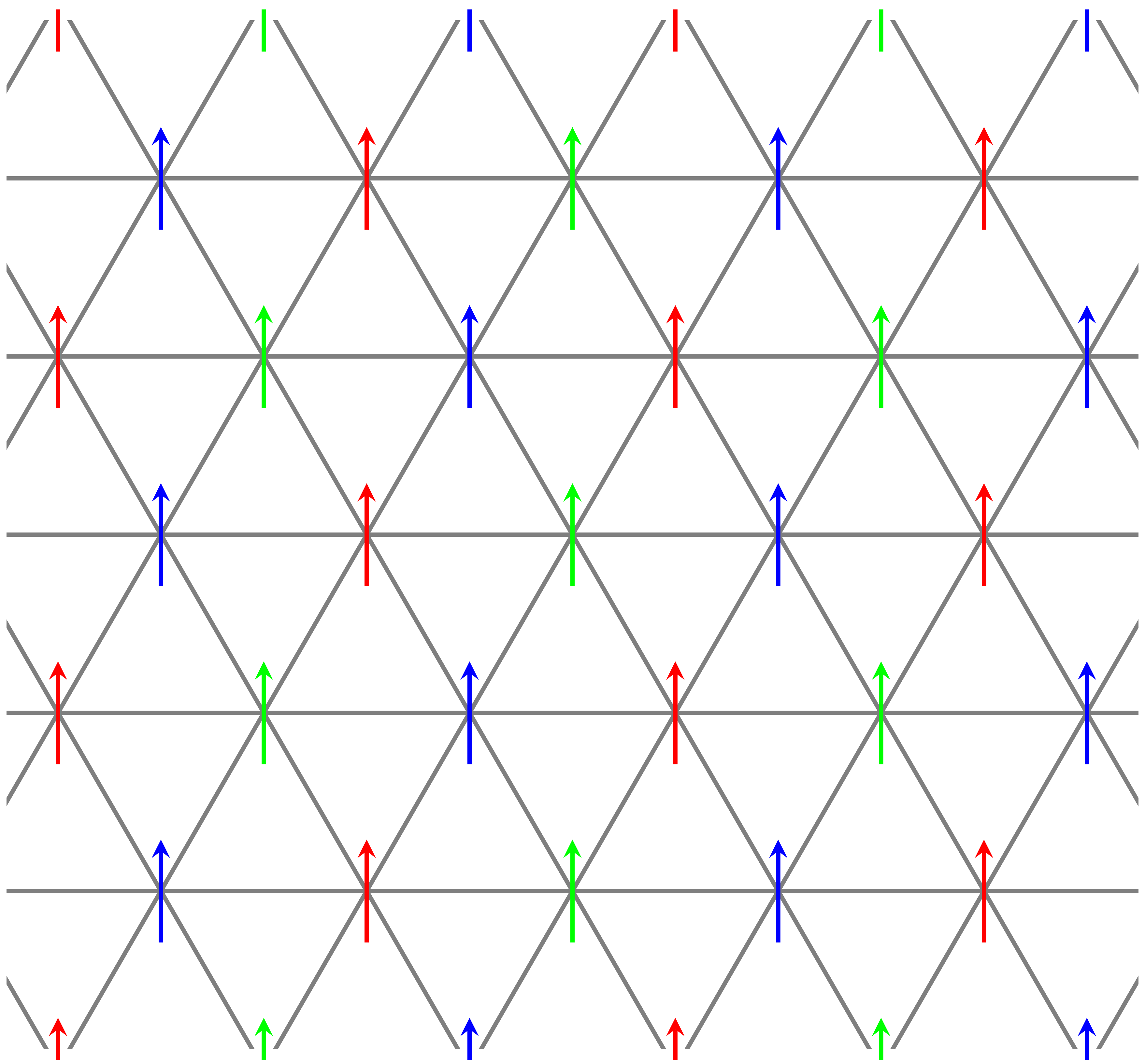
CompPhys24

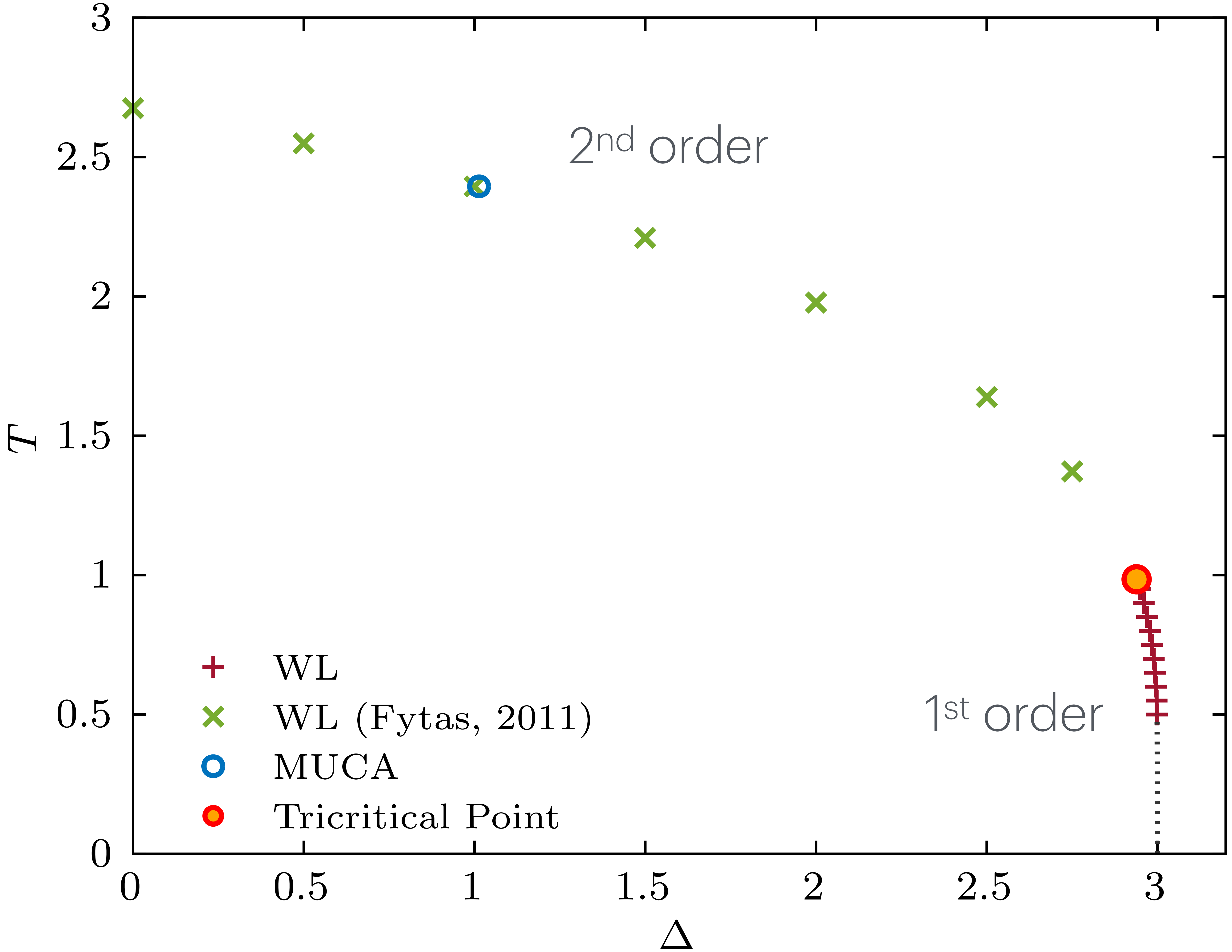
28/11/2024

Triangular Blume-Capel model

$$H = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j + \Delta \sum_i \sigma_i^2$$

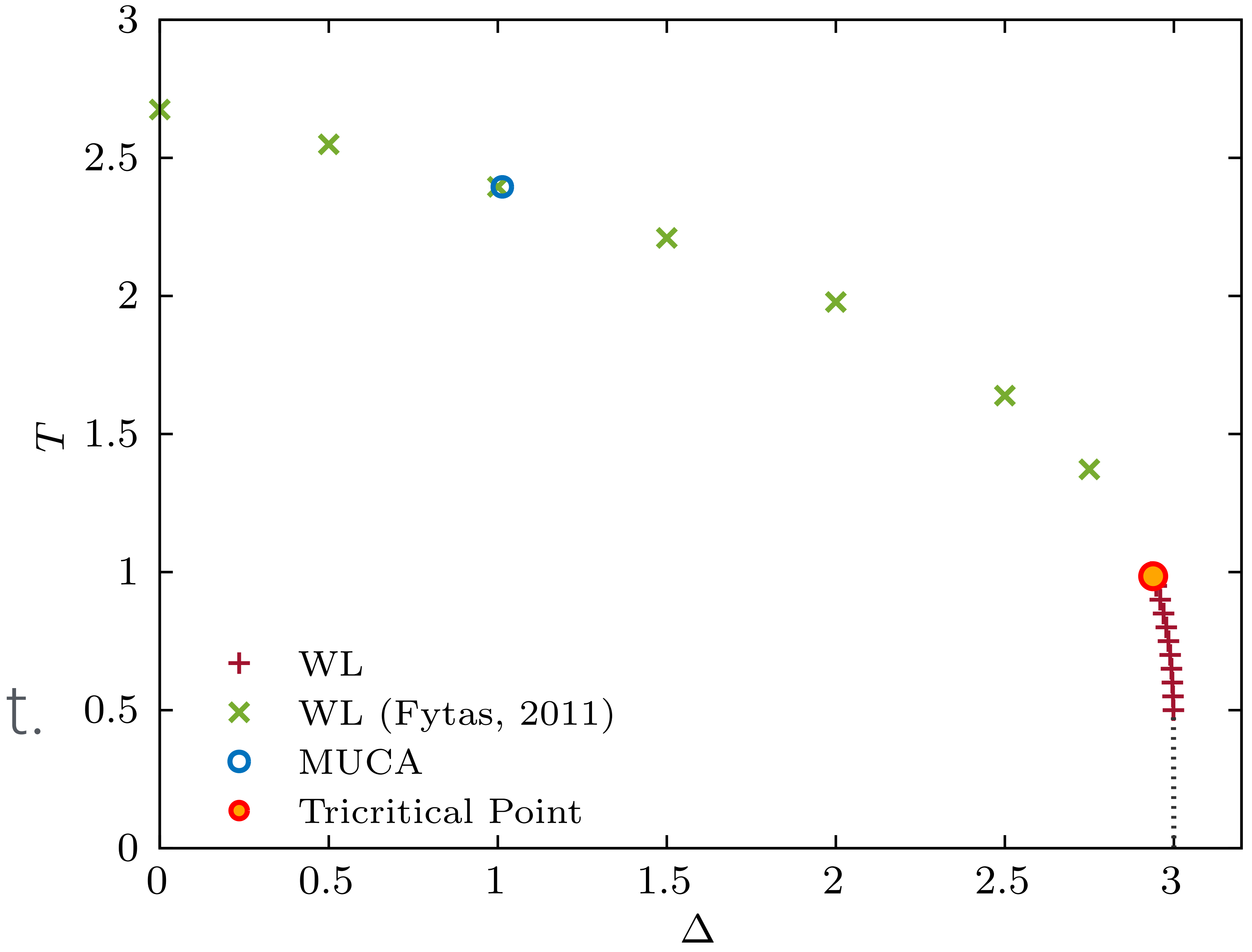
$$H = E_J + \Delta E_\Delta$$





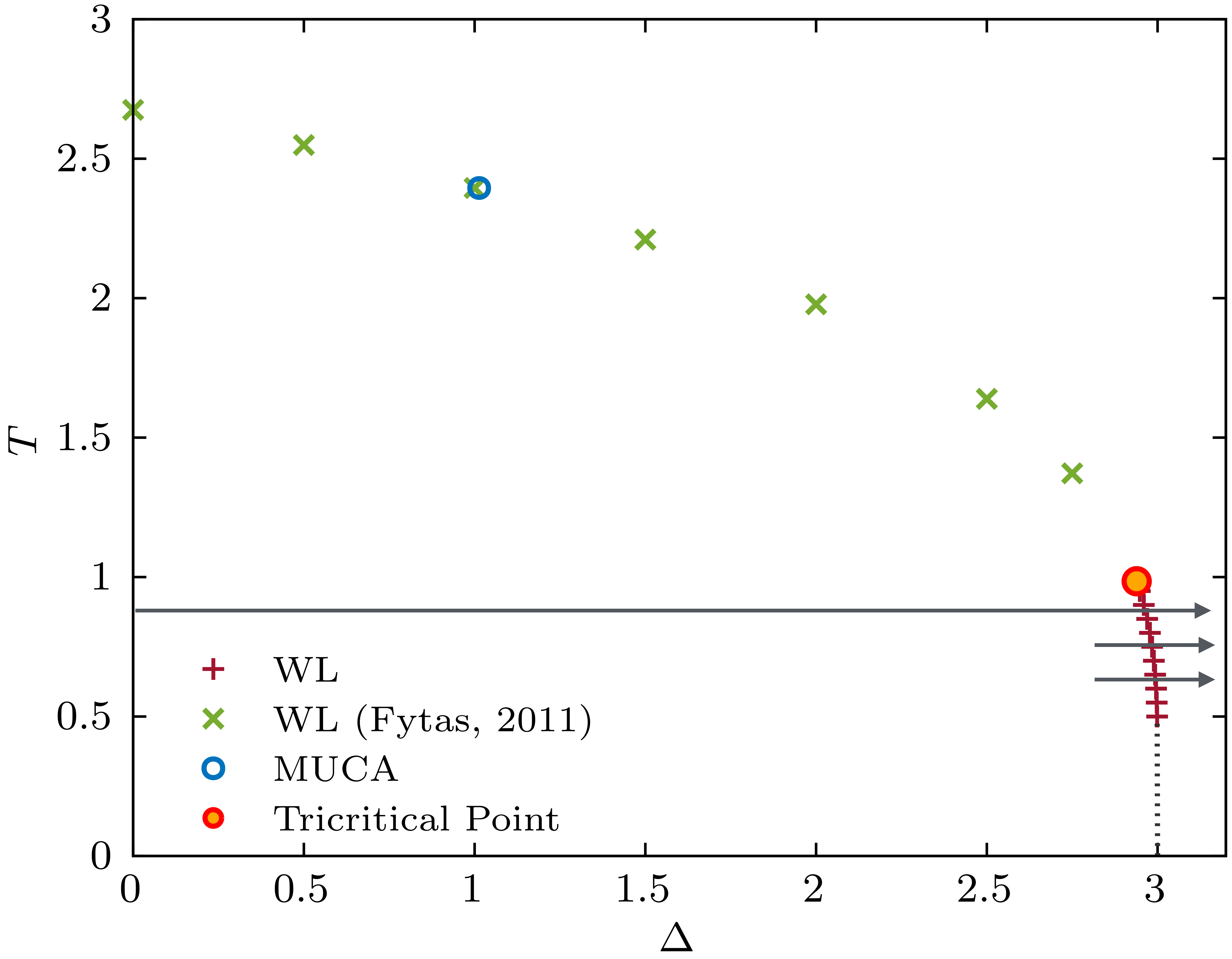
Overview

- **Interface tension** in the 1st order regime:
  - Locating where tension $\rightarrow$ 0.
- **Field mixing**:
  - Constructing the **phase diagram** for small T.
  - Cumulant crossing and location of the multicritical point.
  - Distributions.



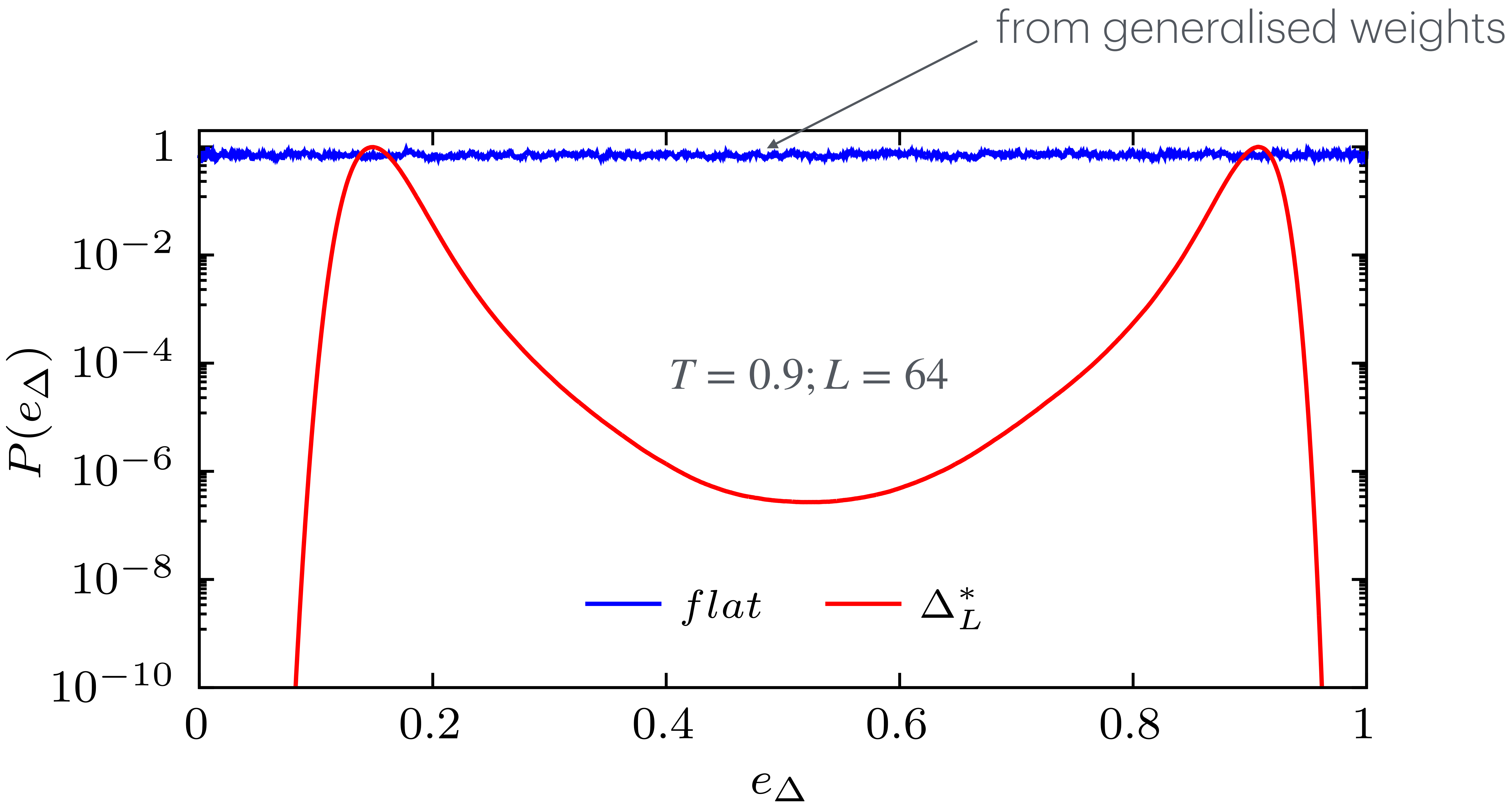
1st order, interface tension, and MUCA

- MUlti-CAnonical (MUCA) simulations.
- Fixed T.
- Generalised weights for E_Δ.
- Reweighting in Δ.
- Parellel on a GPU.

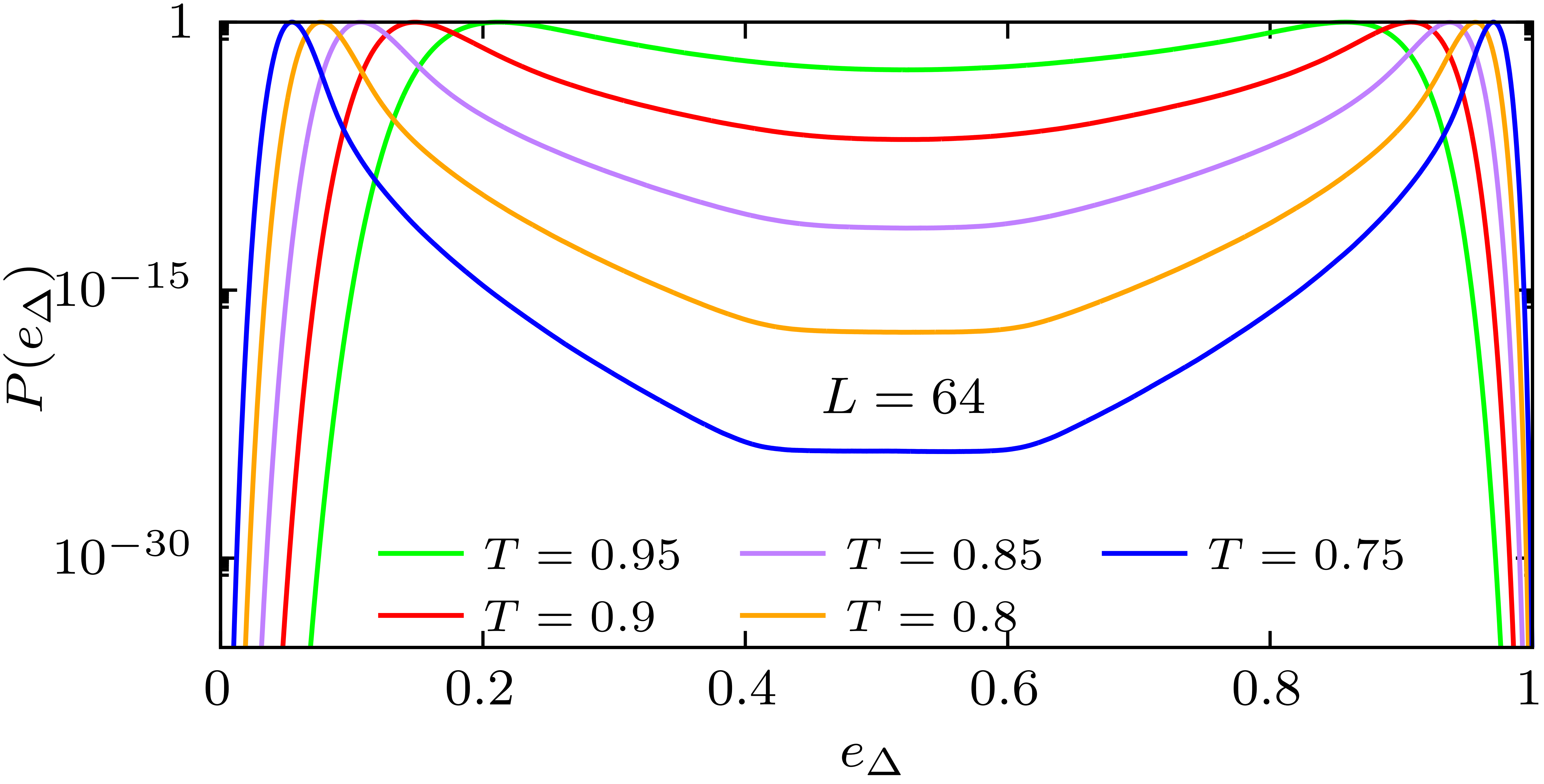


J. Gross et al. Comput. Phys. Commun. **224**, 387 (2018)

Flat histograms and reweighting in Δ



Interface tension

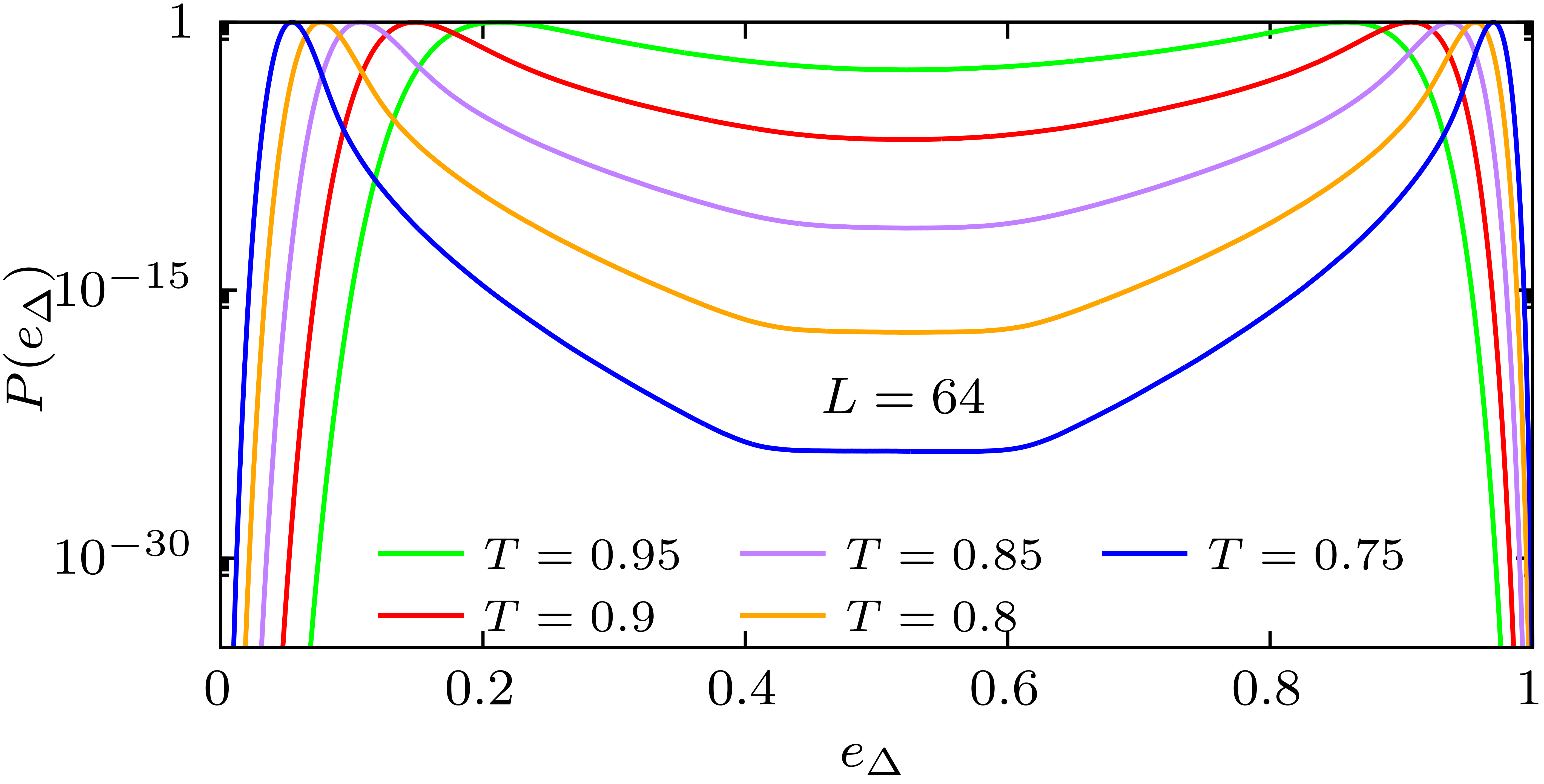


$$\Delta F(L) = \frac{1}{2\beta\Delta} \ln\left(\frac{P_{\max}}{P_{\min}}\right)$$

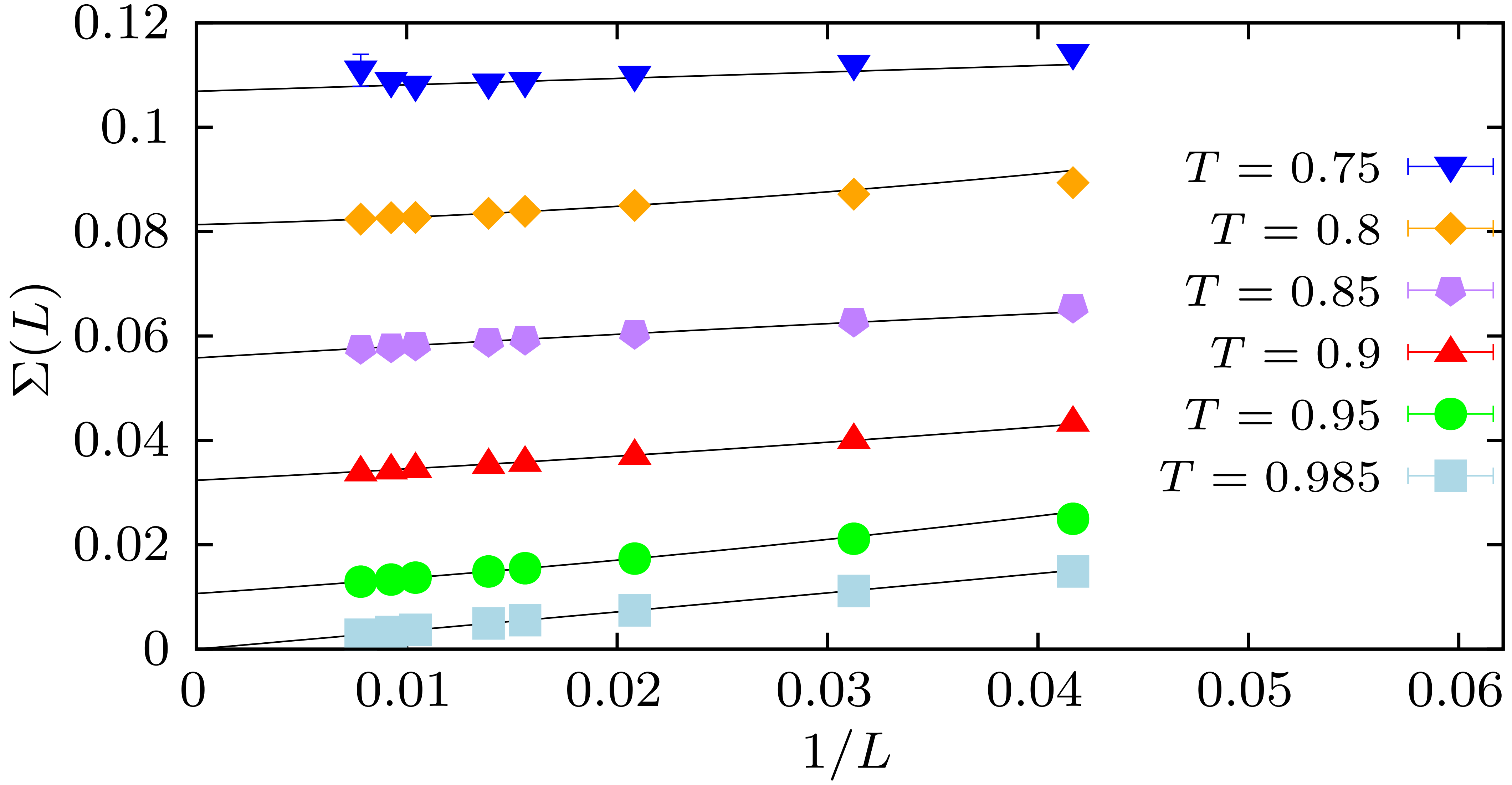
$$\Sigma(L) = \Delta F(L)/L$$

J. Lee and J.M. Kosterlitz, Phys. Rev. B **43**, 3265 (1991)
A. Nußbaumer, E. Bittner, and W. Janke, Phys. Rev. E **77**, 041109 (2008)

Interface tension

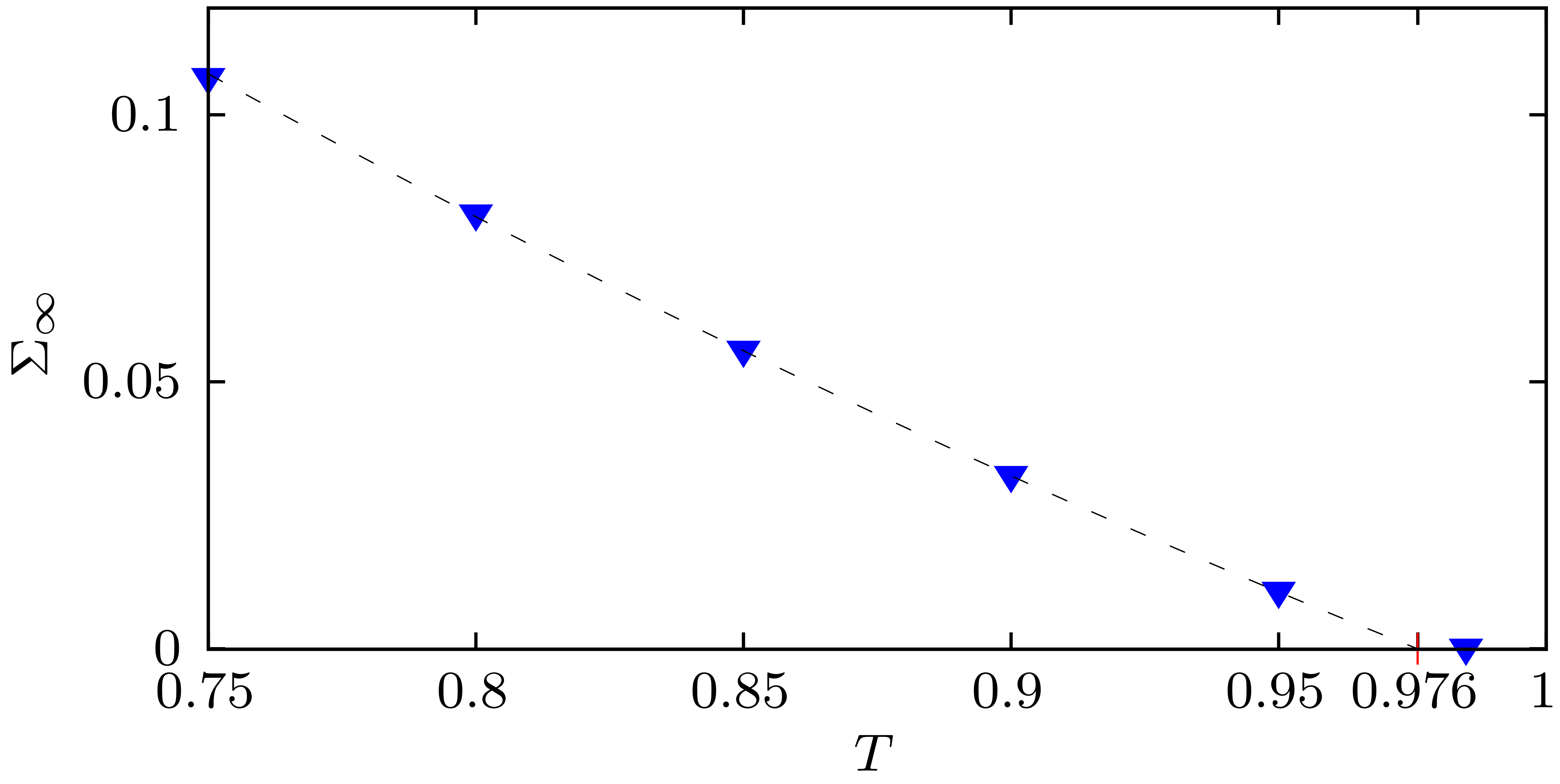


$$\Sigma(L) = \Sigma_\infty + c_1 L^{-1} + \mathcal{O}(L^{-2})$$



$$\Delta F(L) = \frac{1}{2\beta\Delta} \ln\left(\frac{P_{\max}}{P_{\min}}\right)$$

$$\Sigma(L) = \Delta F(L)/L$$



J. Lee and J.M. Kosterlitz, Phys. Rev. B **43**, 3265 (1991)
A. Nußbaumer, E. Bittner, and W. Janke, Phys. Rev. E **77**, 041109 (2008)

The tricritical point

A field mixing study

$$H = E_J + \Delta E_\Delta$$

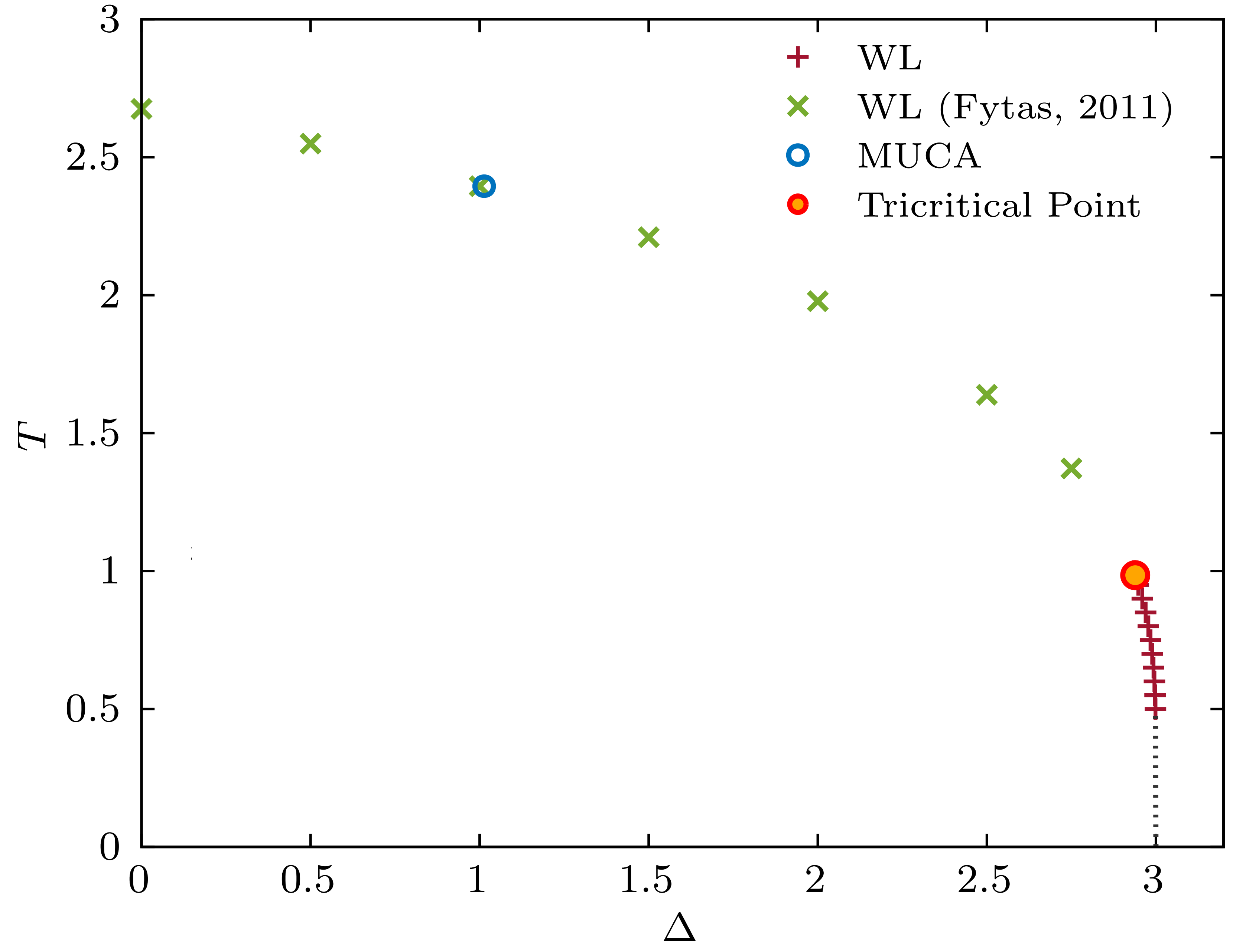
$$\mathscr{Z}(\beta,\mu) = \sum_{\{E_J, E_\Delta\}} g(E_J, E_\Delta) \exp\left(-\beta E_J - \mu E_\Delta\right)$$

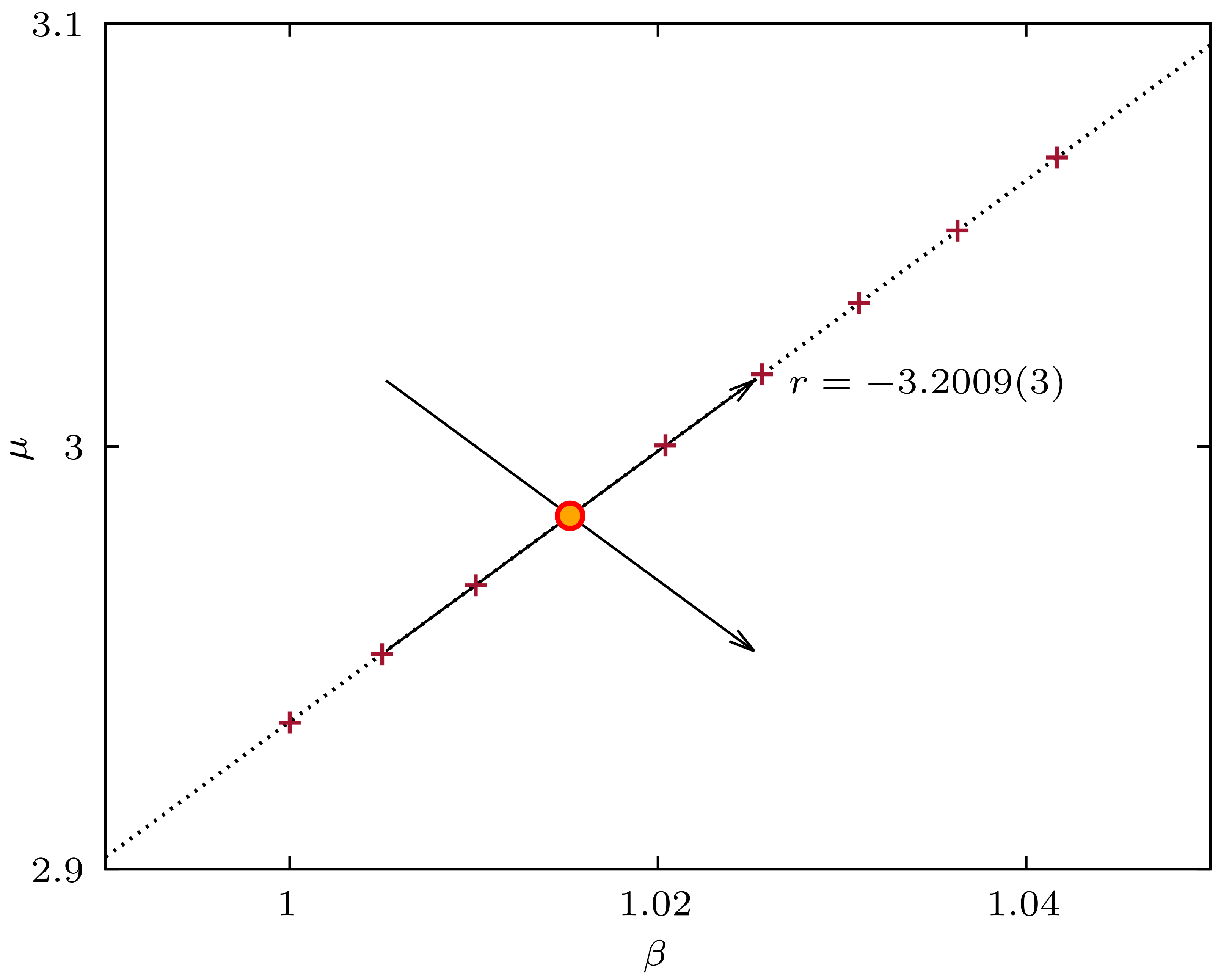
<u>Mixed fields</u>

$$\lambda = (\mu - \mu_t) + r(\beta - \beta_t)$$
$$g = (\beta - \beta_t) + s(\mu - \mu_t)$$

<u>Conjugate variable</u>

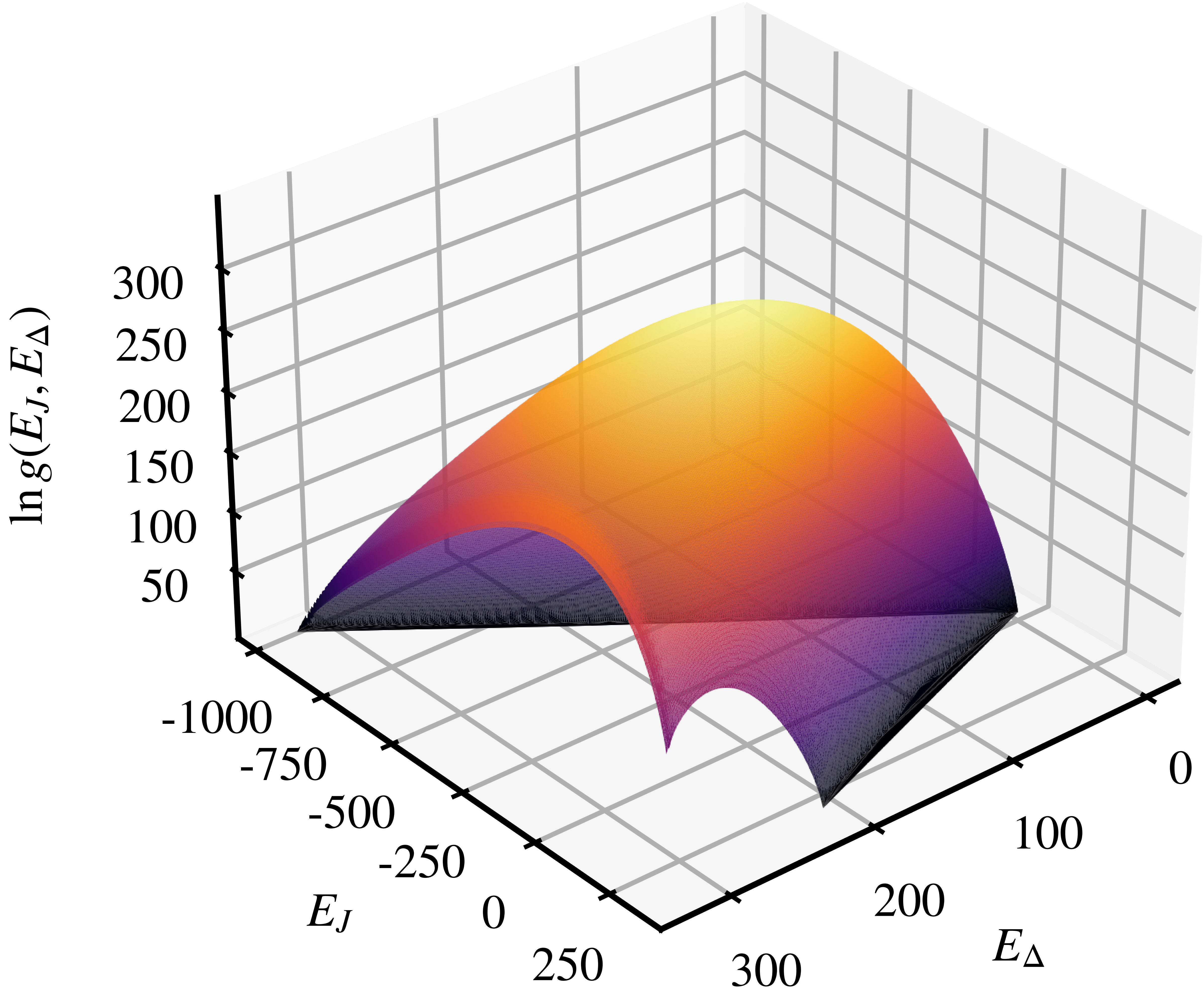
$$\mathscr{Q} = \frac{1}{1-rs}(E_\Delta - sE_J)/L^d$$
$$\mathscr{E} = \frac{1}{1-rs}(E_J - rE_\Delta)/L^d$$



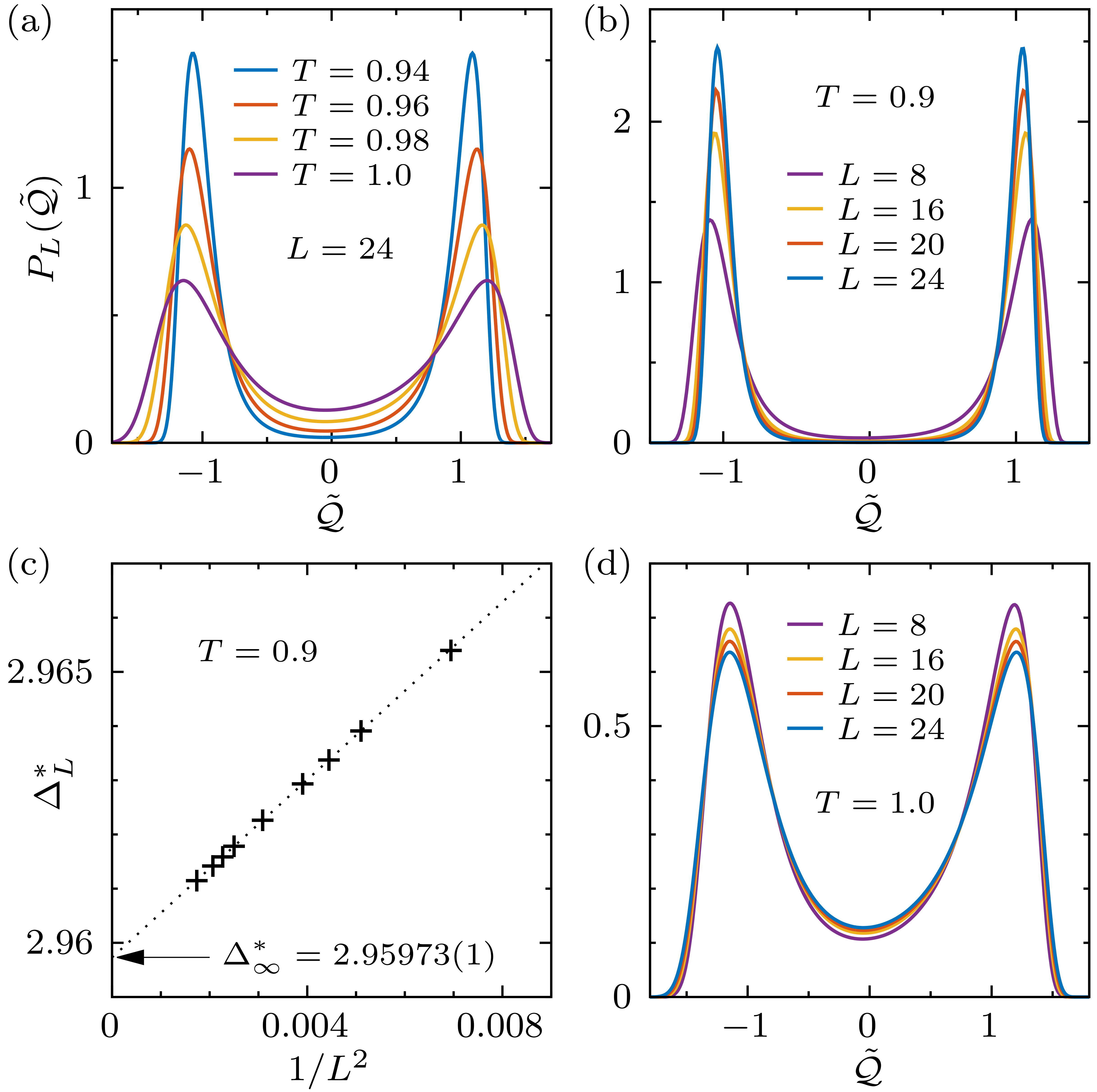


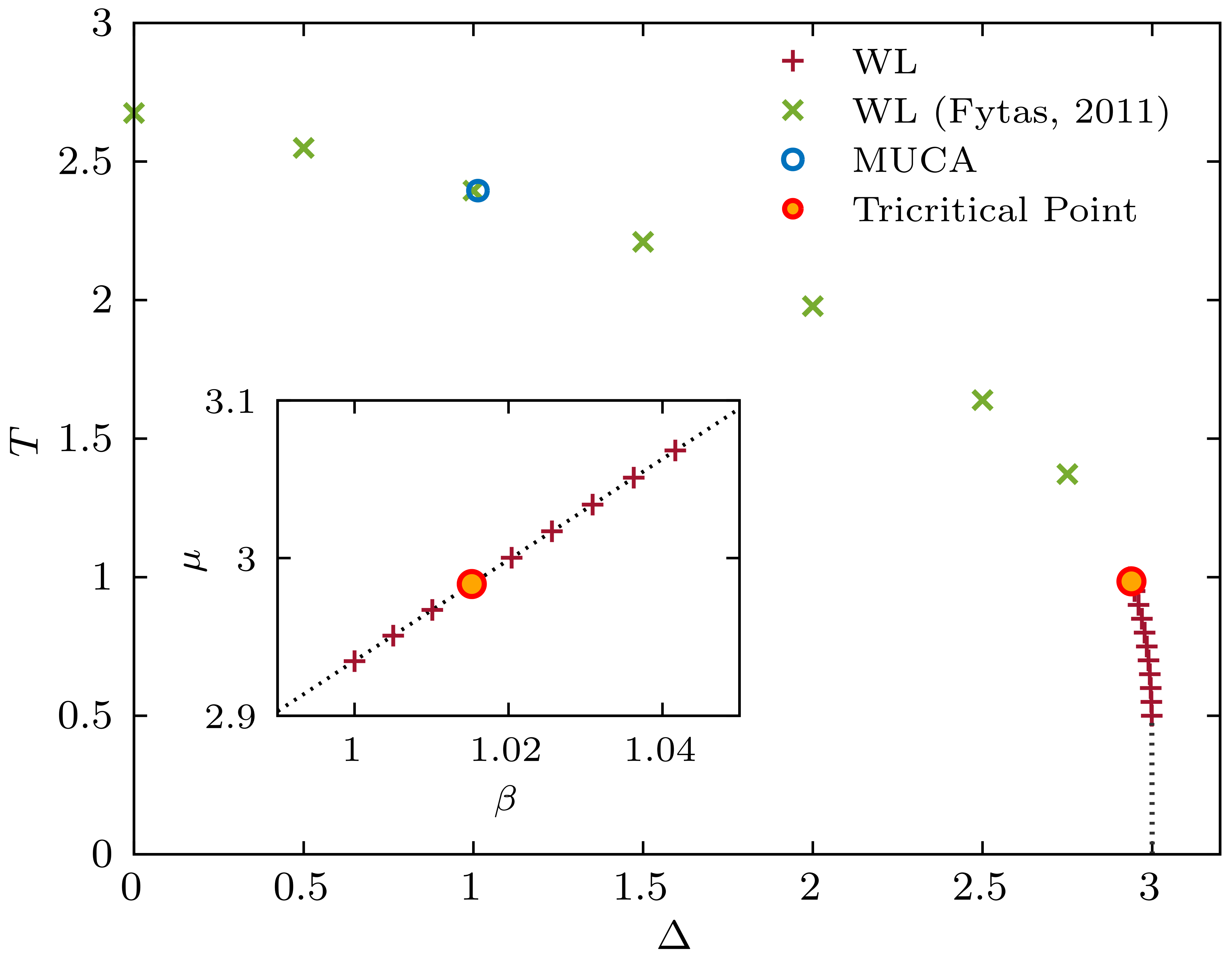
N.B. Wilding and P. Nielaba, Phys. Rev. E **53**, 926 (1996)

Wang-Landau: density of states



Creating the phase diagram

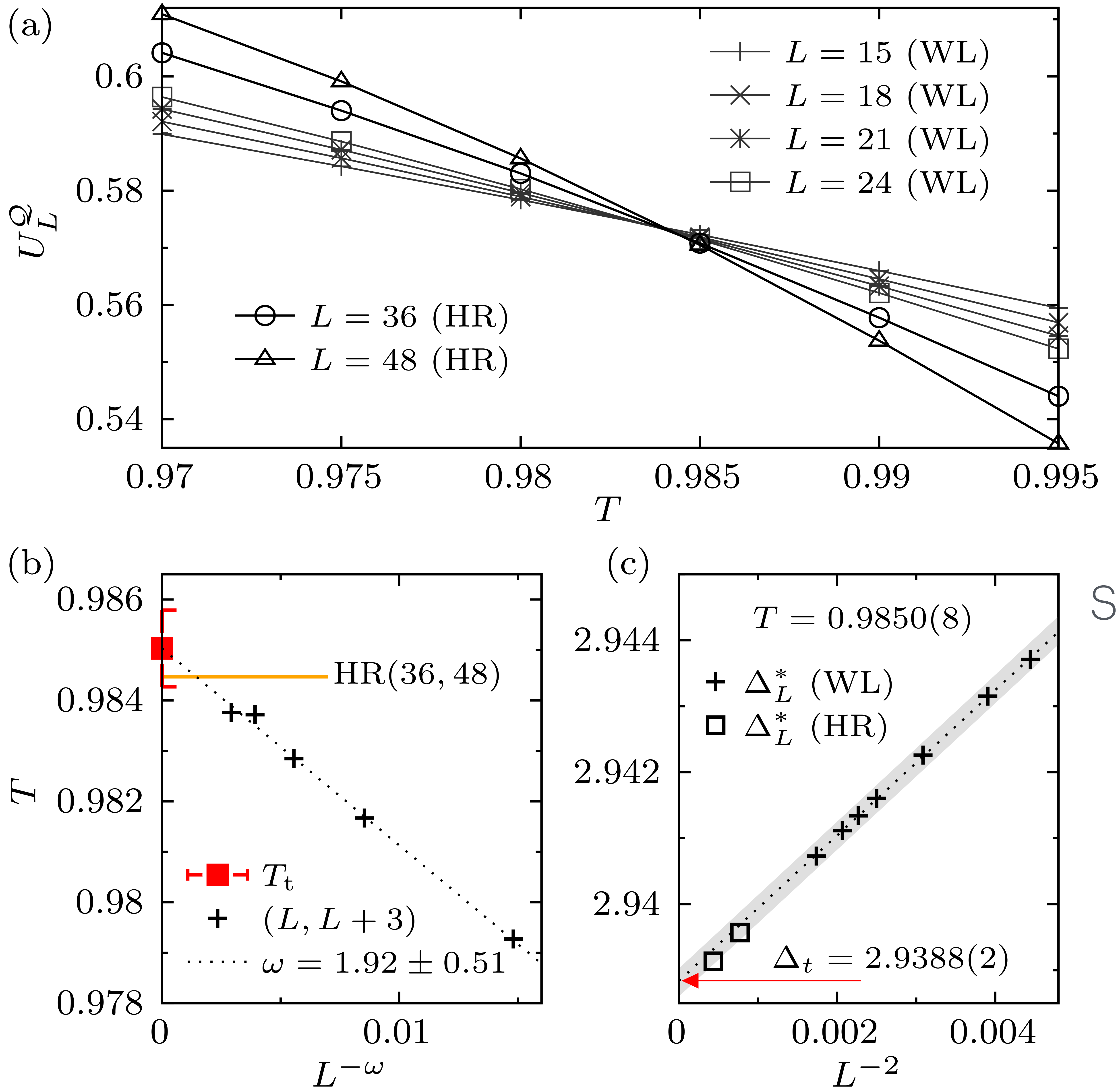




4th order cumulant crossing

$$U_L^{\mathcal{Q}} = 1 - \frac{\langle \tilde{Q}^4 \rangle}{3\langle \tilde{Q}^2 \rangle^2}$$

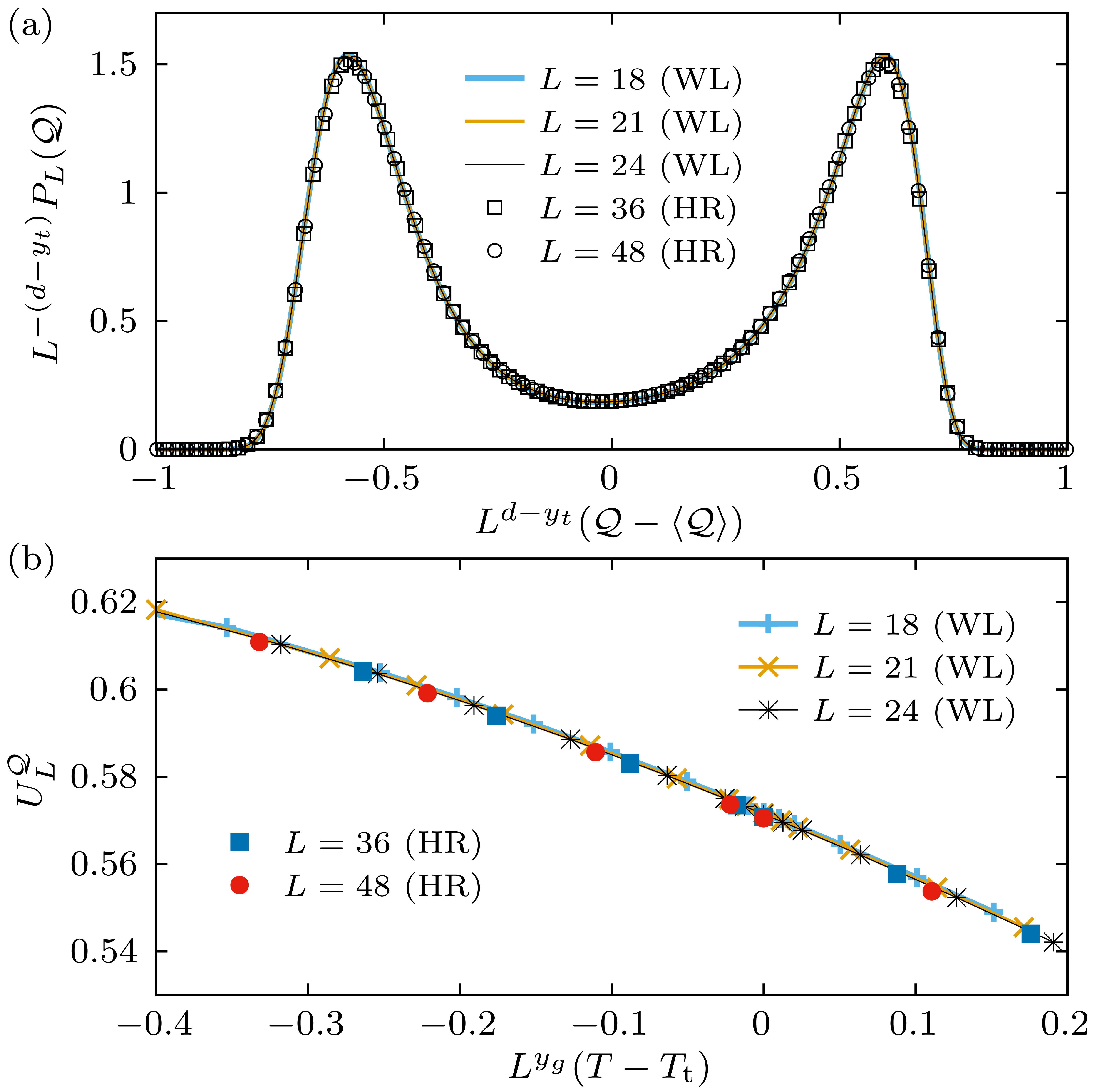
$$T_L = T_\infty + aL^{-\omega}$$



$$U_{\text{cross}}^{\mathcal{Q}} = 0.571(3)$$

Same as Wilding & Nielaba

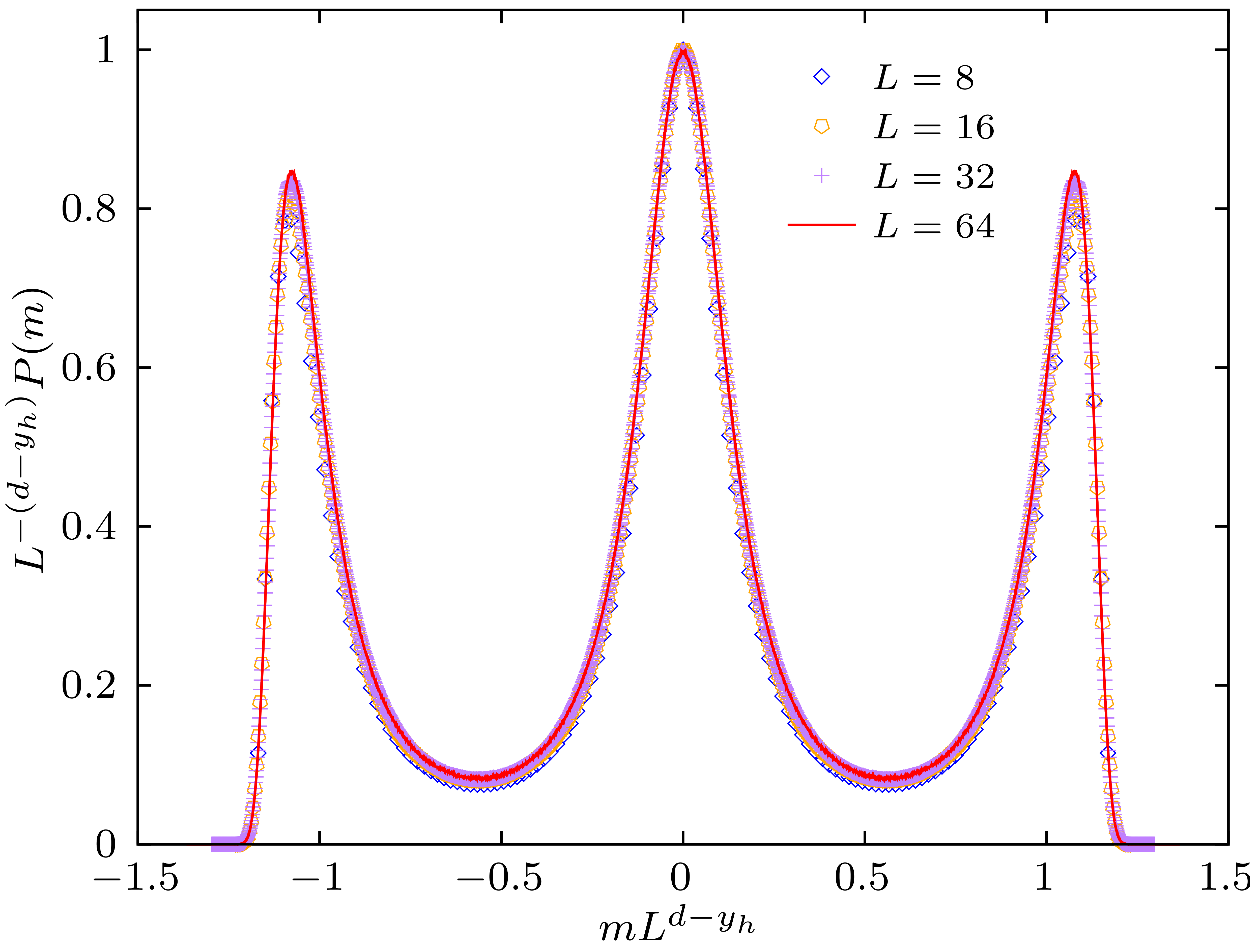
Energy distribution and 4th order cumulant collapse



$y_t = 9/5$

$y_g = 4/5$

Magnetisation distribution



$y_h = 77/40$

Discussion

https://arxiv.org/abs/2411.11689

- Triangular Blume-Capel model.
- Field mixing using Wang-Landau to locate the tricritical point.
- Distributions of m and $\mathcal{Q}$ collapse.
- Computed the interface tension behaviour along the 1st order line.

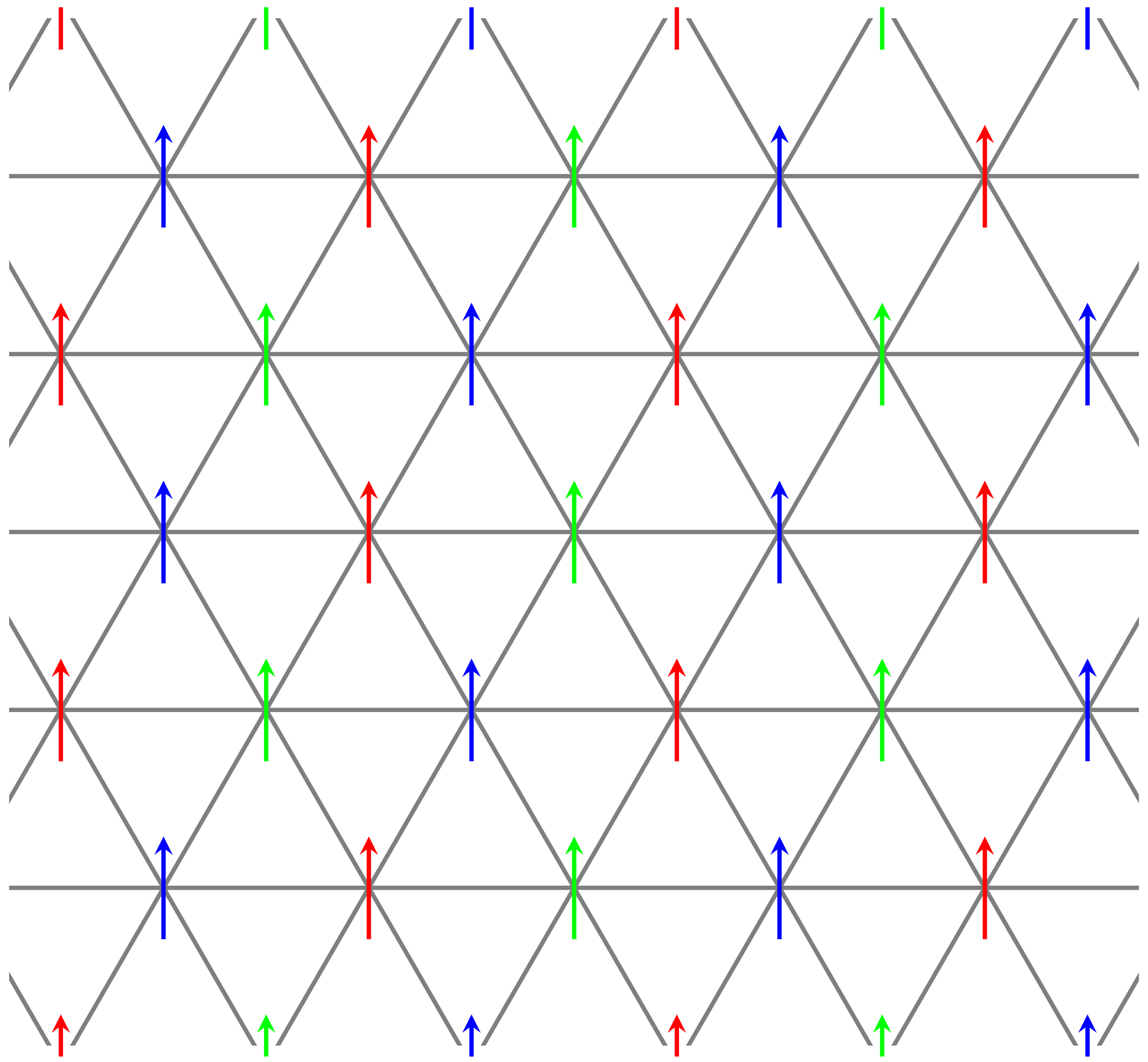
Outlook

- Apply the methods in the three-spin interactions case (Baxter-Wu).
- Study the pentacritical point.

Extra Slides

Motivation

Baxter-Wu and multicriticality



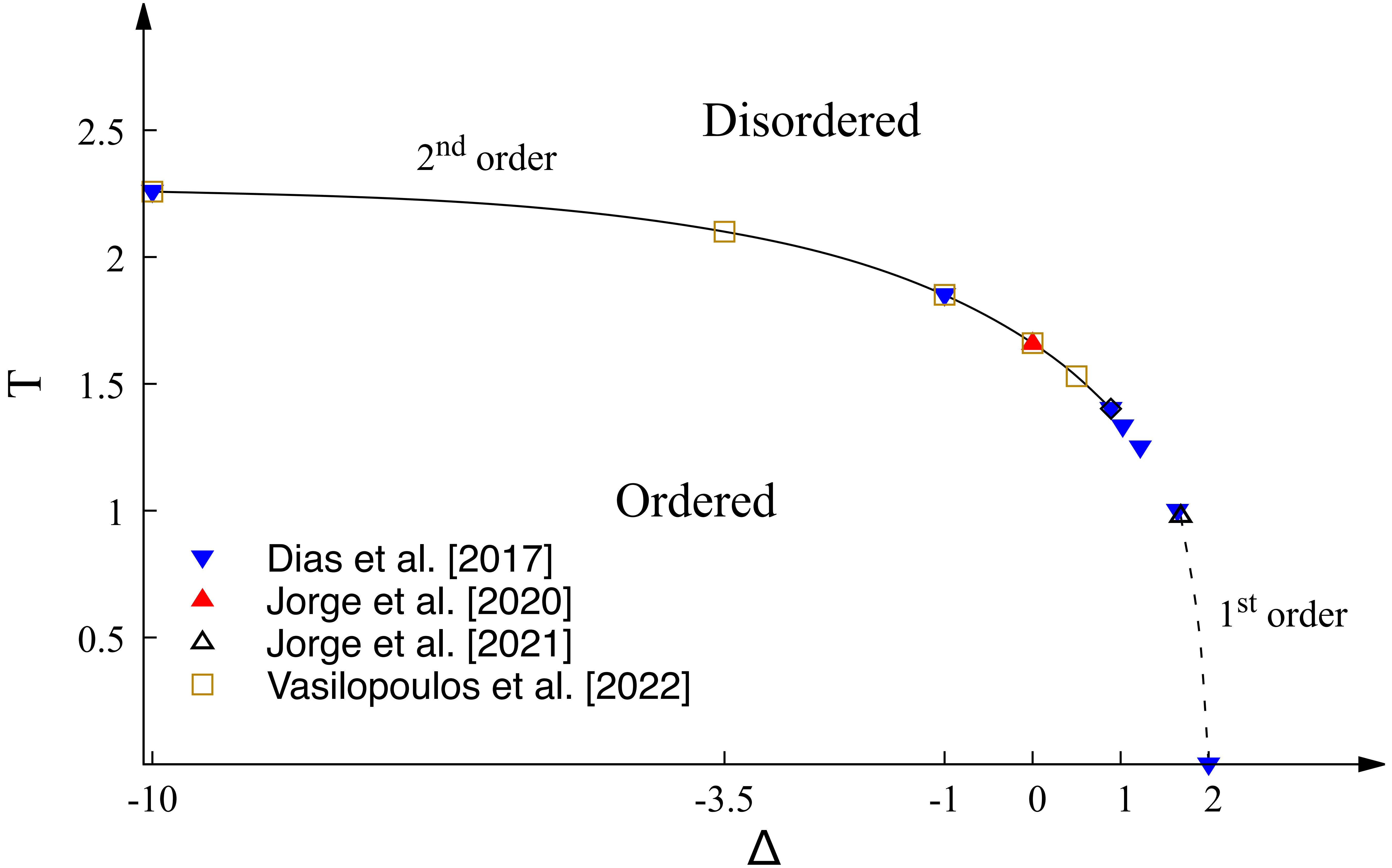
- Triangular lattice.

- Three-spin interactions:

$$H = -J\sum_{ijk}\sigma_i\sigma_j\sigma_k + \Delta\sum_i \sigma_i^2 = E_J + \Delta E_\Delta \, .$$

- Pentacritical point location?

- Field mixing: N.B. Wilding and P. Nielaba, Phys. Rev. E **53**, 926 (1996).



Methods

Metropolis

- Pick a spin.

- Choose a new candidate state excluding the current one.

- Flip with probability:

$$p = \begin{cases} \exp\left\{-\beta\Delta E\right\}, & \Delta E > 0 \\ 1, & \Delta E \leq 0 \end{cases}$$

- PRNG: Mersenne Twister 19937 from C++ Random library since C++11 (Boost).

Methods

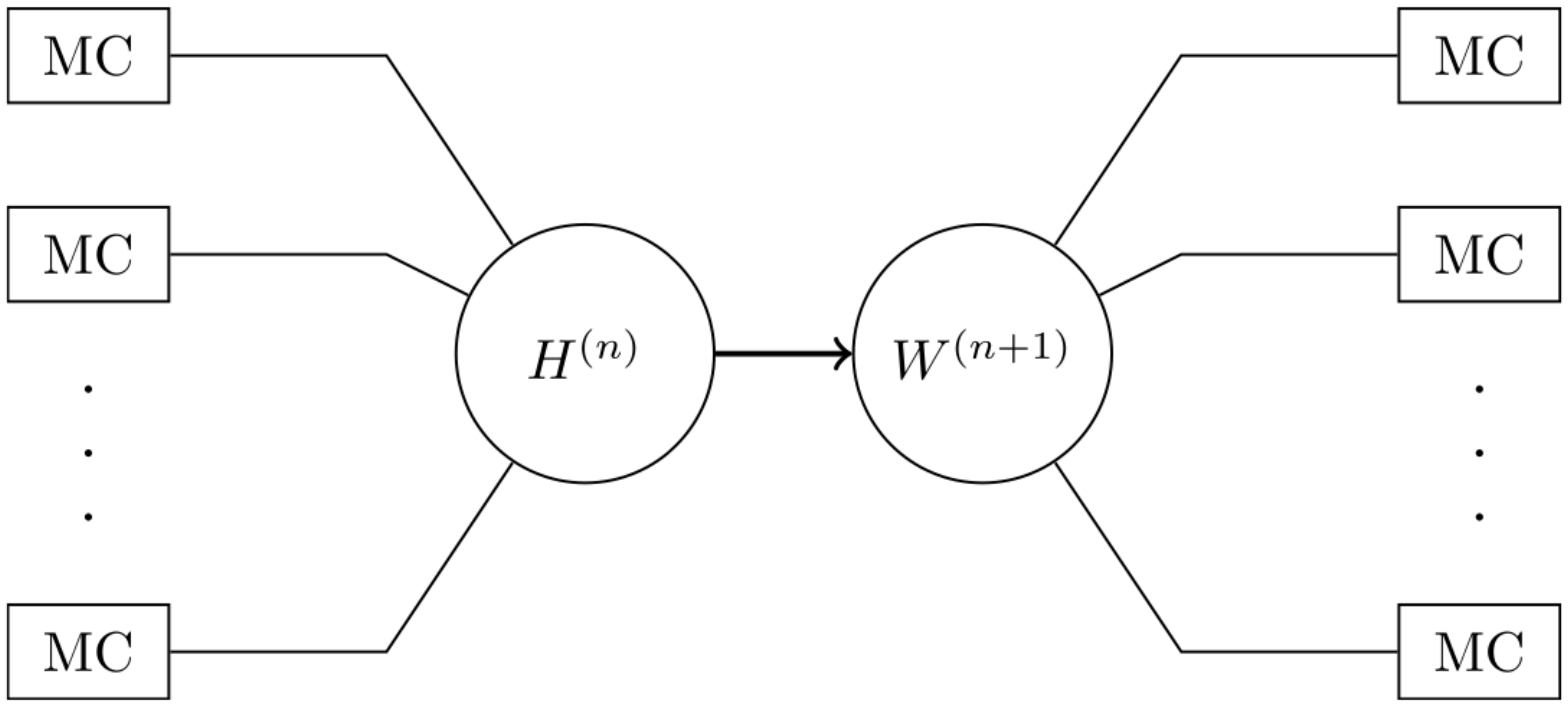
MUCA

- GPU implementation with CUDA [Gross, Zierenberg, Weigel, and Janke 2018].
- Pick a random spin and a candidate state for it (excluding current state).
- Flip with probability:

$$p = \min\left\{1, \frac{W^{(n)}(E'_\Delta)\exp\{-\beta E'_J\}}{W^{(n)}(E_\Delta)\exp\{-\beta E_J\}}\right\}$$

- Accumulate histogram of E_Δ. Update weights:

$$W^{(n+1)}(E_\Delta) = W^{(n)}(E_\Delta)/H^{(n)}(E_\Delta)$$



J. Gross et al. Comput. Phys. Commun. **224**, 387 (2018)

MUCA

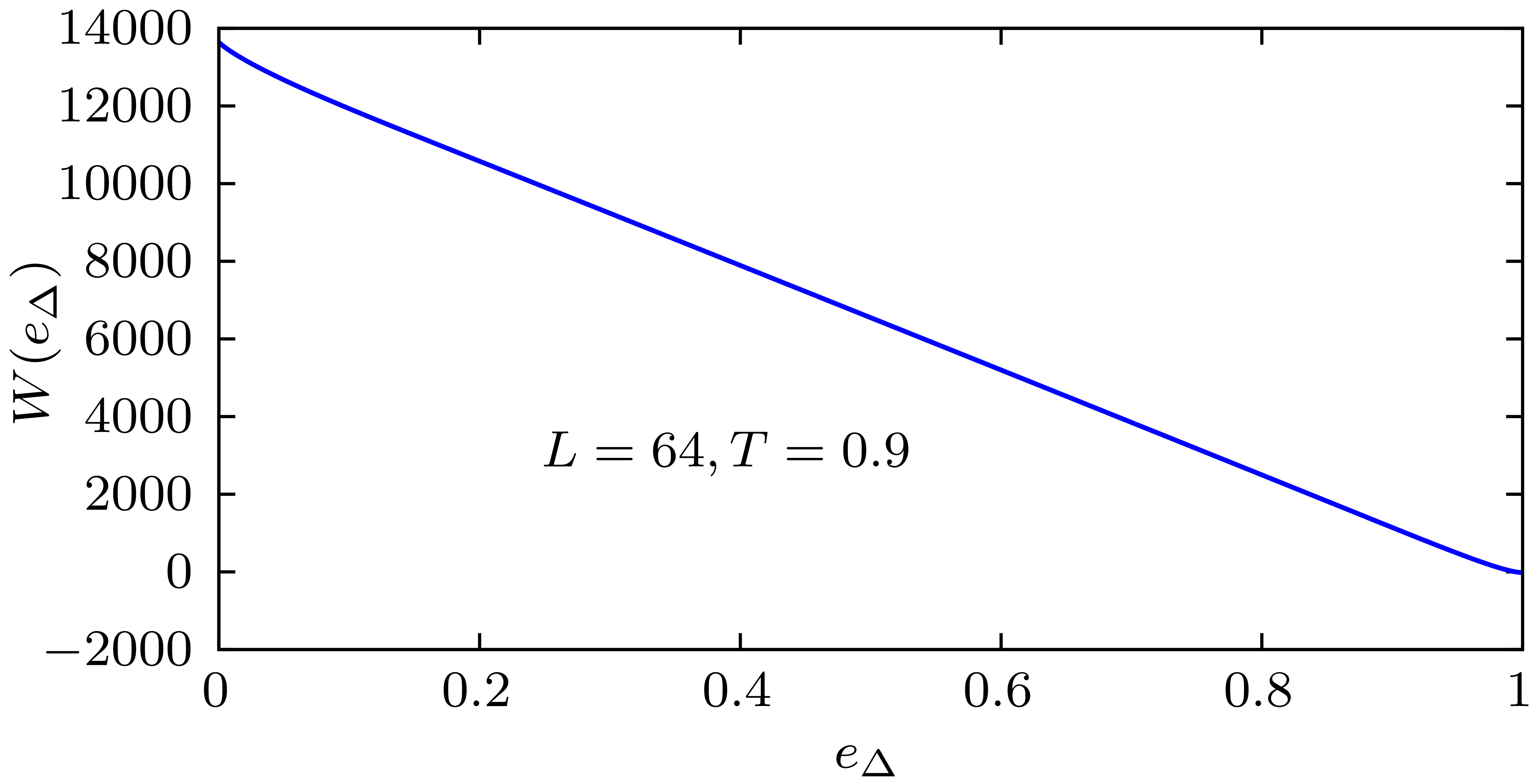
Details

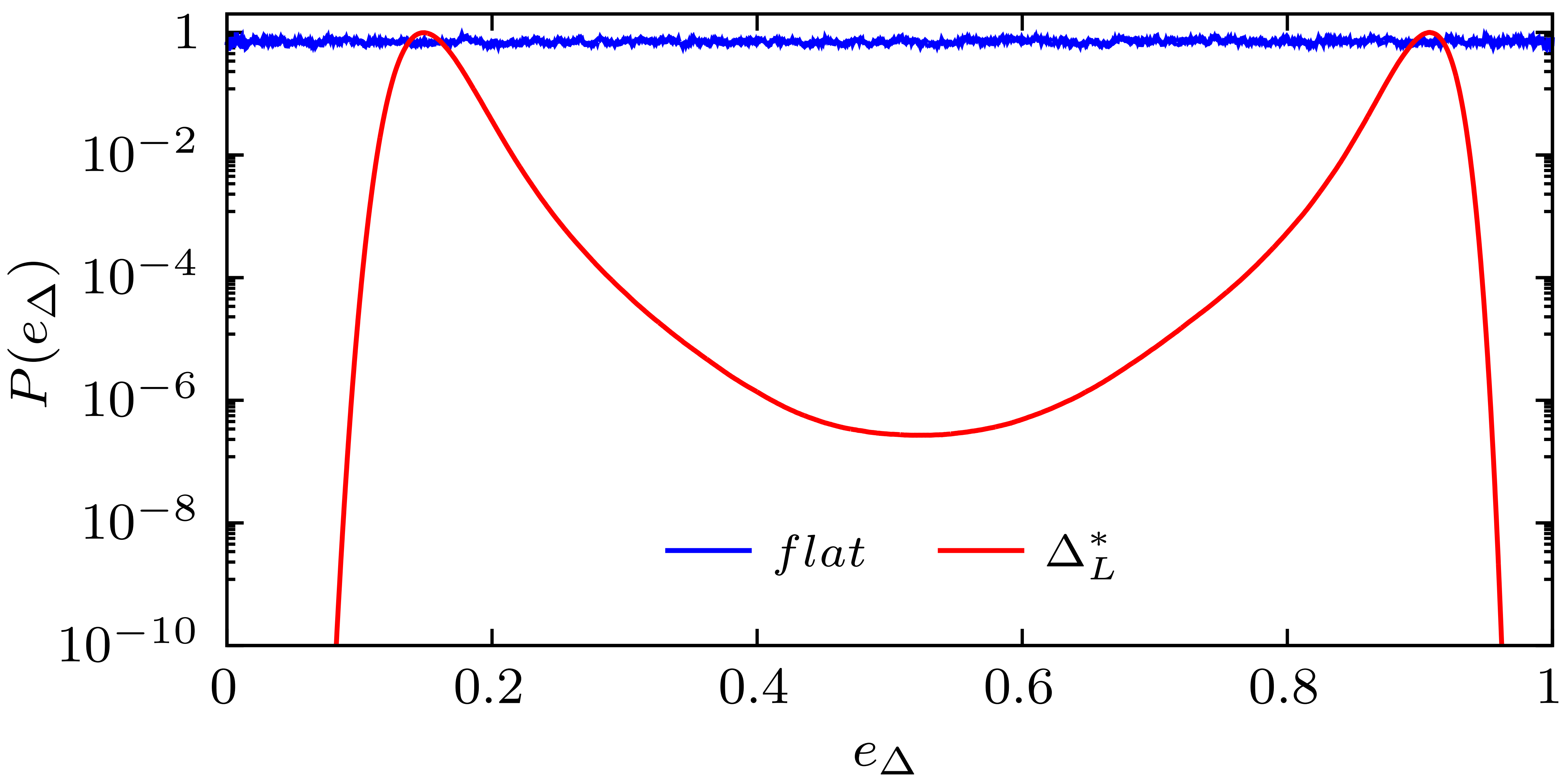
- PRNG: phillox32.
- Nvidia TURING RTX2080 or PASCAL GTX1080T 47,104 and 57,344 systems respectively.
- Jackknife bins: 32 - 128.

Generalised weights and flat histograms

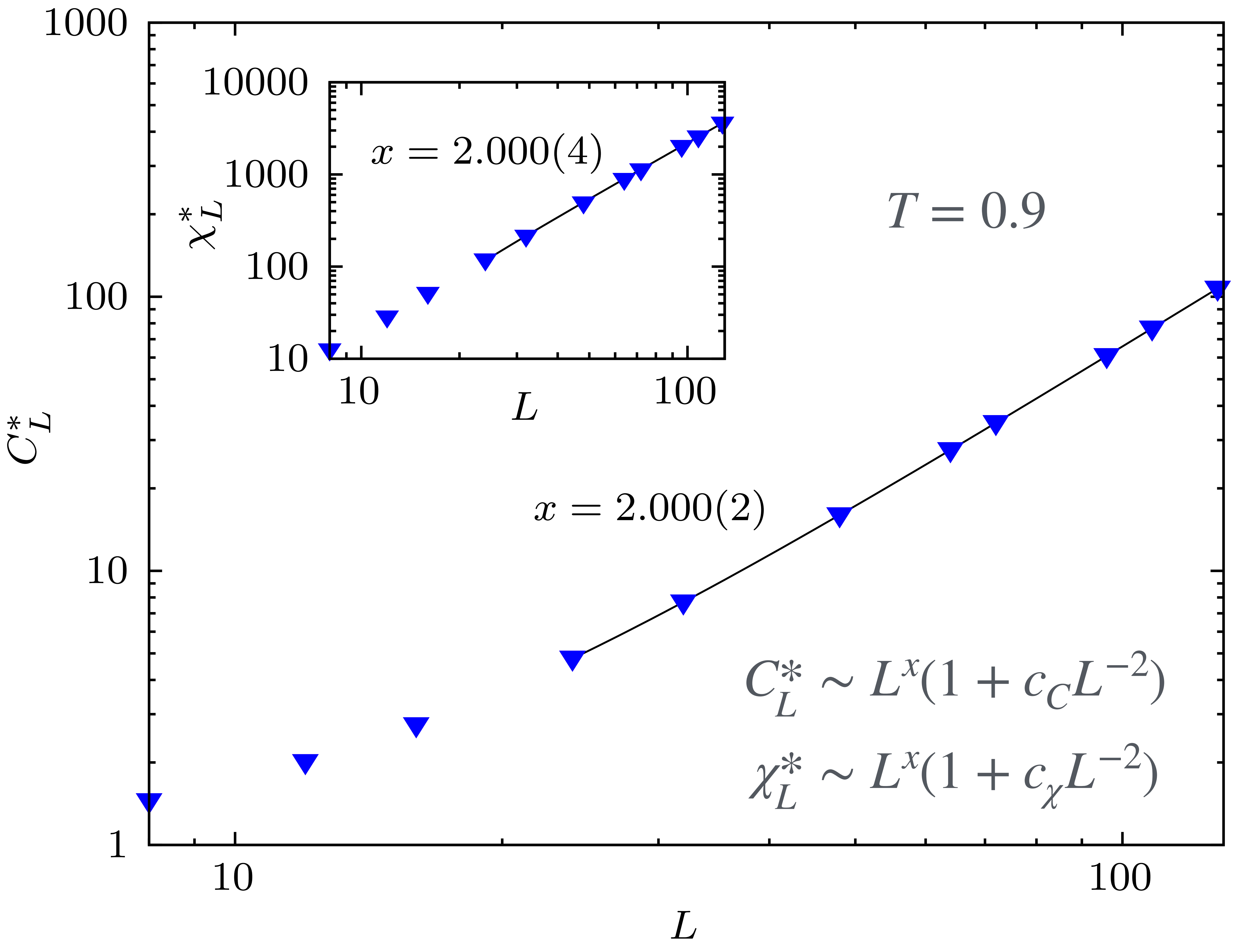
$$\mathscr{Z}_{\text{MUCA}} = \sum_{\{E_J, E_\Delta\}} g(E_J, E_\Delta) e^{-\beta E_J} W(E_\Delta)$$

$$W(E_\Delta) \propto \frac{\mathscr{Z}_{\text{MUCA}}}{\sum_{E_J} g(E_J, E_\Delta) e^{-\beta E_J}}$$



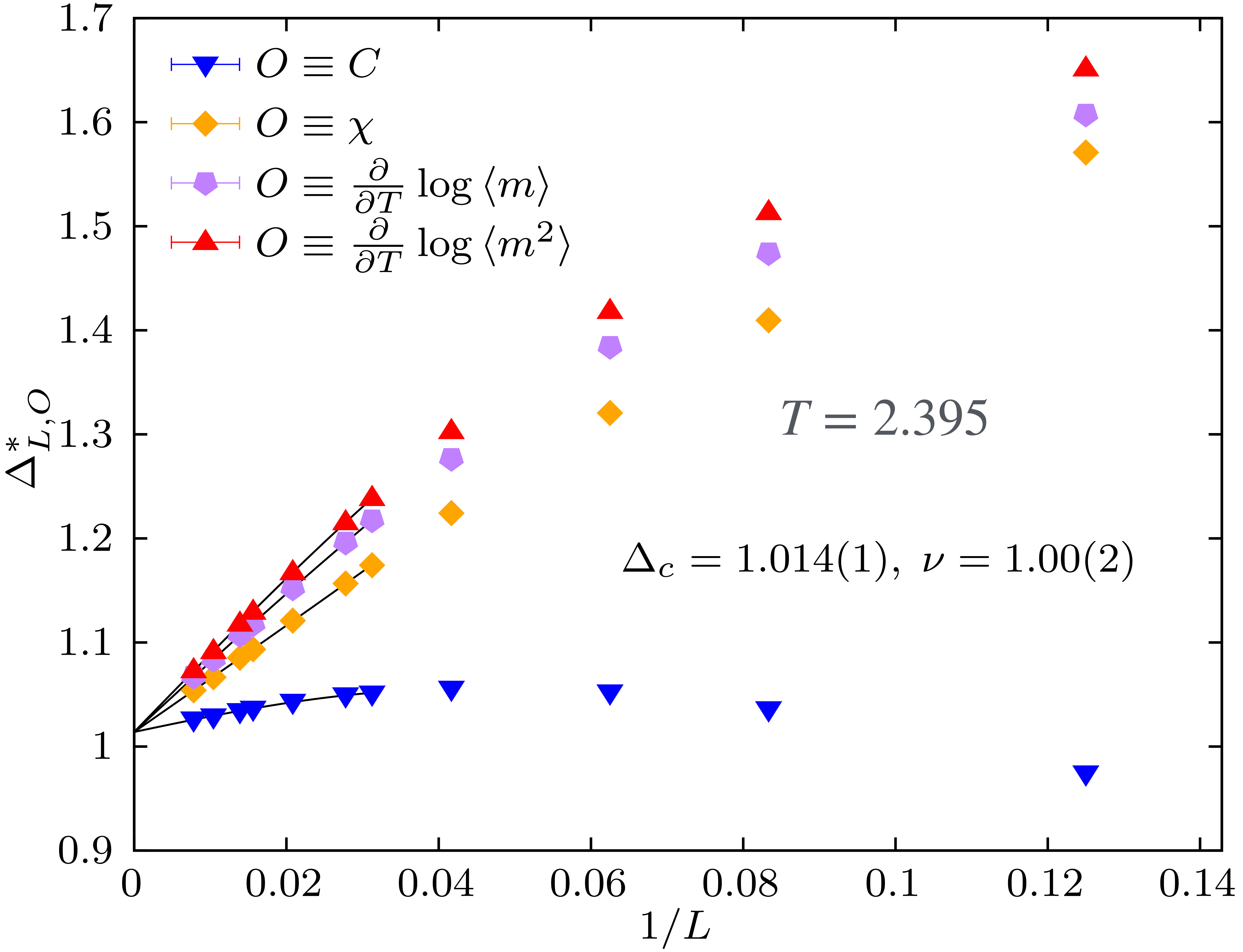


First order



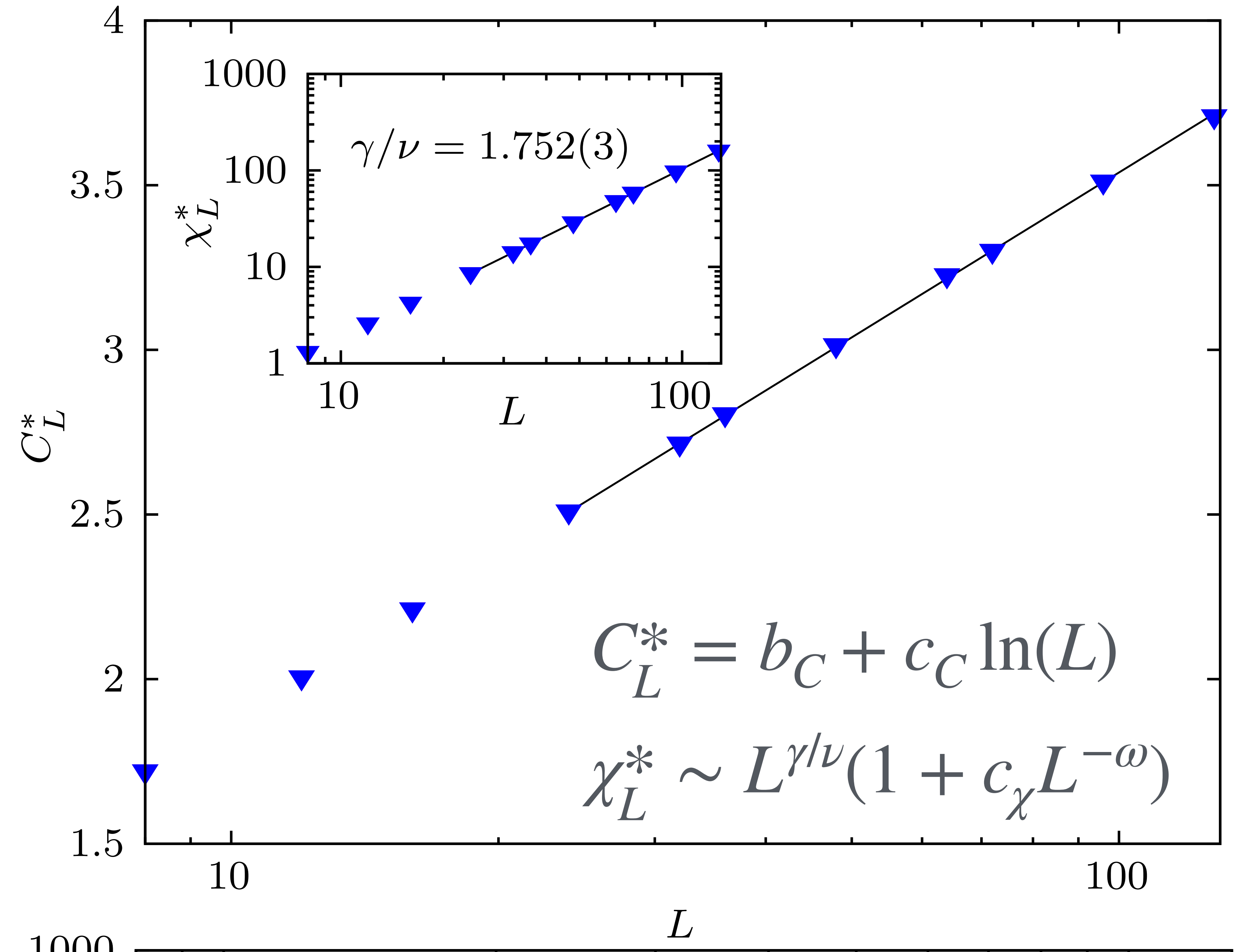
1000
100
10
1
10
100
L
C_L^*
10000
1000
100
10
10
100
L
χ_L^*
$x = 2.000(4)$
$T = 0.9$
$x = 2.000(2)$
$C_L^* \sim L^x(1 + c_C L^{-2})$
$\chi_L^* \sim L^x(1 + c_\chi L^{-2})$

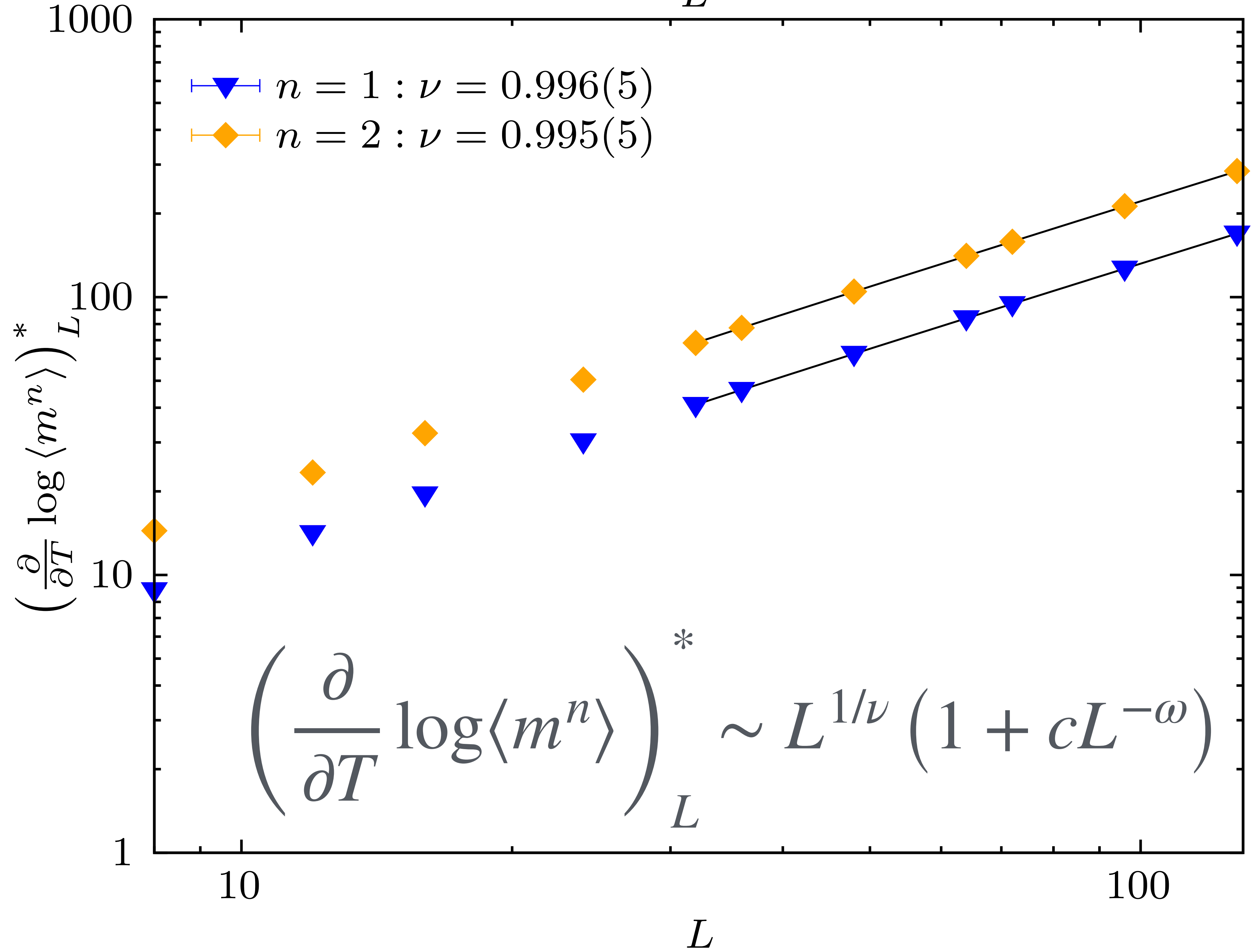
Second order



$$\Delta^*_{L,O} = \Delta_c + bL^{-1/\nu}\left(1 + cL^{-\omega}\right)$$

$$\omega = 1.75$$





Methods

WL

- Pick a random spin and a candidate state for it (excluding current state).

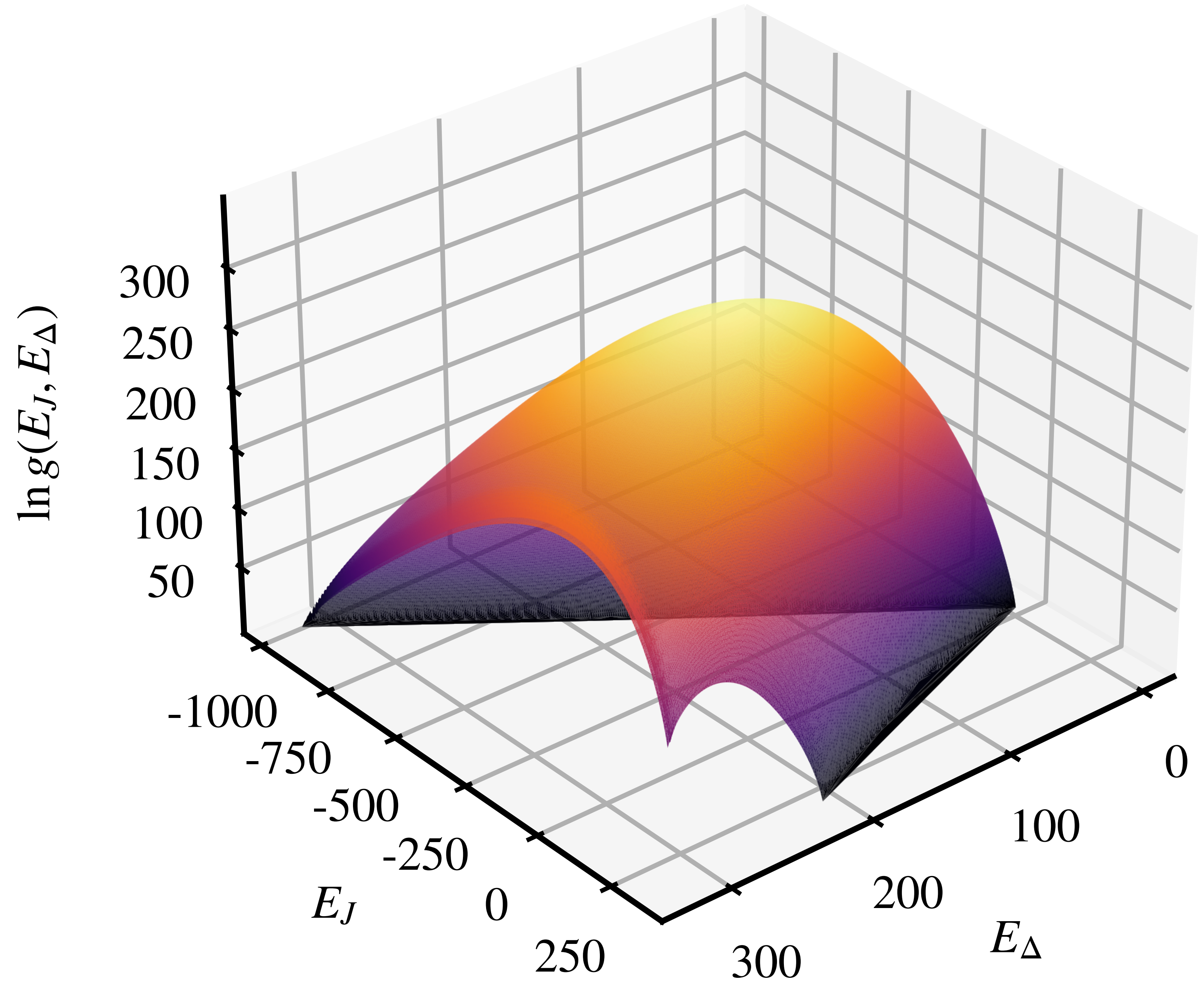
- Flip with probability:

$$p = \min \left\{ 1, \frac{g^{(i)}(E_J, E_\Delta)}{g^{(i)}(E'_J, E'_\Delta)} \right\}$$

- Accumulate histogram and update weights:

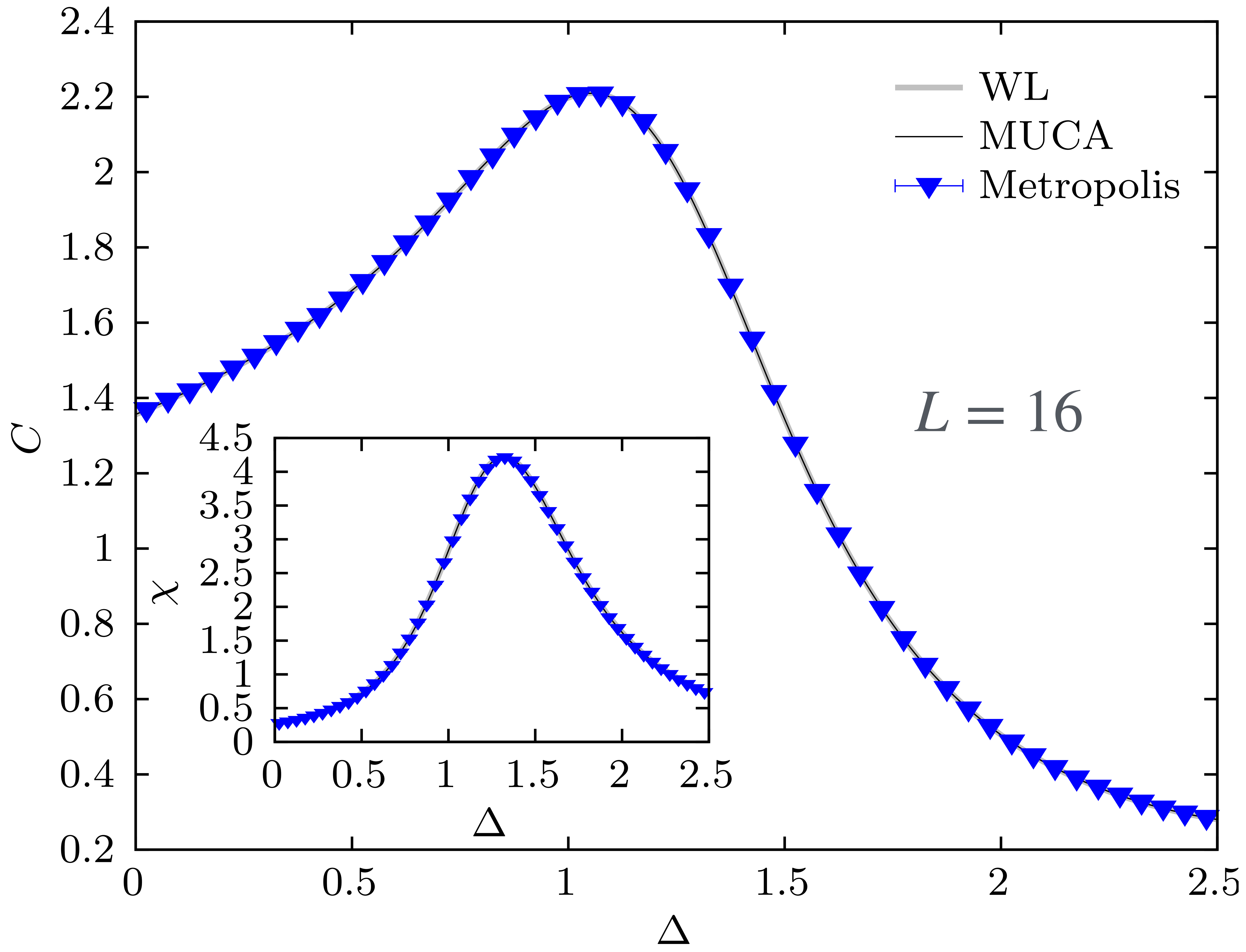
$$g^{(i+1)}(E_J, E_\Delta) = g^{(i)}(E_J, E_\Delta) * \text{factor}$$

- If the histogram is flat, update factor $\leftarrow \sqrt{\text{factor}}$.



Methods

Comparison



Locating minima

MUCA

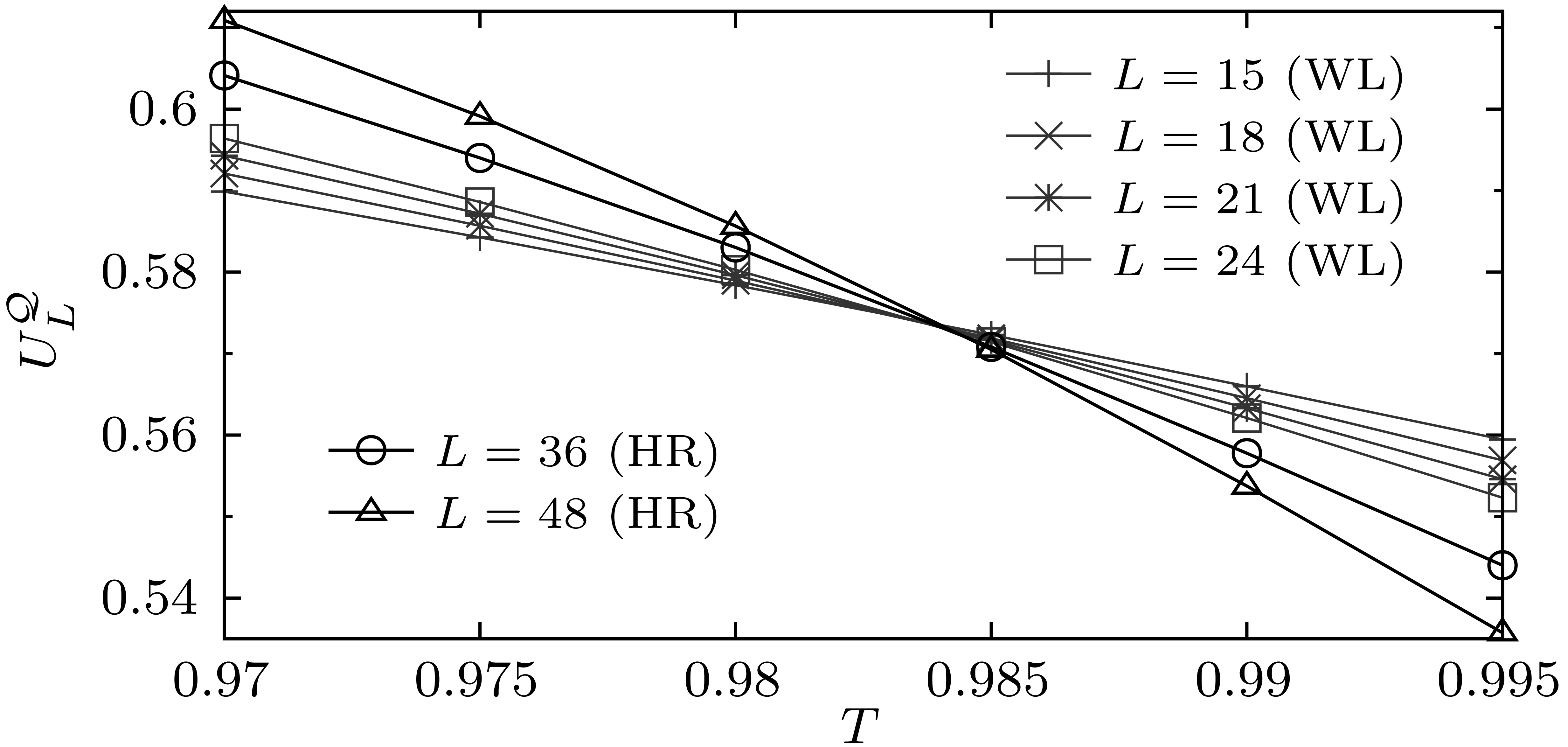
- Reweight:

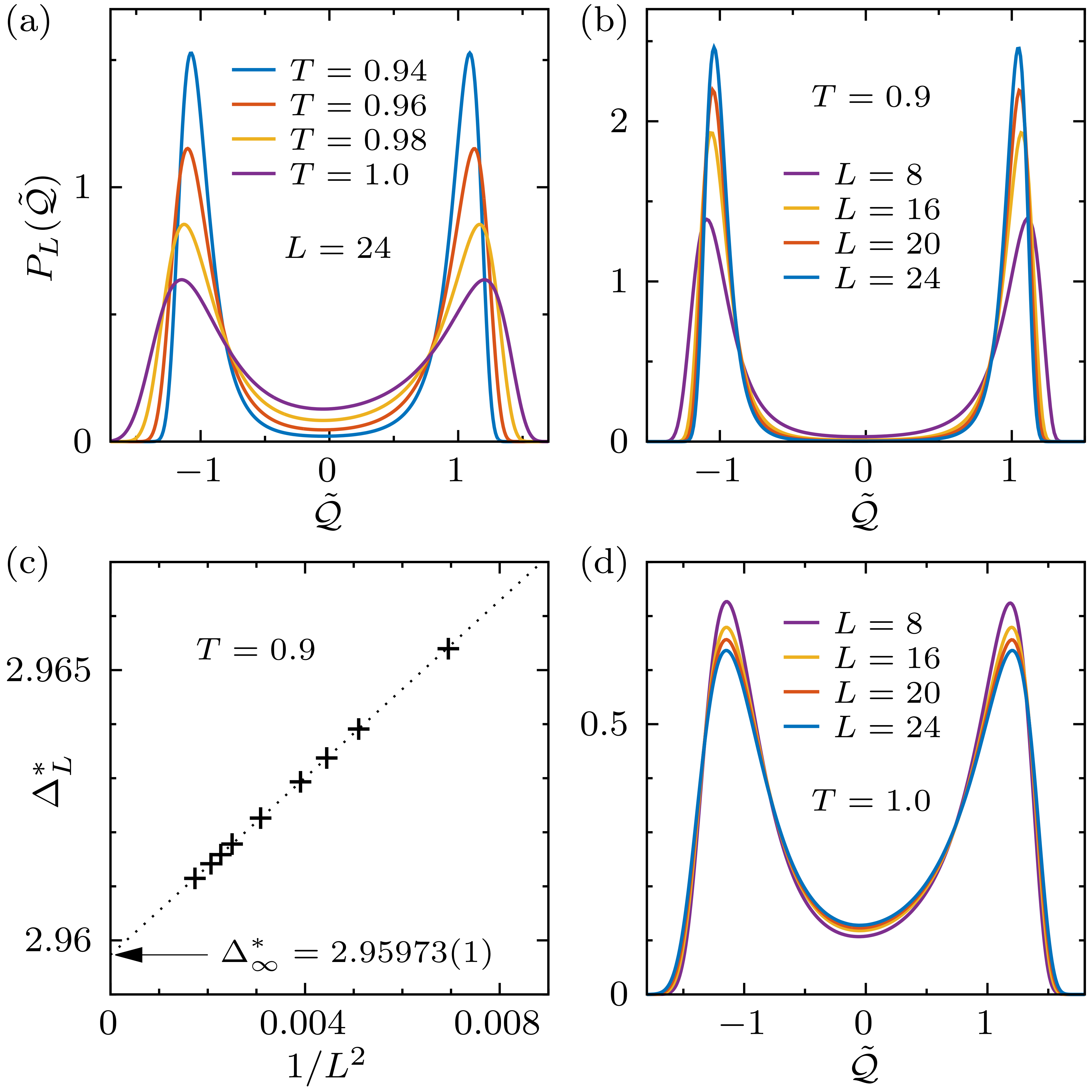
$$\langle O \rangle_\Delta = \frac{\left\langle O \;\; \exp\{-\beta\Delta \; E_\Delta\} W^{-1}(E_\Delta) \right\rangle_{\text{MUCA}}}{\left\langle \exp\{-\beta\Delta \; E_\Delta\} W^{-1}(E_\Delta) \right\rangle_{\text{MUCA}}}$$

- Use Brent algorithm from GSL to find minimum.
- Use openmp to speed the jackknife analysis.
- Use MPFR to avoid numerical issues from the large weights.

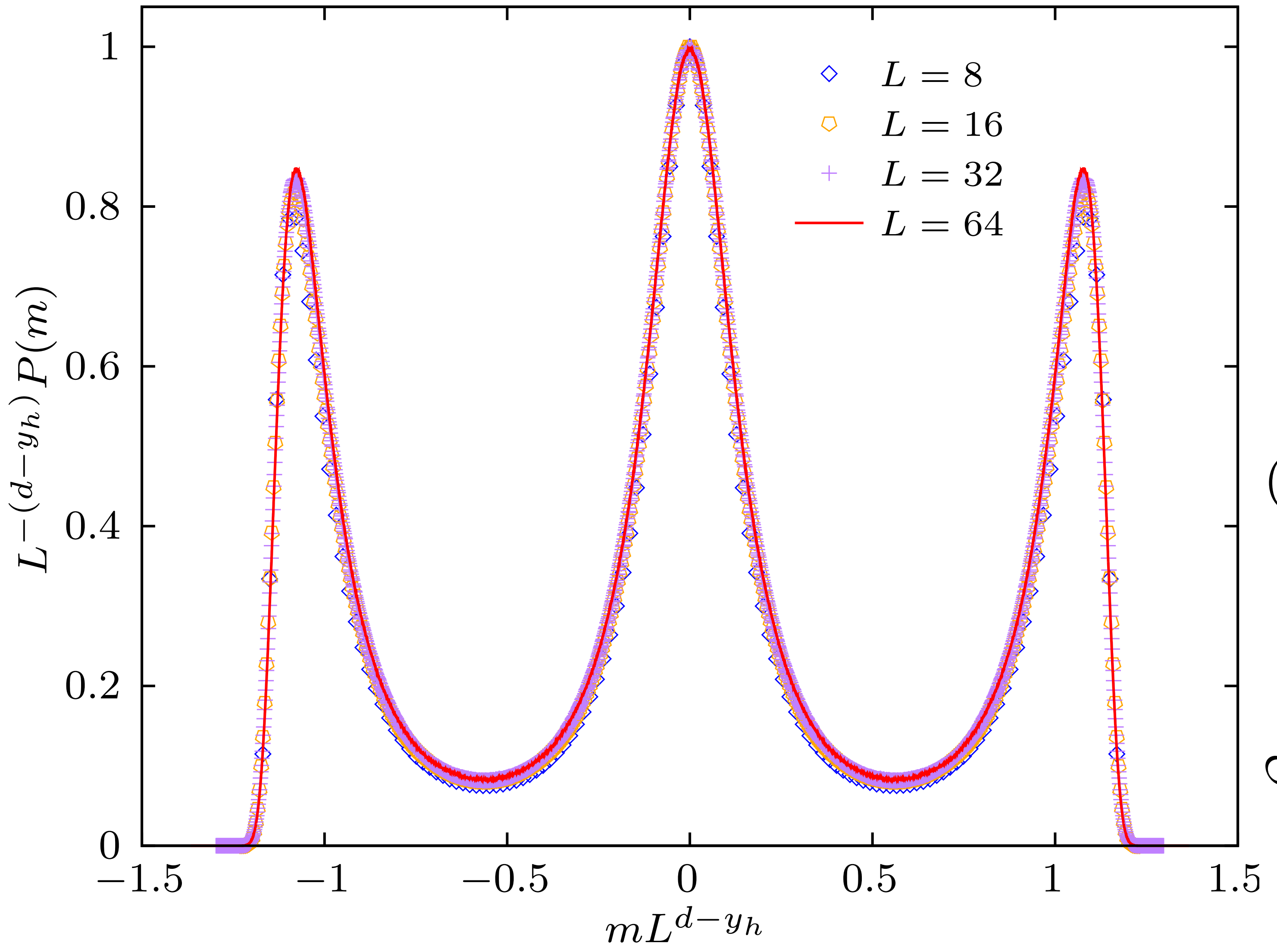
Creating the cumulant curves

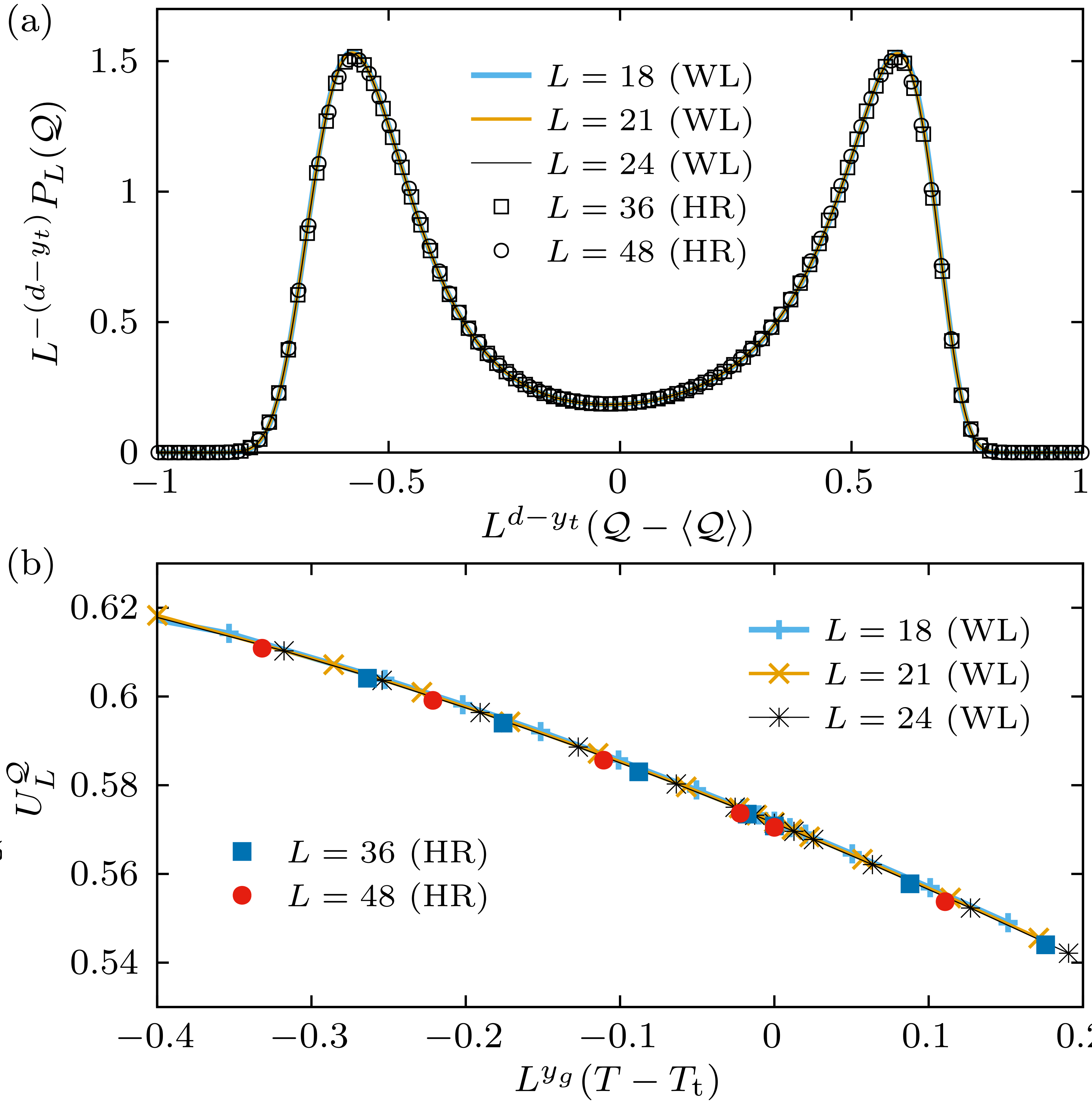
- Solve for equal population and equal height in $P_L(\tilde{Q})$.
- Calculate limiting values from Δ_L^* and s_L^*.
- Calculate $1 - \frac{1}{3}\frac{\langle Q^4 \rangle}{\langle Q^2 \rangle^2}$ in the specified values.

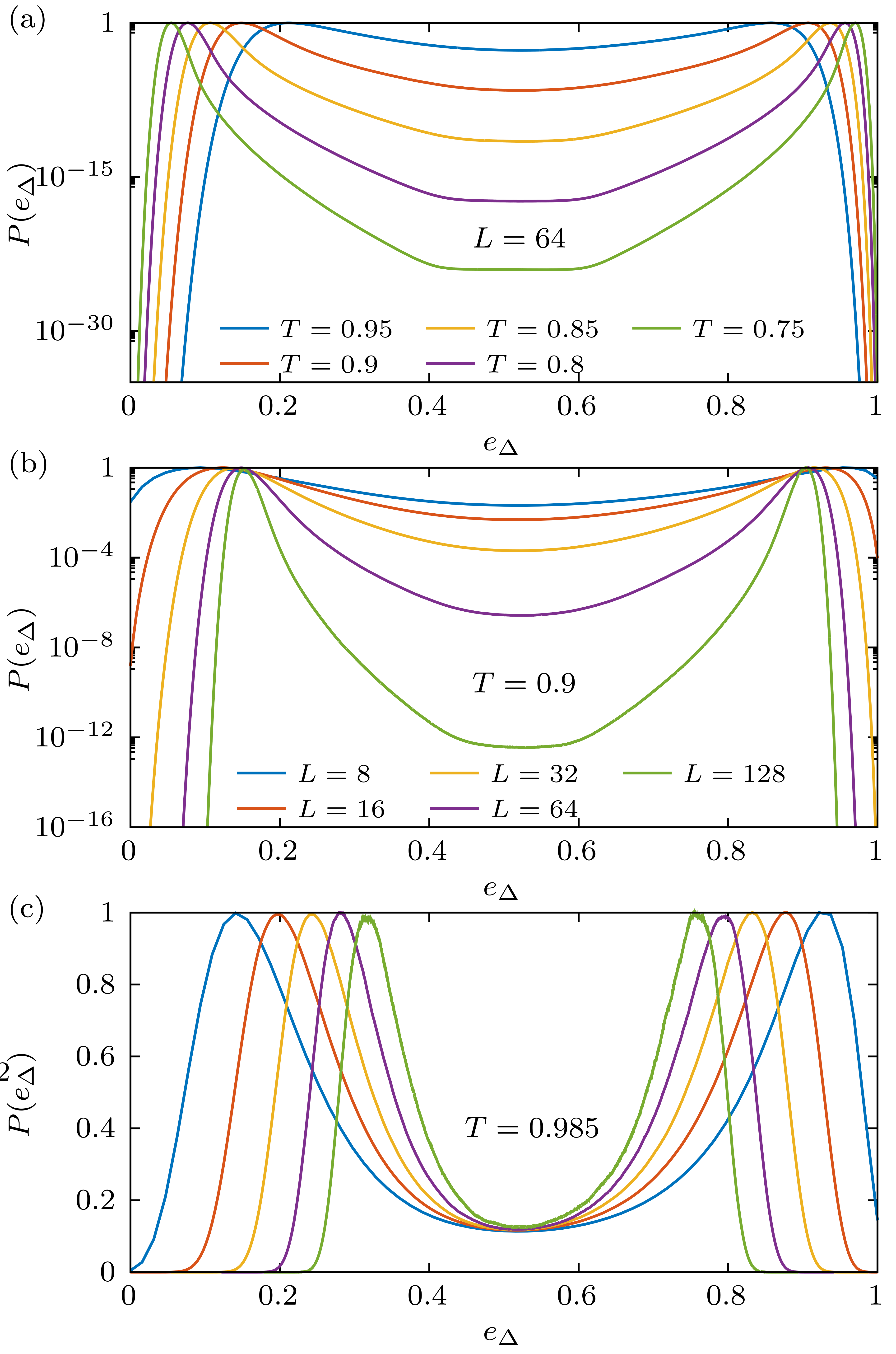




Distributions







Exponents

$\alpha_t/\nu_t = 1.6059(8)$

$\alpha_t/\nu_t = 1.5950(2)$