Machine-learned density of states for the doped Hubbard model

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TRA MATTER

TRANSDISCIPLINARY RESEARCH AREA

The generalized density of states method

Generalized DoS: [K. Langfeld, B. Lucini (2014)]

$$S(\phi) = S_r(\phi) + i\mu S_i(\phi)$$

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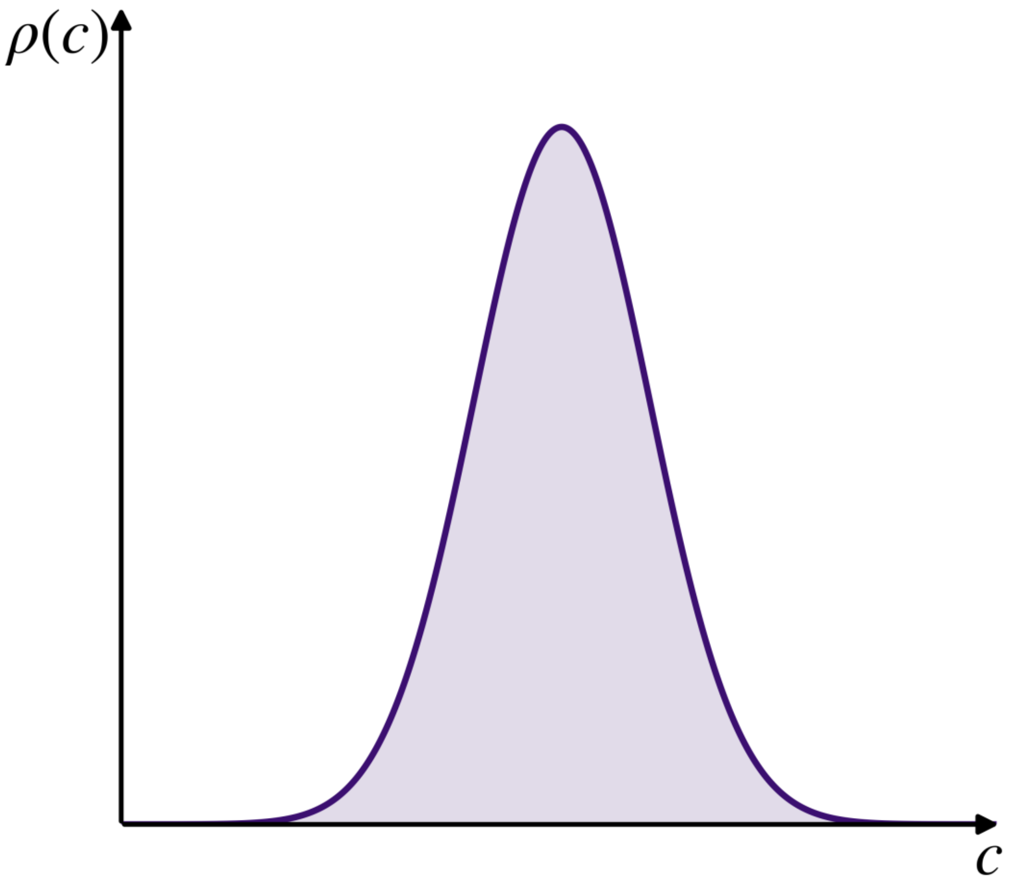

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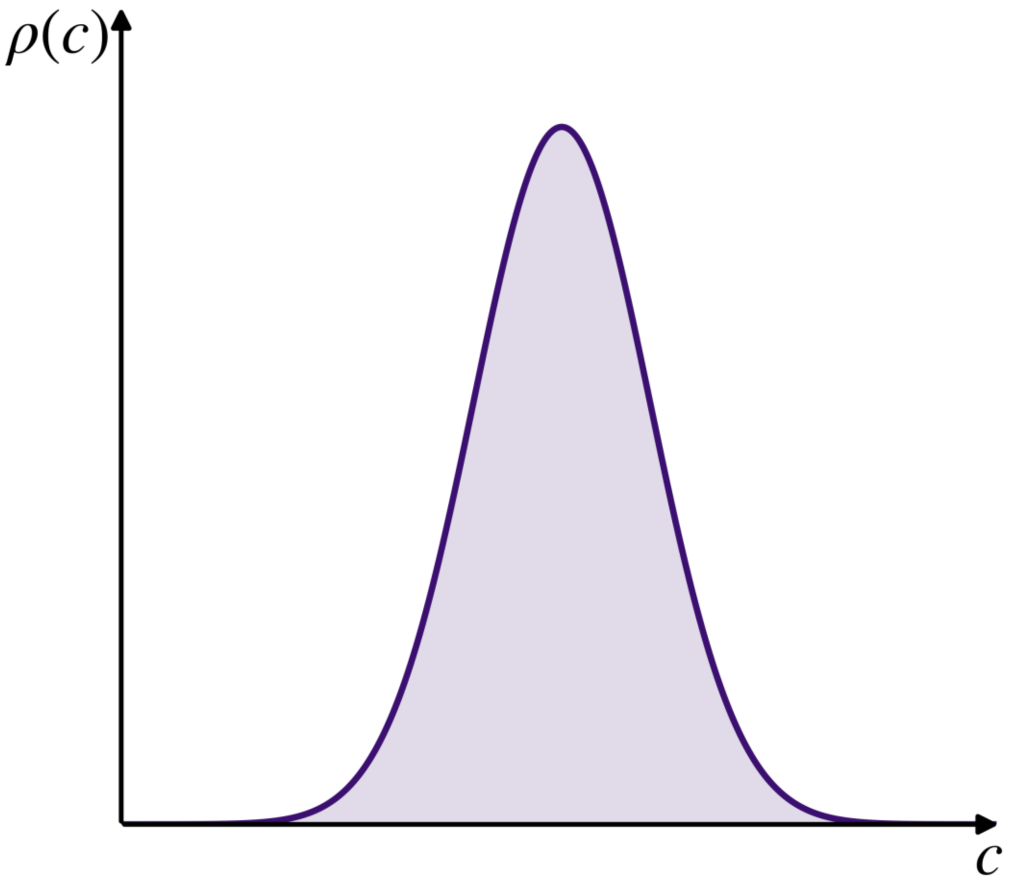

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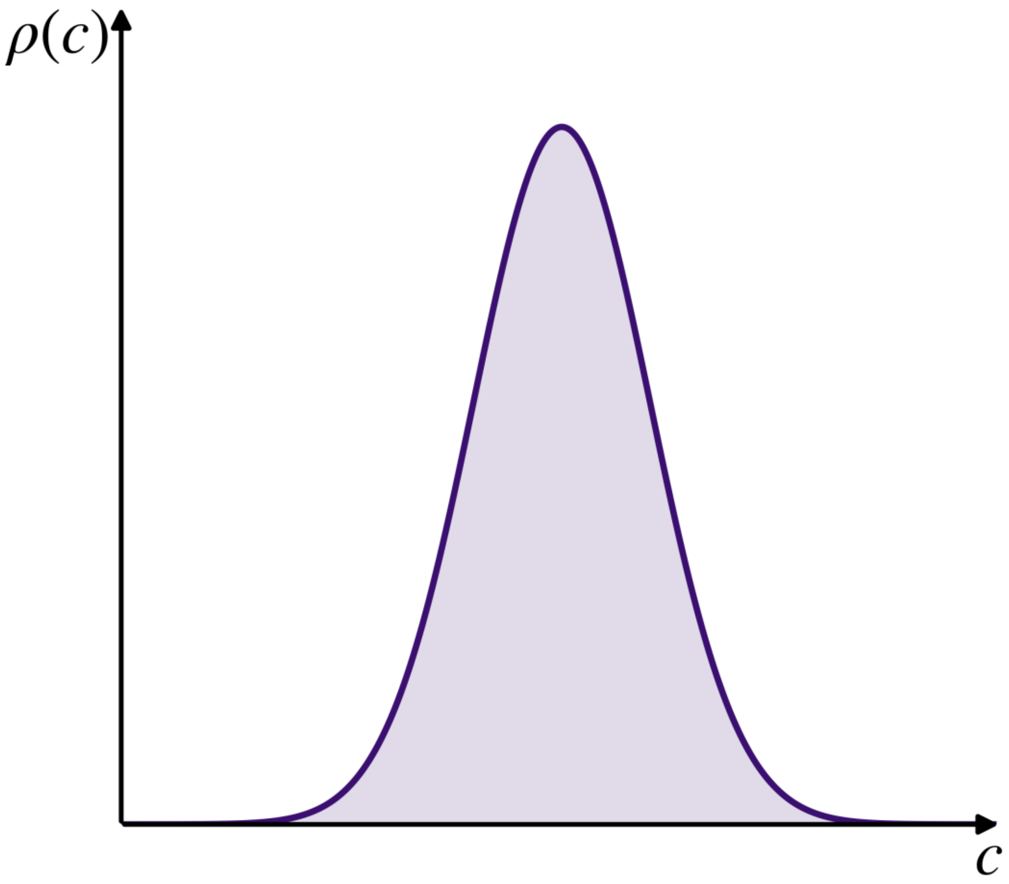

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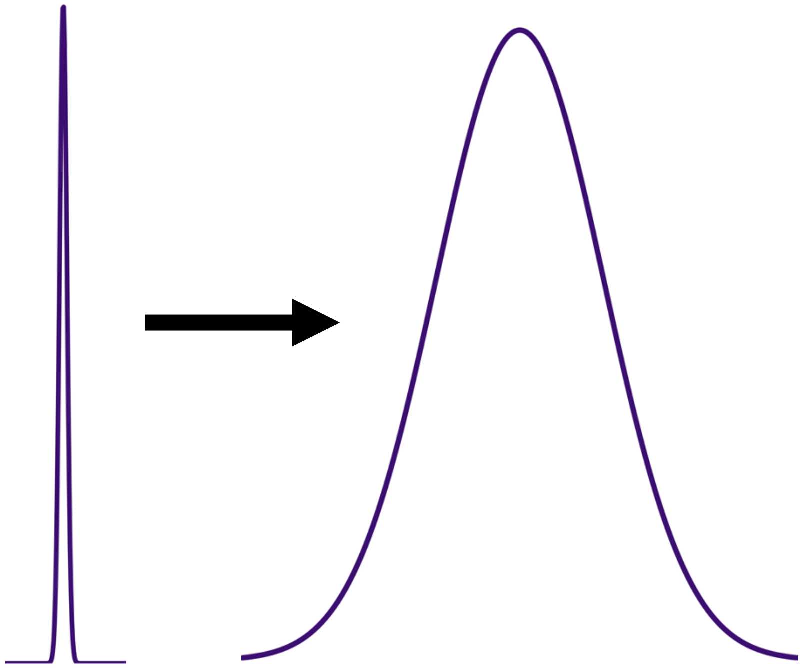

Machine-learned density of states

Original ML-DoS; Application to 2D ϕ^4: [J. M. Pawlowski, J. M. Urban (2023)]
Application to U(1) 2D: [S. Singh, L. Funcke (PoS Lattice 2026)]

P-regularize the δ-function:

$$\rho_P(c) = \int \mathcal{D}\phi \; e^{-S_r(\phi)} \boxed{e^{-\frac{P}{2}(c-S_i(\phi))^2 - \log \mathcal{N}}}$$

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$$=: \int \mathcal{D}\phi \; e^{\boxed{-S_{c,P}(\phi)}}$$

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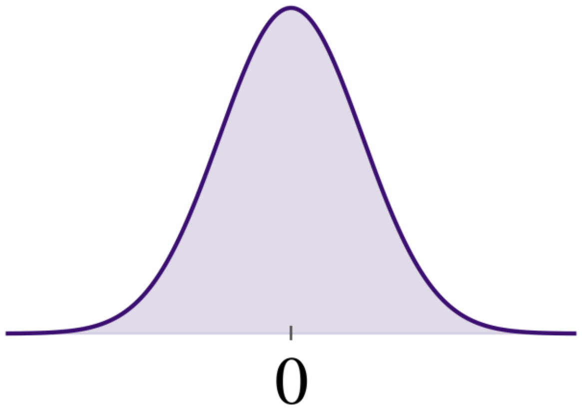
$$= \left\langle e^{-S_{c,P}(\phi)-log\; q_P(\phi|c))}\right\rangle_{\phi\sim q_P(\phi|c)}$$

Conditional Normalizing flow

Original ML-DoS; Application to 2D two-component ϕ^4: [J. M. Pawlowski, J. M. Urban (2023)]

Prior



$$\phi \sim p_0$$
$$c \in [0, c_{max}]$$

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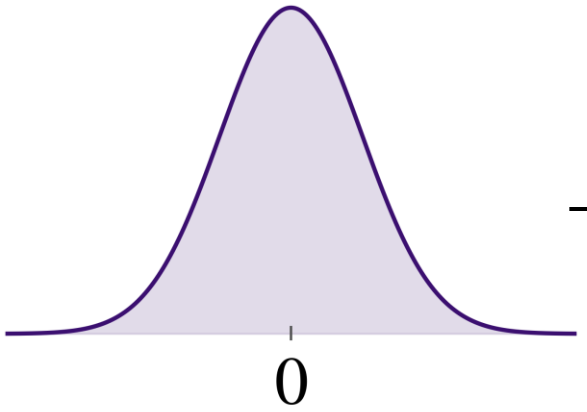

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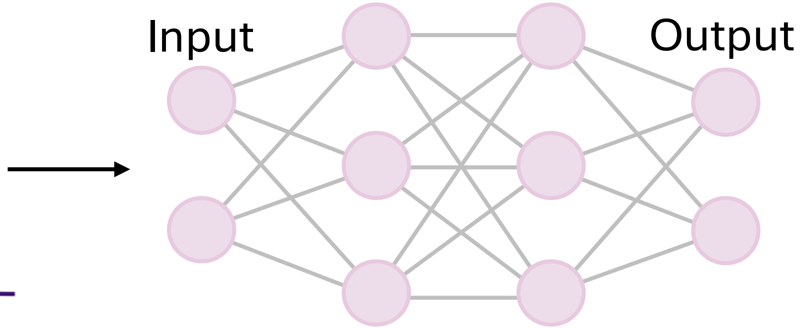
Neural Network



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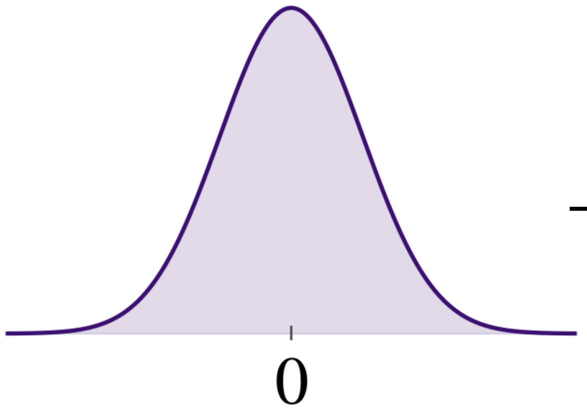

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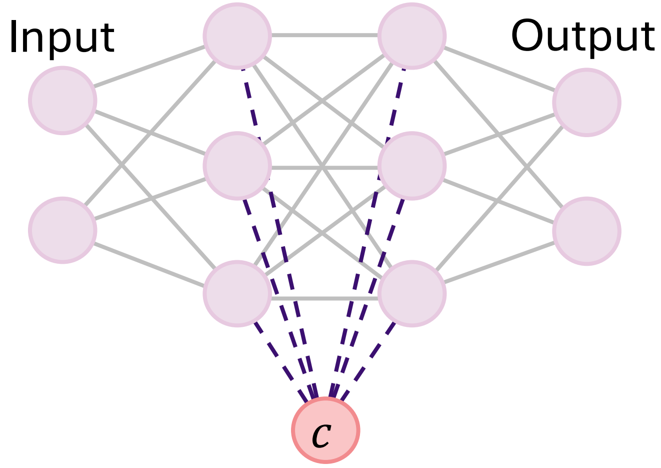

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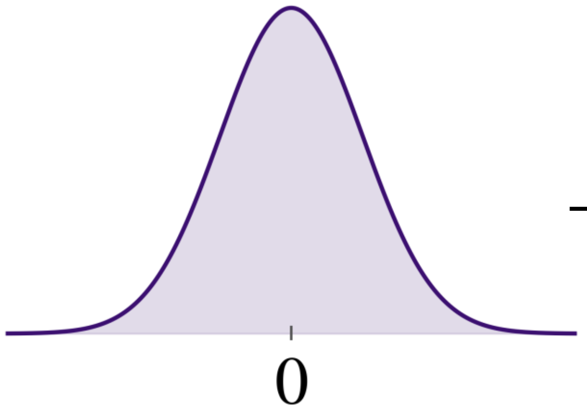

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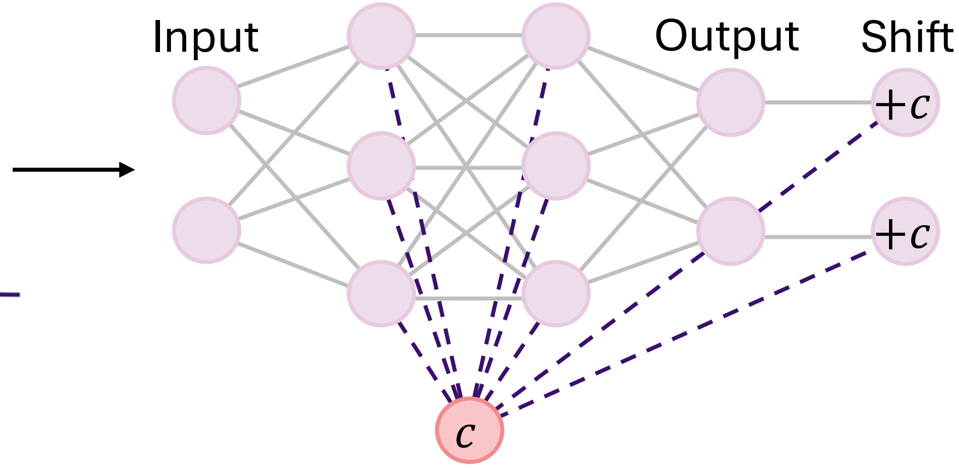

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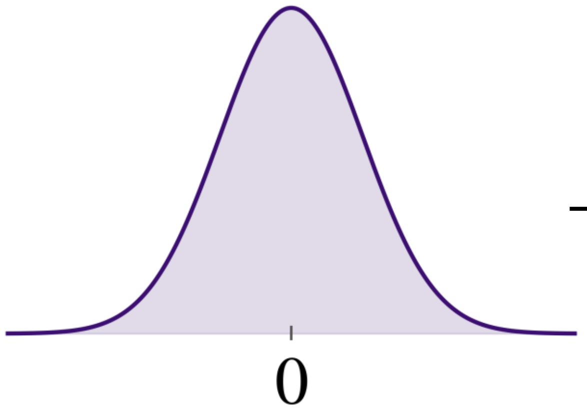

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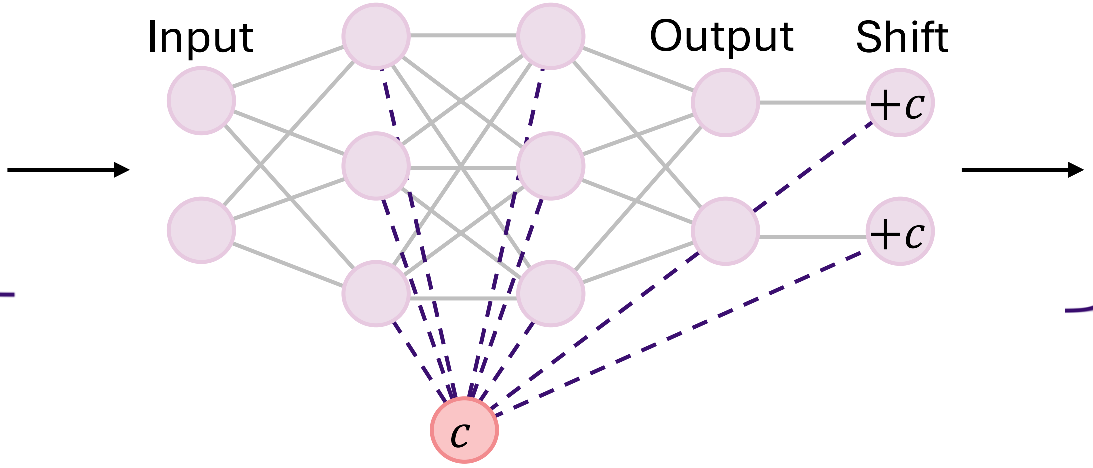
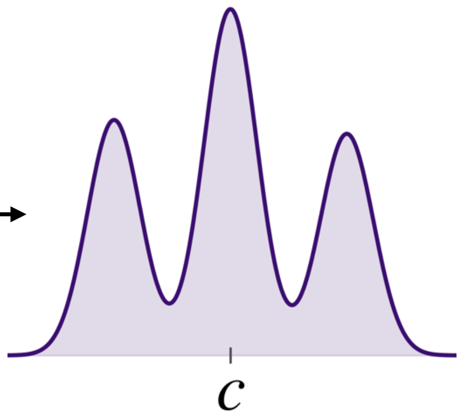


Learned distribution



$\langle \phi \rangle \approx c$

The Hubbard Model

Work in the charge basis:

$$S = \frac{1}{2\widetilde{U}} \sum_{x,t} {\phi_{x,t}}^2 - \log \det(\mathrm{M}[i\phi, \mu]\mathrm{M}[-i\phi, -\mu])$$

LLR Hubbard: [M. Körner, K. Langfeld, D. Smith, L. v. Smekal, PRD (2020)]

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$\Phi = \frac{1}{V} \sum_{x,t} \phi_{x,t}$ $V = N_x \cdot N_t$

$$\phi_{x,t} \to \phi_{x,t} + i\mu$$

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Phase!

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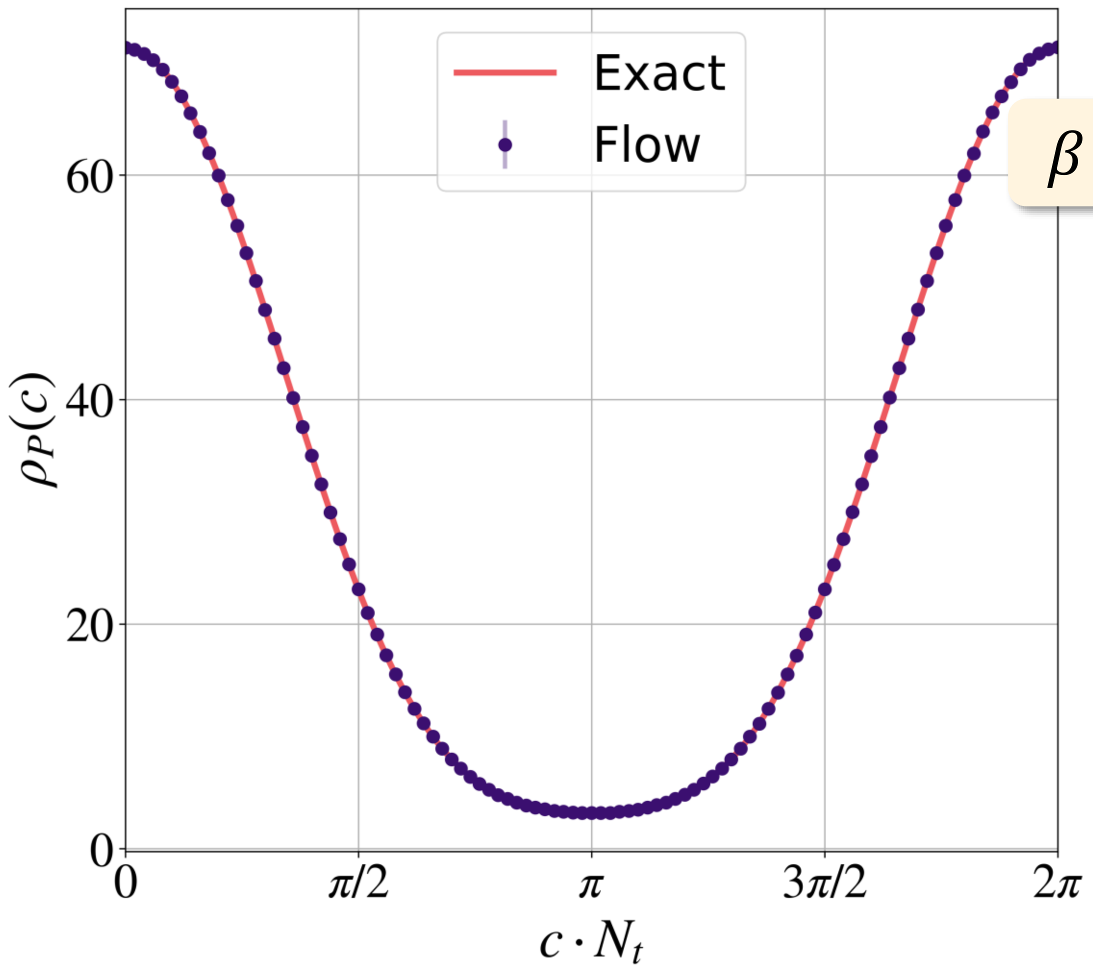
DoS results from flow

<u>What we keep fixed:</u>

- $N_x = 2 \rightarrow$ proof-of-principle demonstration
- $U = 1$
- $P = 1000$
- Use diagonal disc. for training

DoS results from flow



$\beta = 1, N_t = 1$

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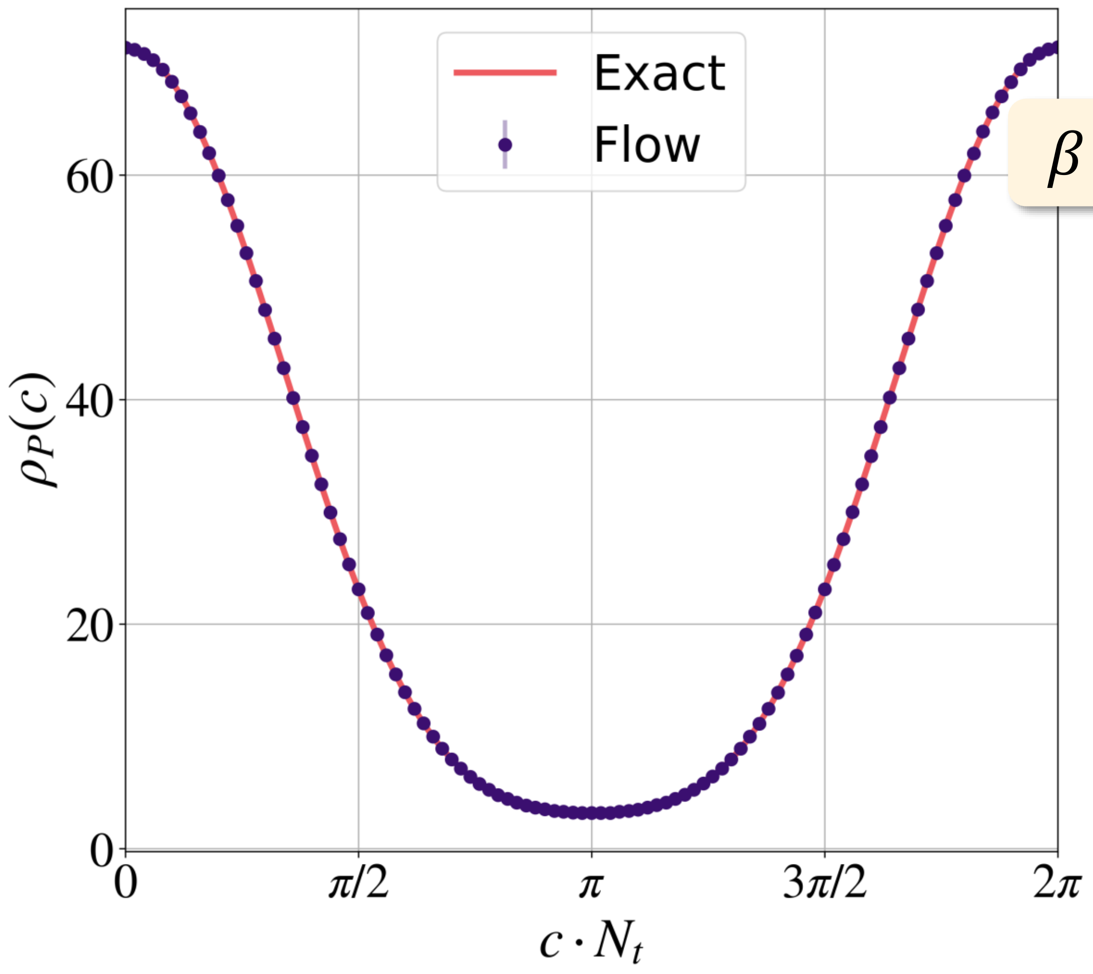

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$$\rho_{P,exact}(c) = \int \mathcal{D}\phi \; e^{-S_{c,P}(\phi)}$$

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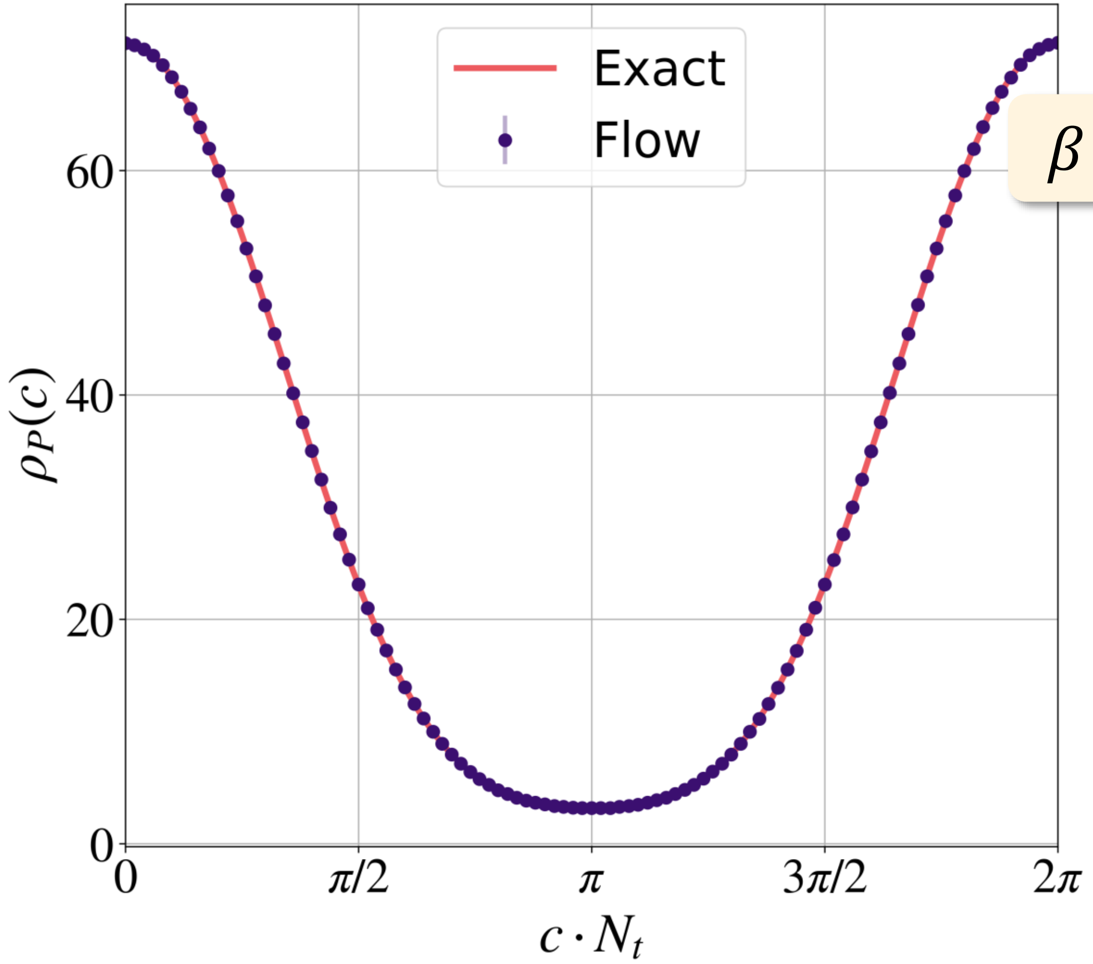

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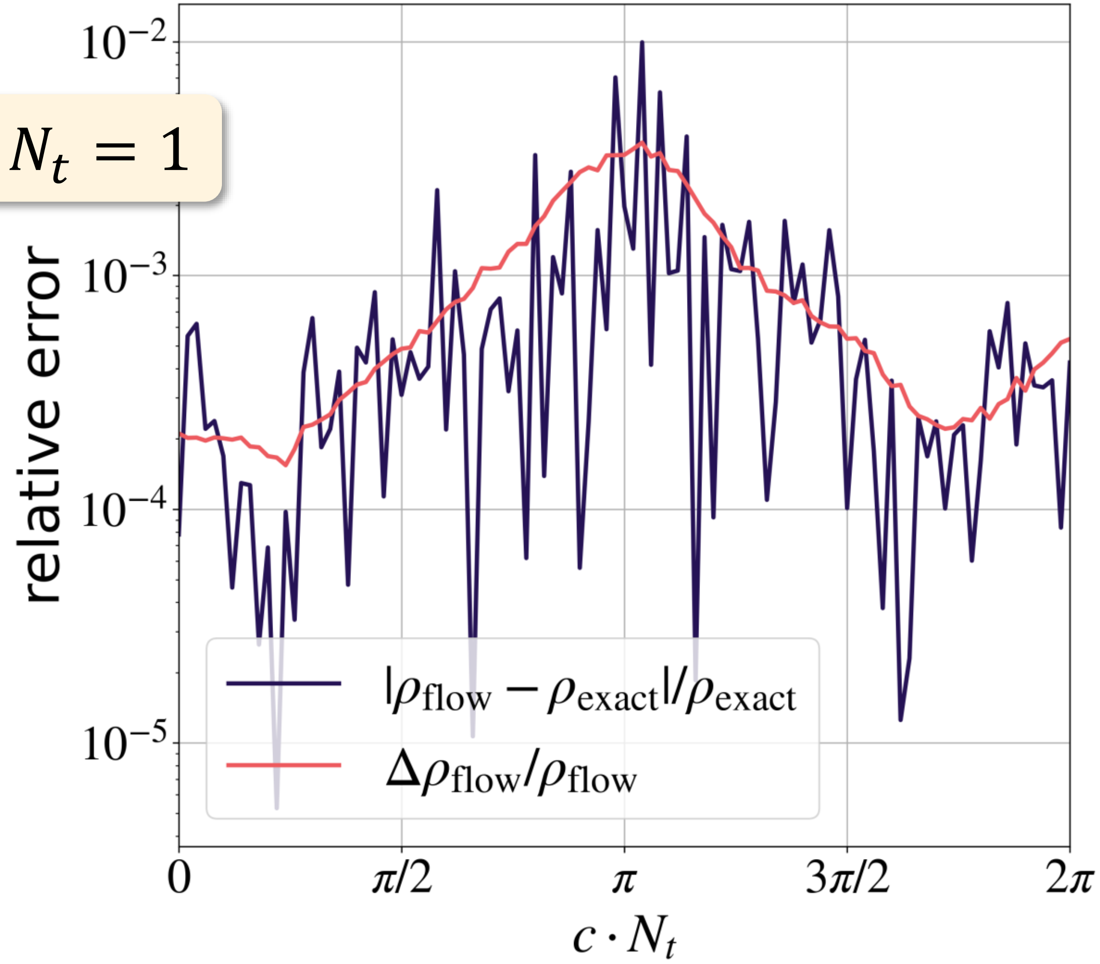

Partition function

$$Z_{true} = e^{\frac{\omega^2}{2\gamma}} \int D\phi \; e^{-S_r(\phi) - i\omega\Phi - \frac{\gamma}{2}\Phi^2}$$

$\gamma = \frac{V}{\tilde{U}}$ and $\omega = \gamma\delta\mu$

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$$Z_{true} = e^{\frac{\omega^2}{2\gamma}} \int D\phi\, e^{-S_r(\phi) - i\omega\Phi - \frac{\gamma}{2}\Phi^2} = \sqrt{\alpha}\, e^{\frac{\alpha\omega^2}{2\gamma}} \int dc\, \rho_P\, e^{-\alpha(i\omega c + \frac{\gamma}{2}c^2)}$$

Correction factor: $\alpha = \frac{P}{P-\gamma}$

$$Z_P = e^{\frac{\omega^2}{2\gamma}} \int dc\, \rho_P(c) e^{-i\omega c - \frac{\gamma}{2}c^2}$$

Semi-analytic approach

Semi-anlytic approach for DoS: [K. Langfeld (2016)]

Fourier decomposition of the DoS:

$$\rho_P(c) = \sum_{k=0}^{N_x} a_k \cos(k N_t c)$$

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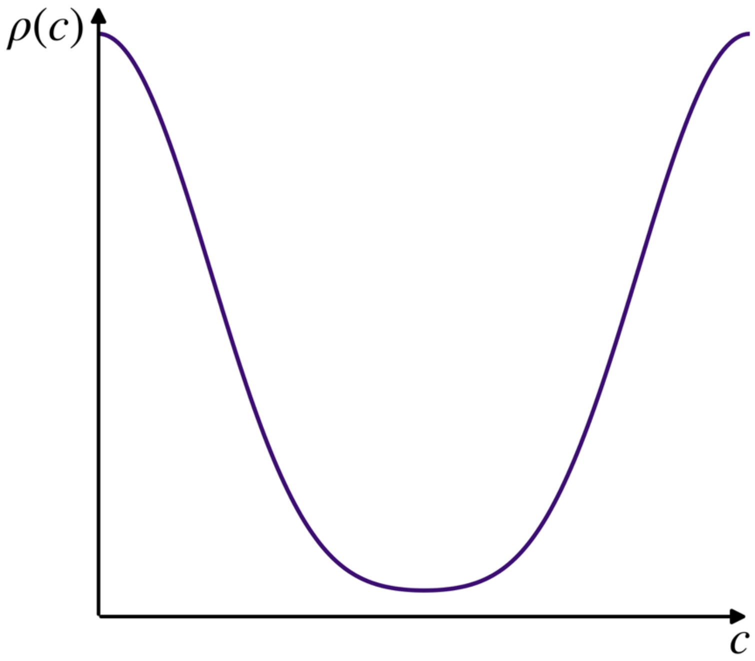

Semi-analytic approach

Fourier decomposition of the DoS:

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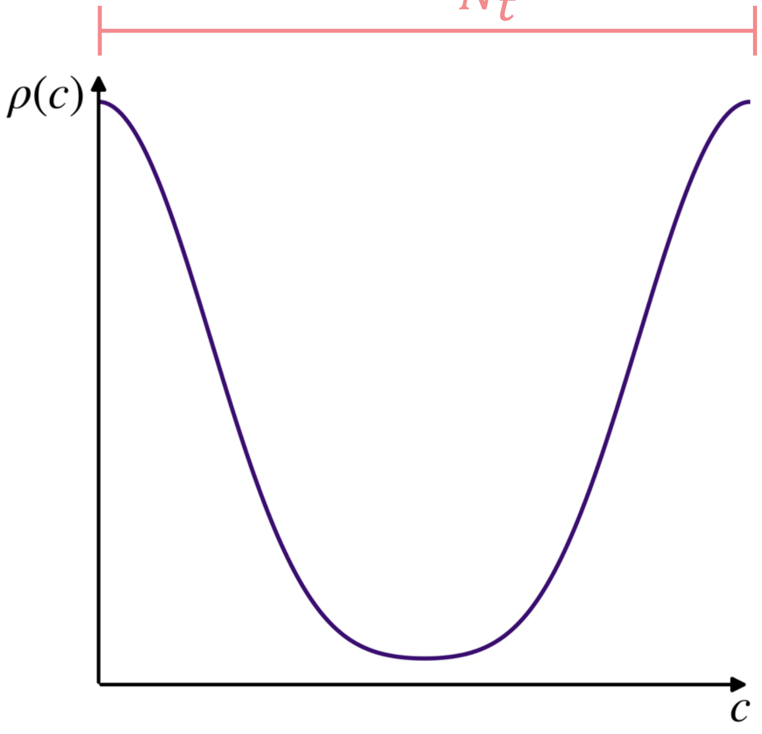
$$T = \frac{2\pi}{N_t}$$



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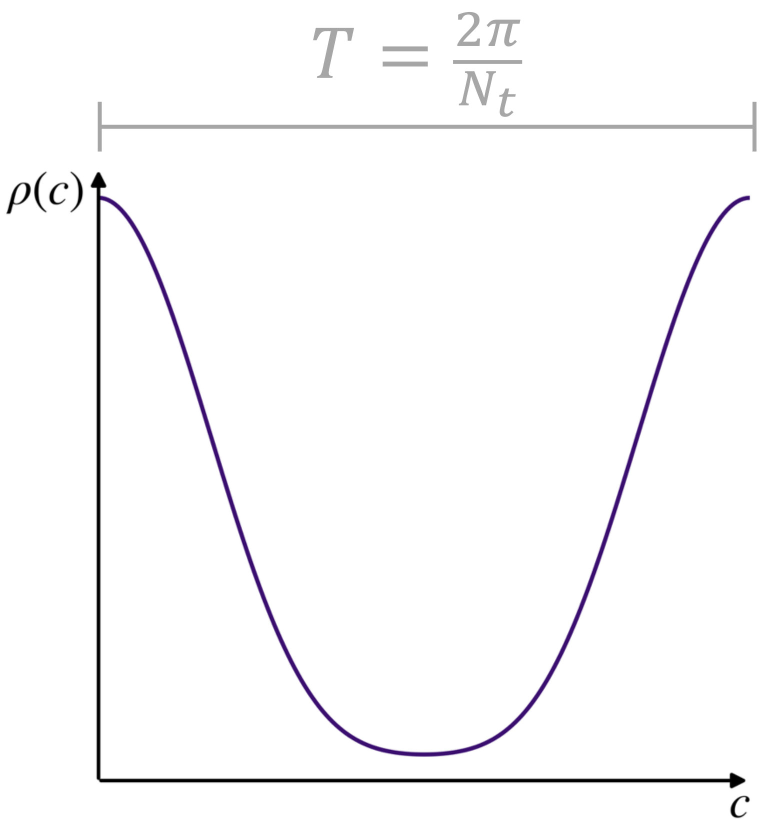
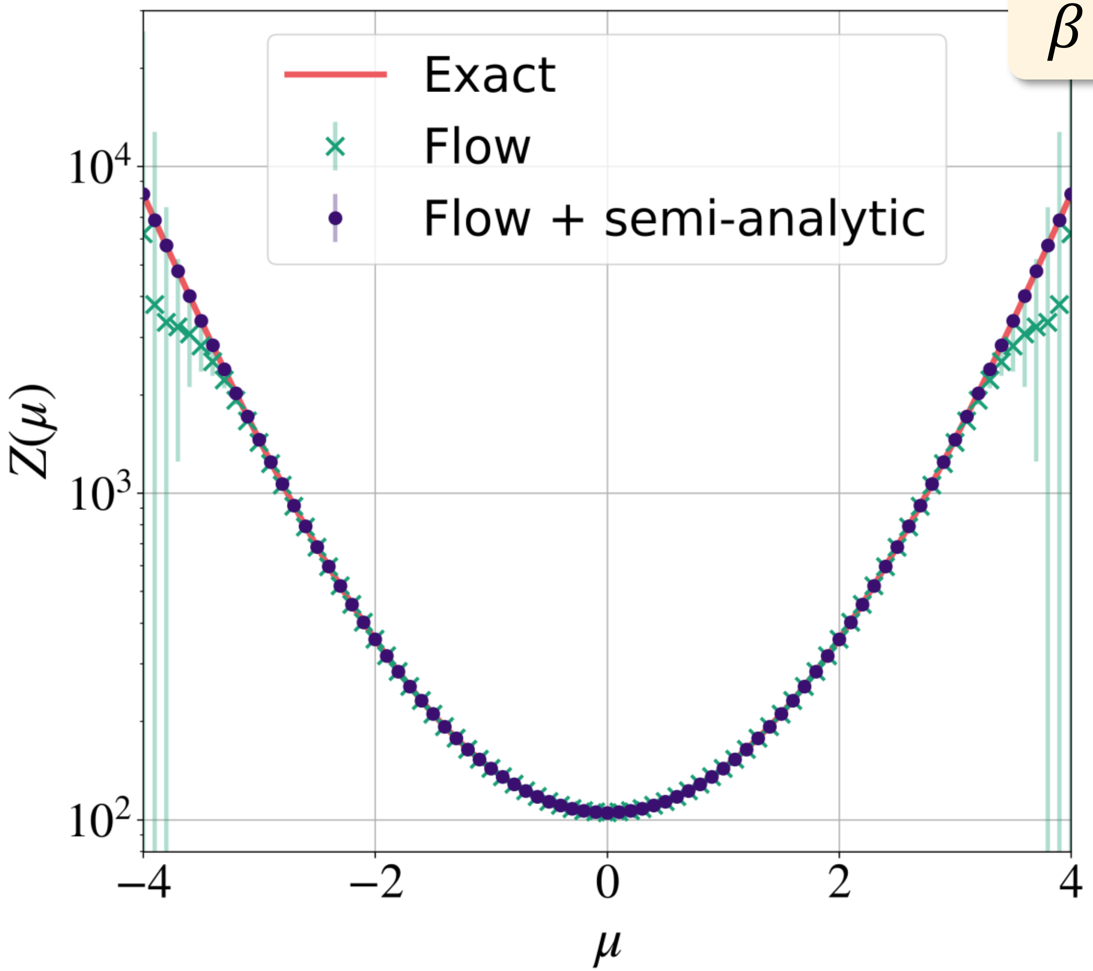
$$Z_{true} = \sqrt{\frac{2\pi}{\gamma}} \sum_{k=0}^{N_x} a_k e^{\frac{-k^2 N_t^2}{2\alpha\gamma}} \cosh(\mu\beta k)$$



Partition function results



$\beta = 1, N_t = 1$

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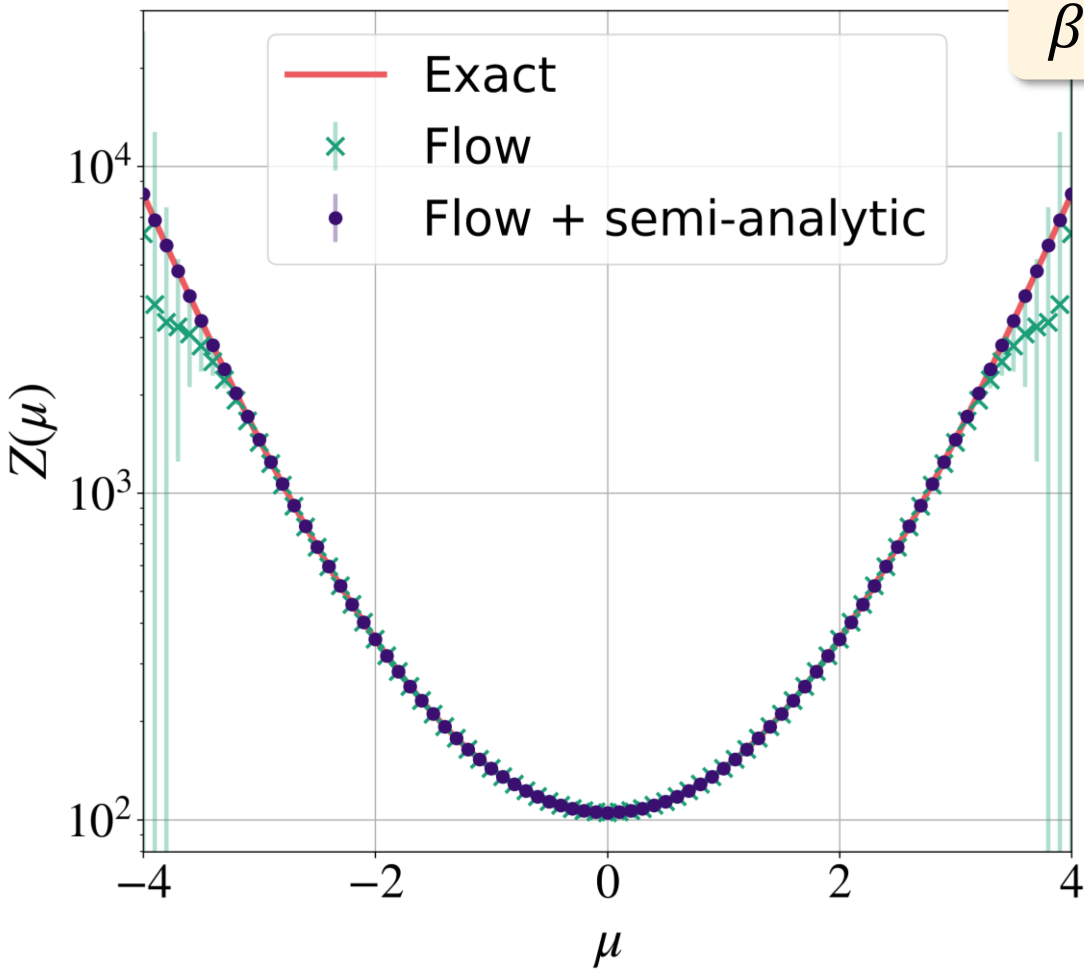

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$$Z_{exact} = \int \mathcal{D}\phi \; e^{-S(\phi)}$$

Charge density

$$Q = \frac{1}{\beta}\frac{d}{d\mu}\ln Z$$

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learn $\rho_P(c)$ once → get a_k

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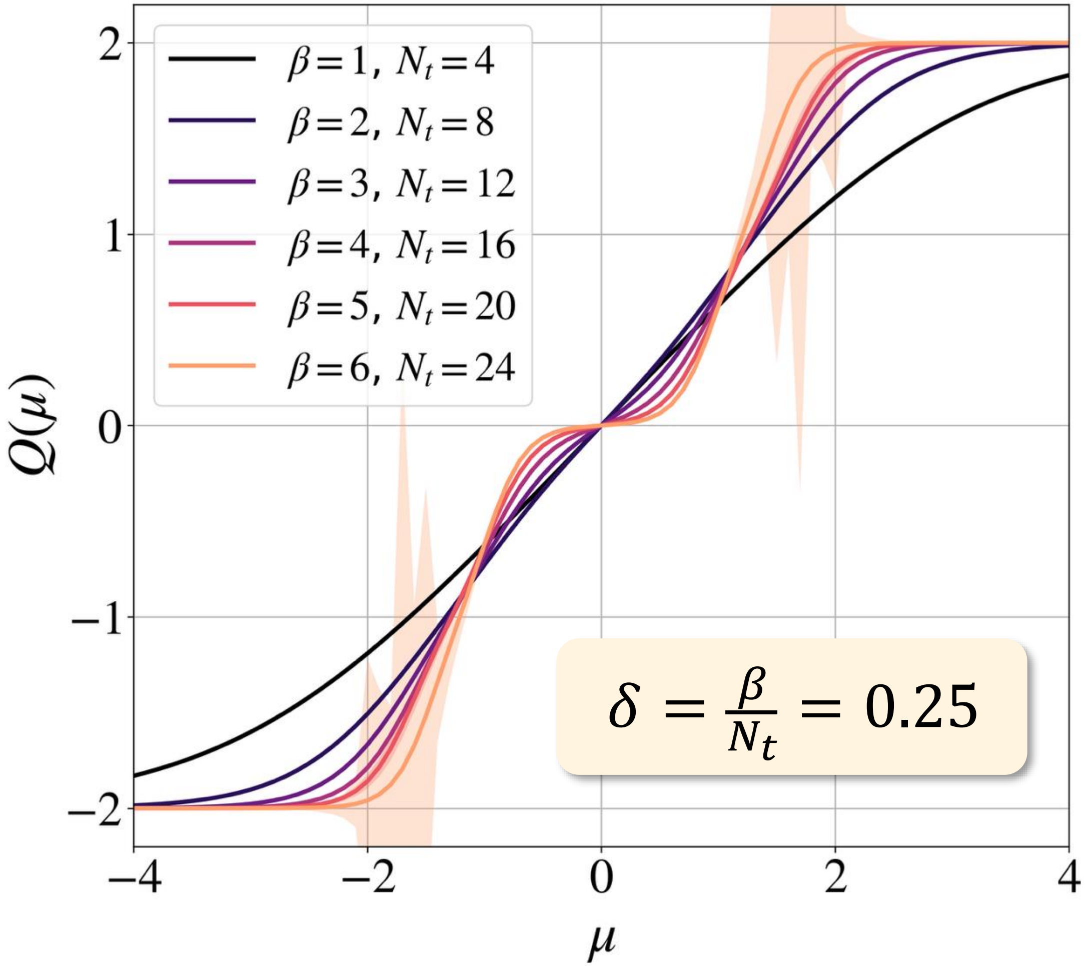
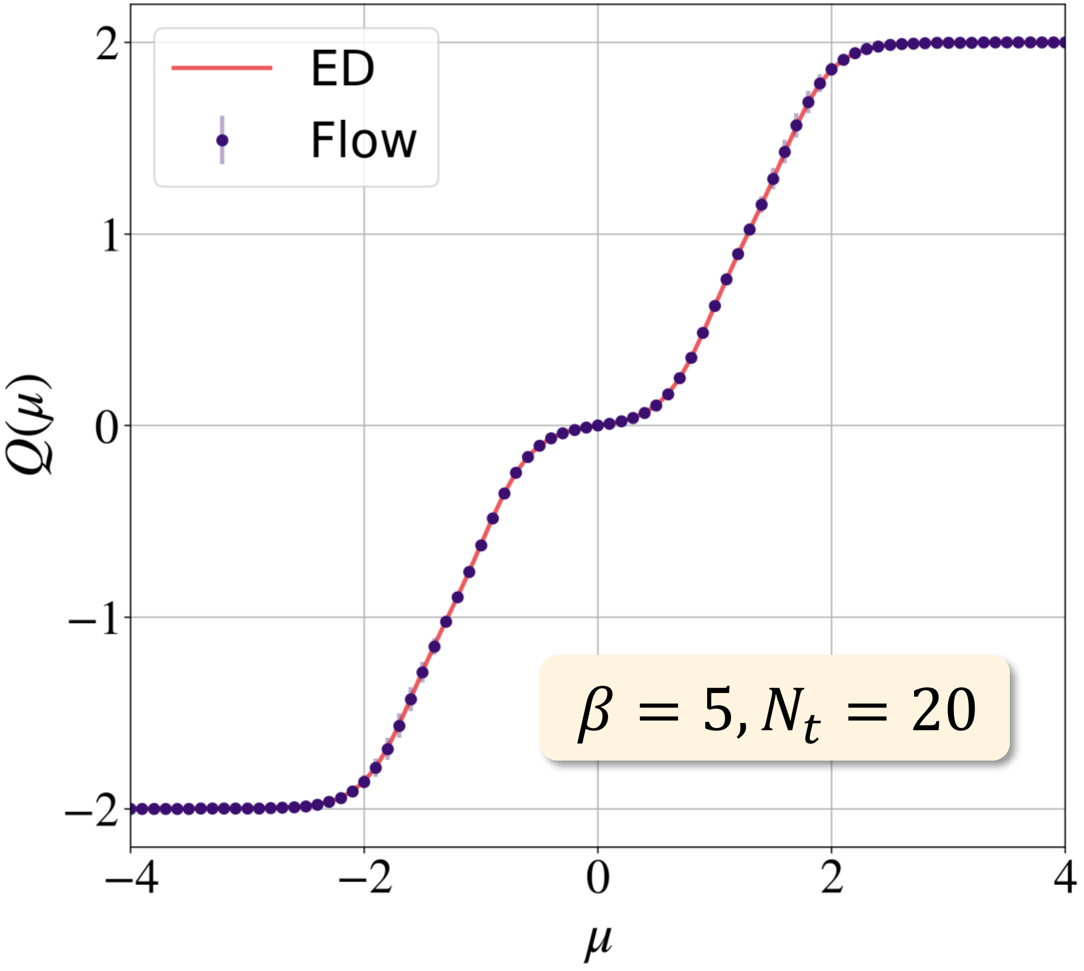
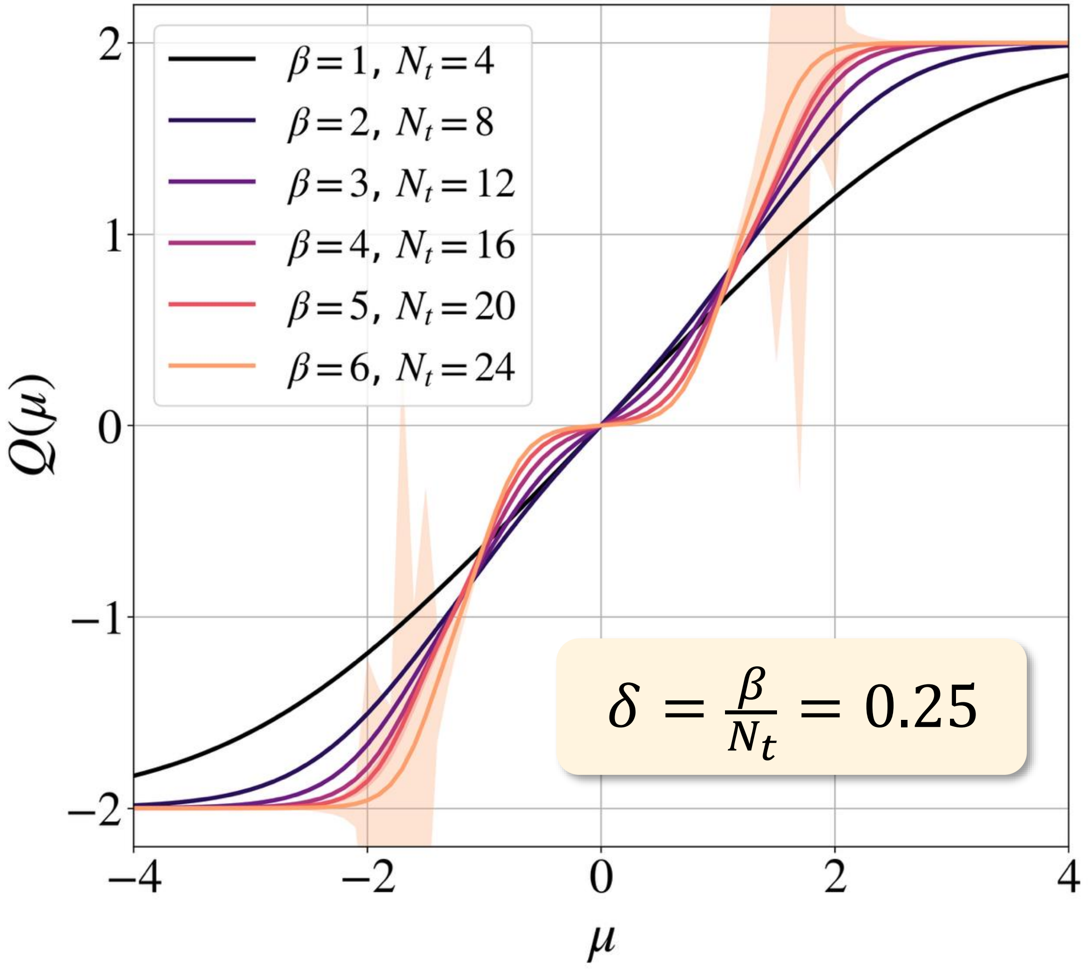


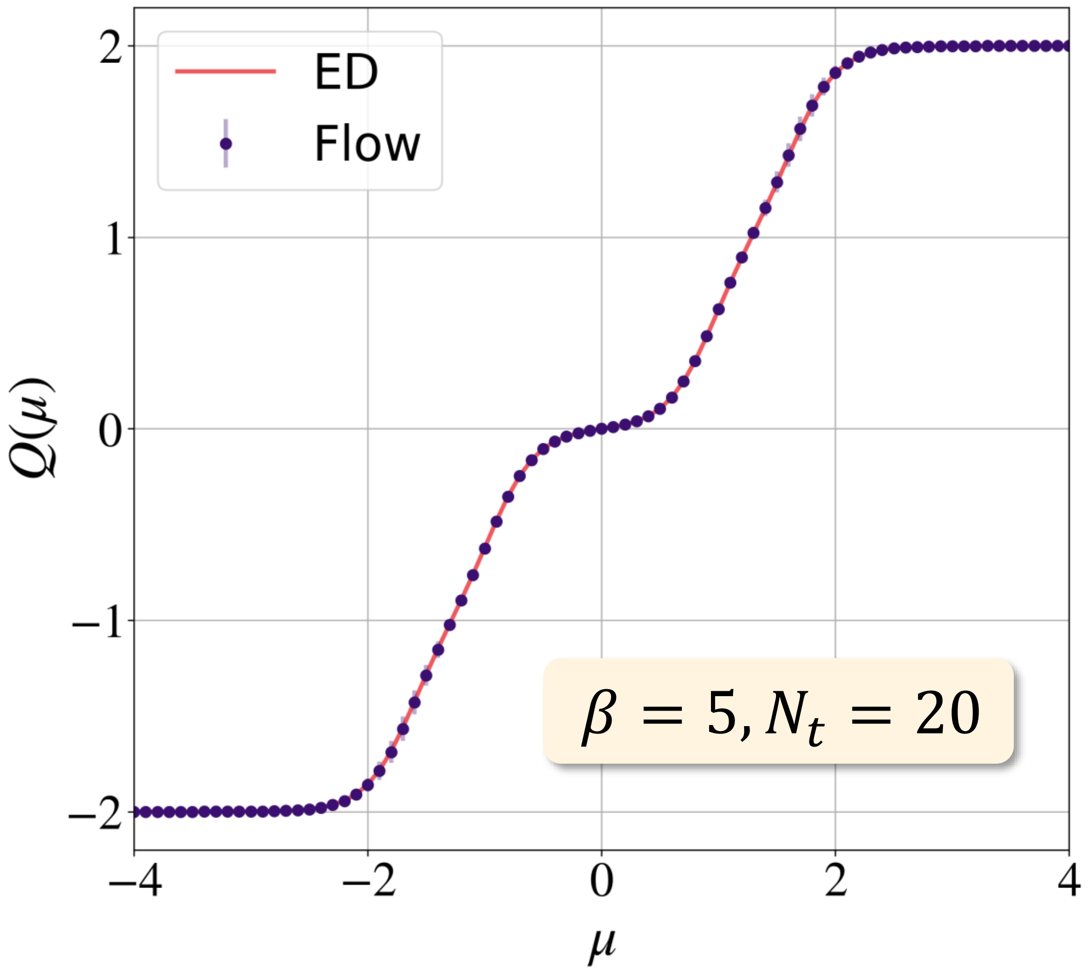
$\delta = \frac{\beta}{N_t} = 0.25$

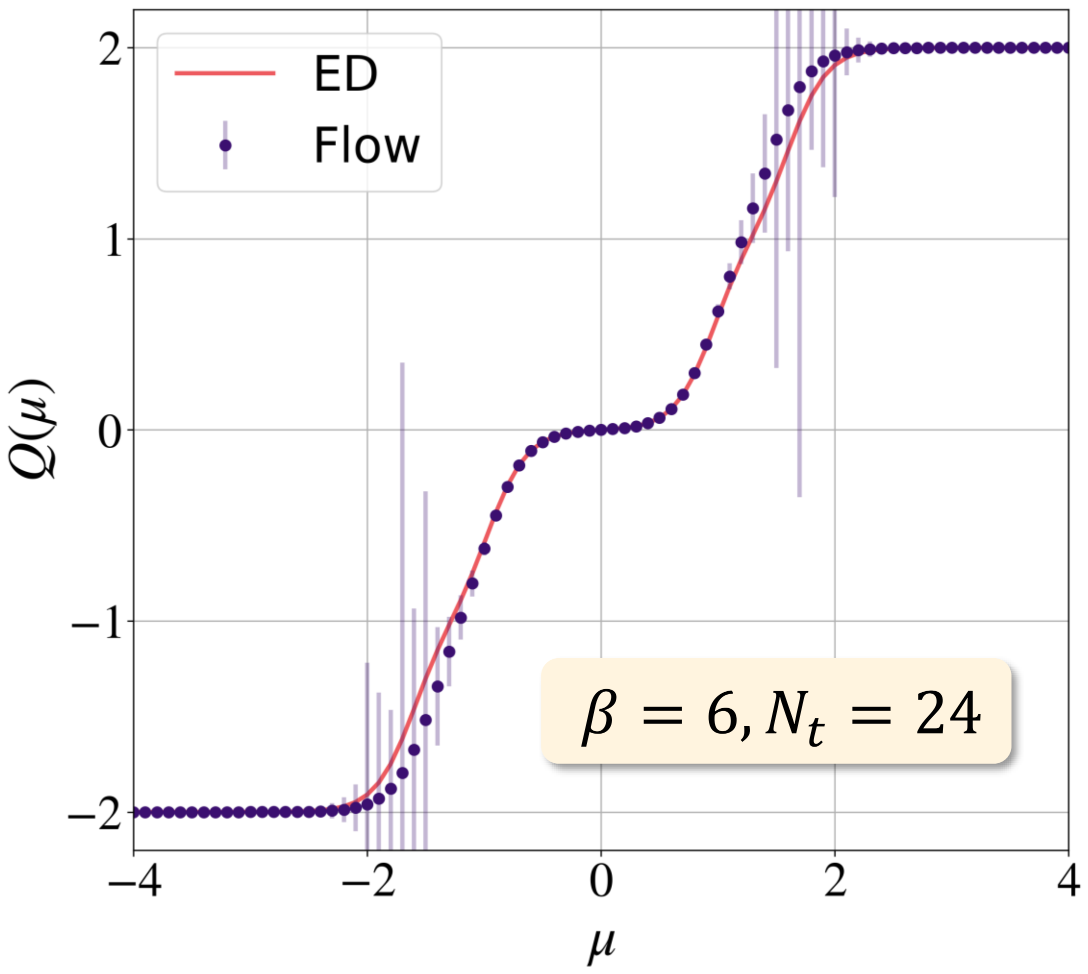
Charge density



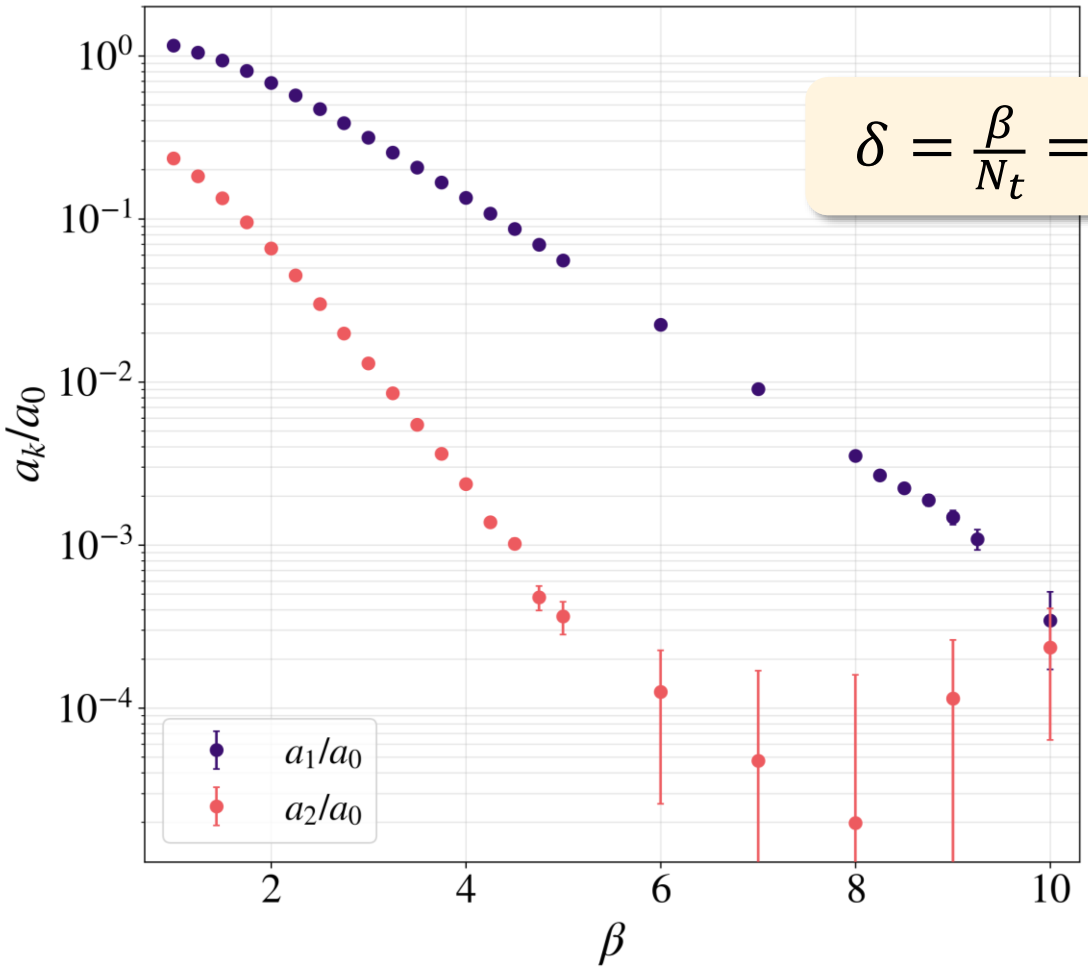


Charge density





Extrapolation of the a_k



$$\delta = \frac{\beta}{N_t} = 0.25$$

get a_k from noisy $\rho_P(c)$

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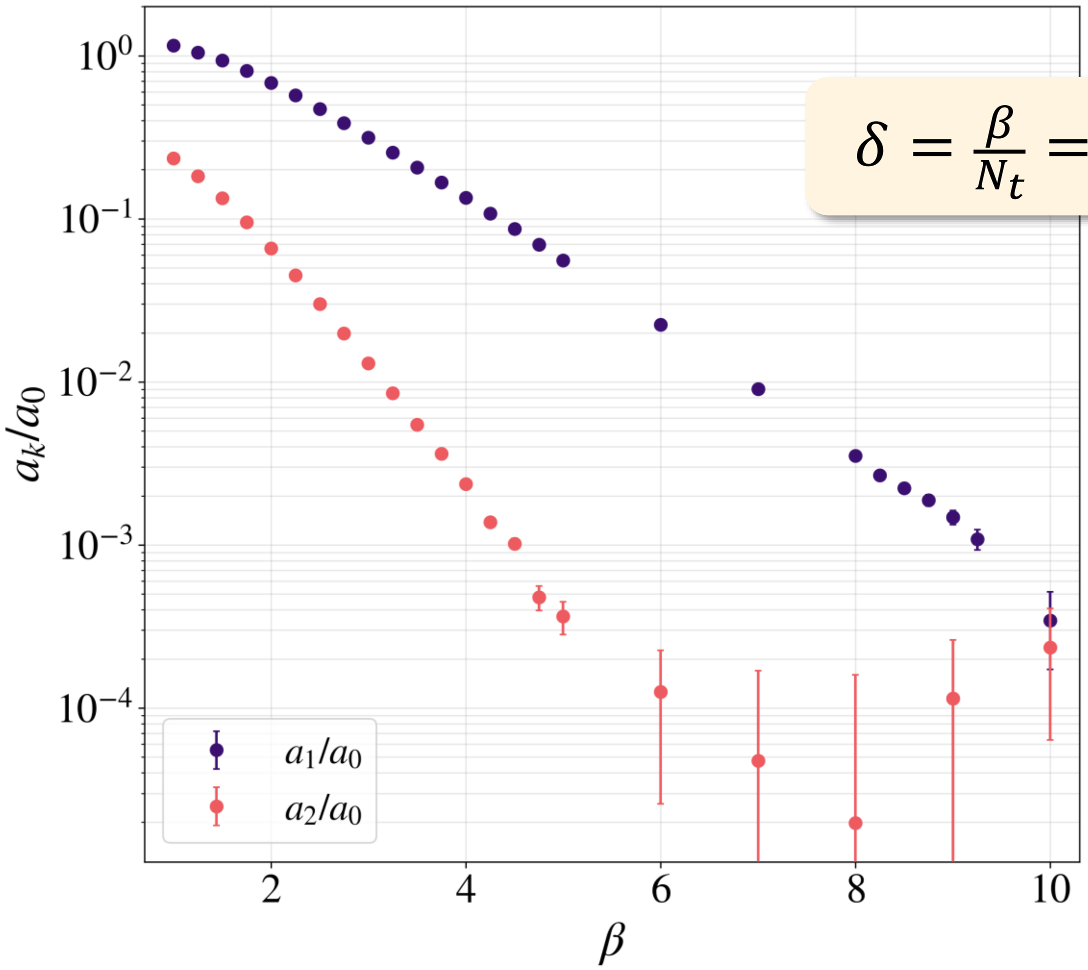

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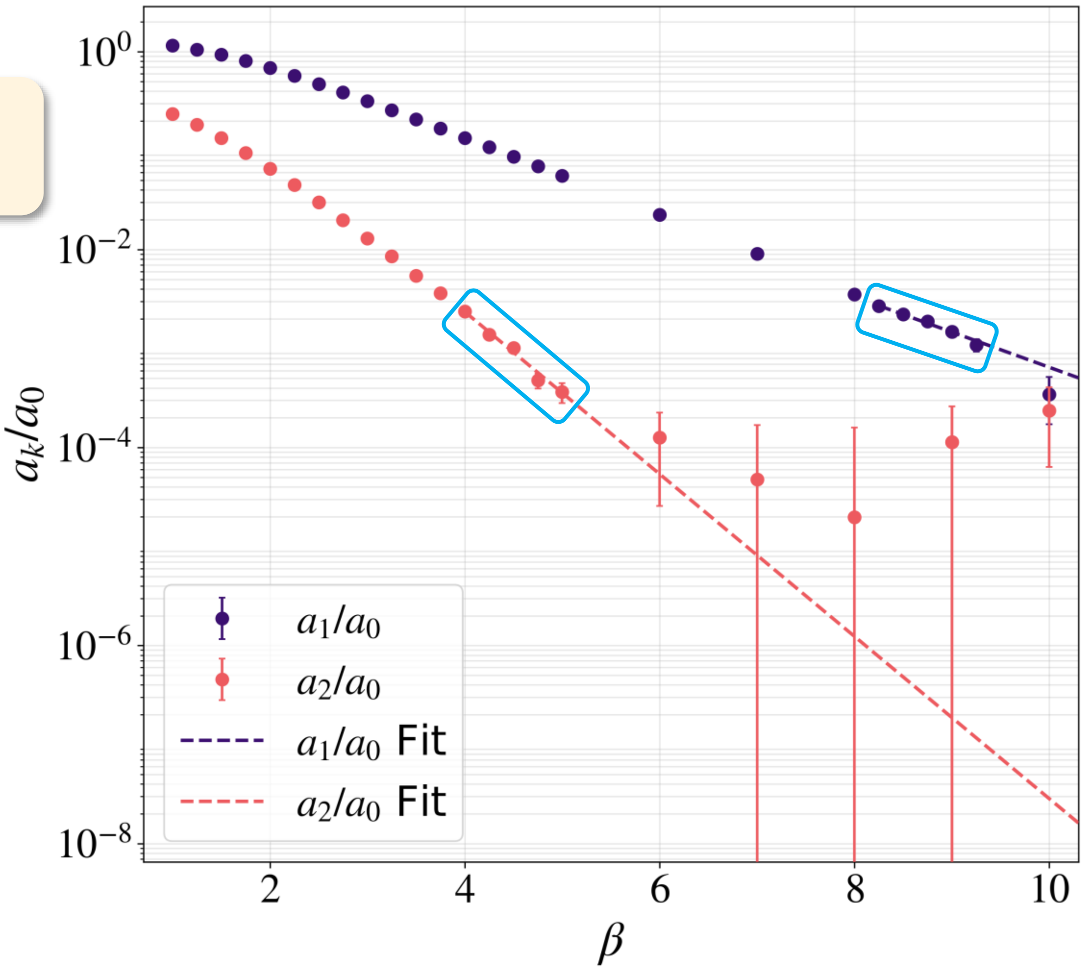
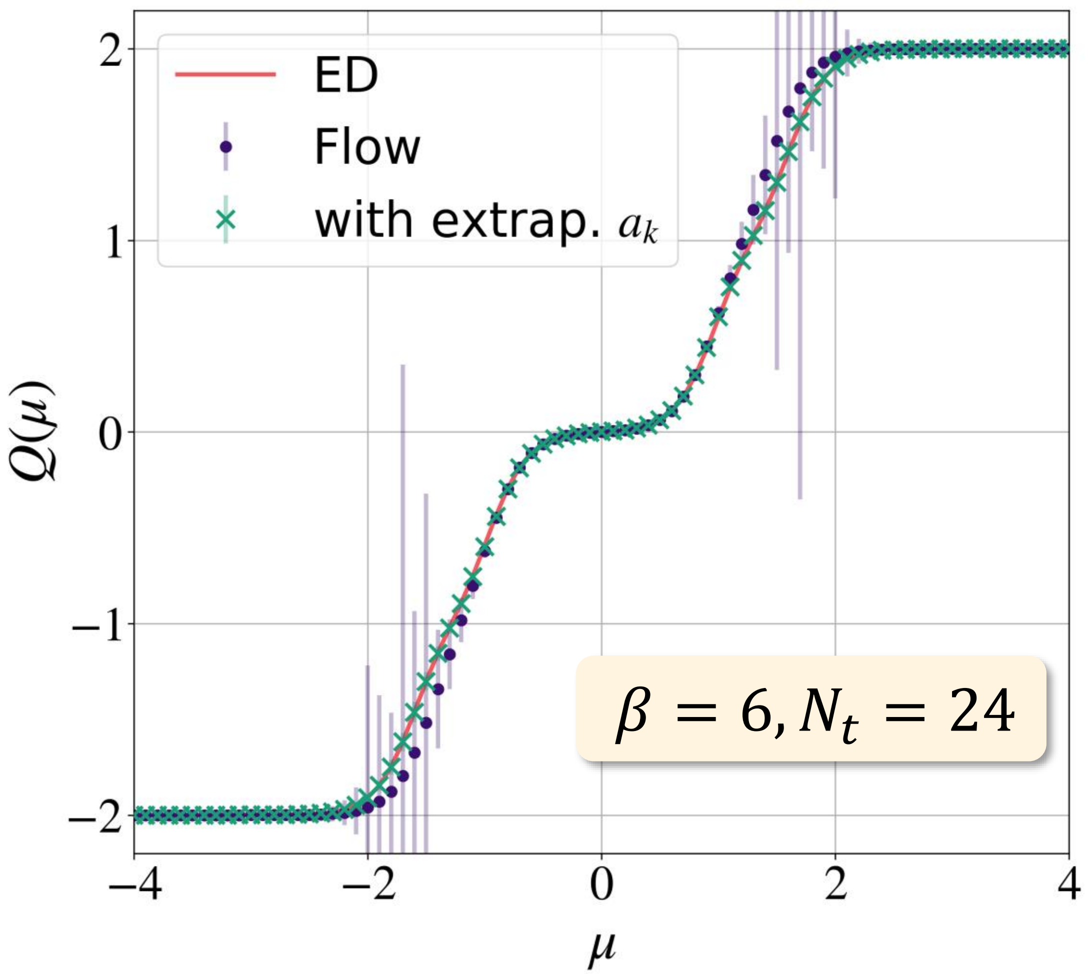
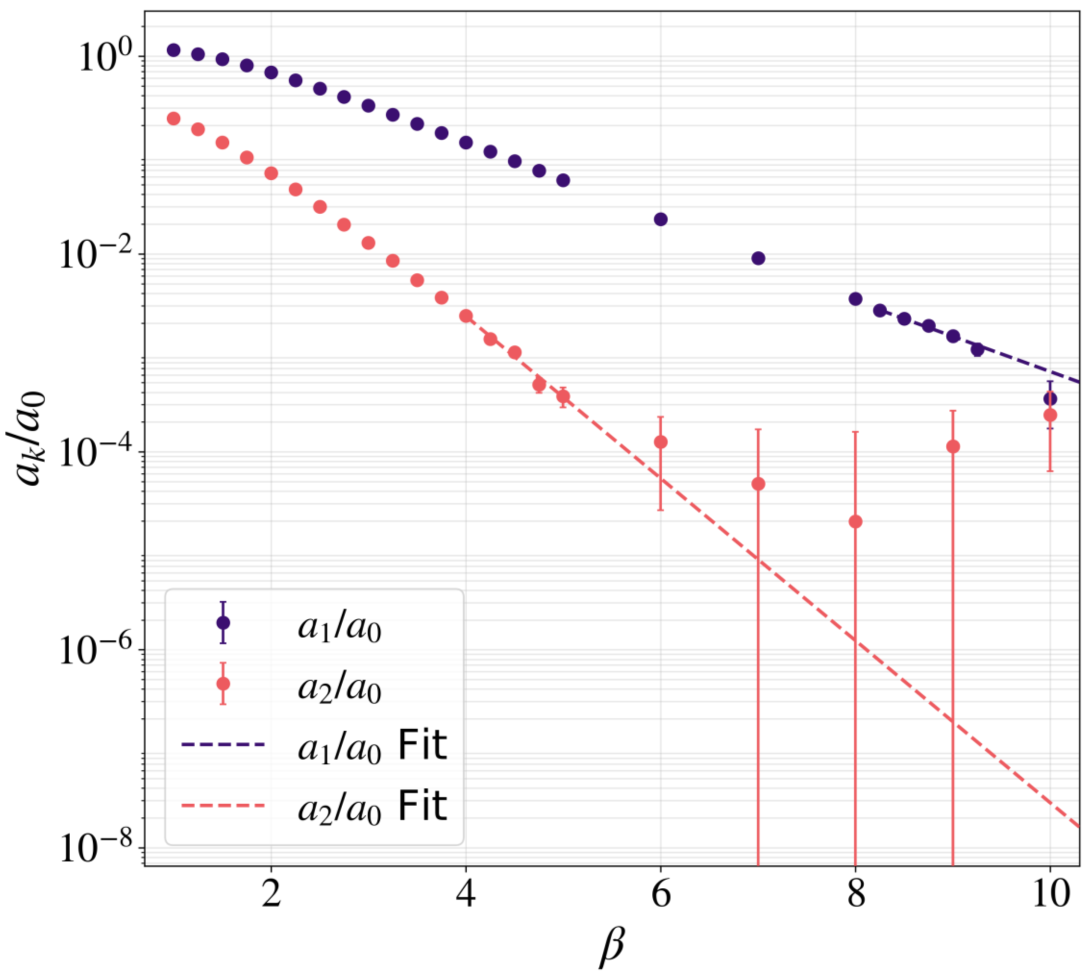
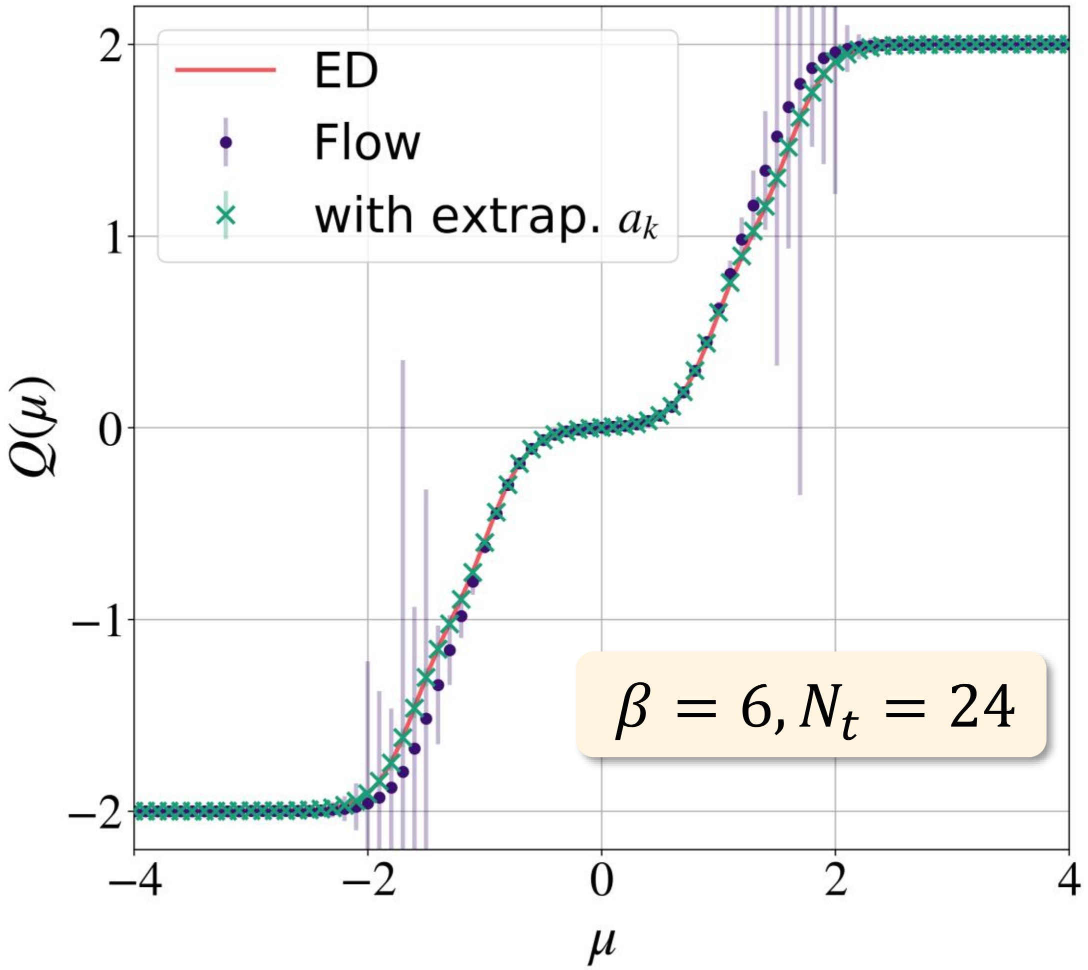


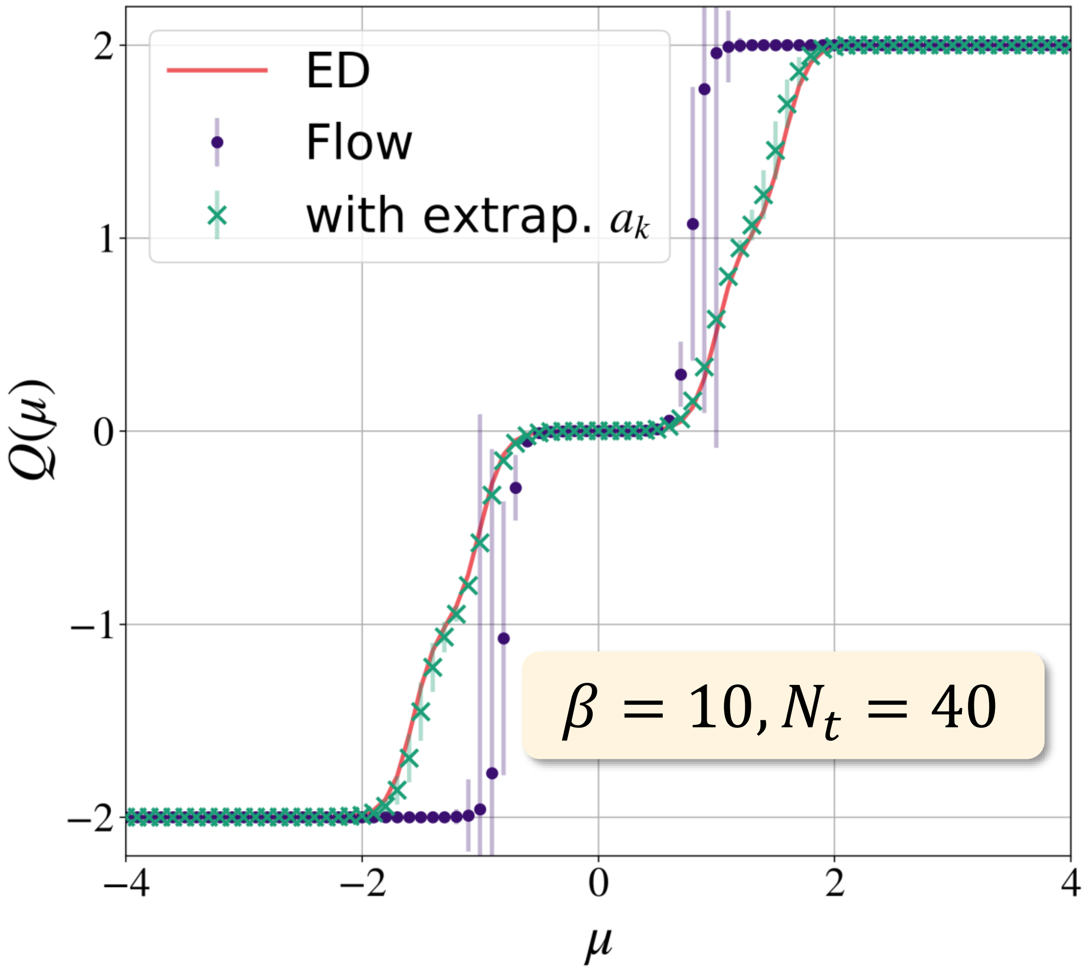
Extrapolation of the a_k





Extrapolation of the a_k





Summary

Numerical results

- Applied the generalised DoS method to the Hubbard model

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→ Match ED until $\beta = 10, N_t = 40$

Outlook

- Improve NN, e.g. incorporate symmetries
- Go to higher N_x

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Simran Singh

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Janik Kreit

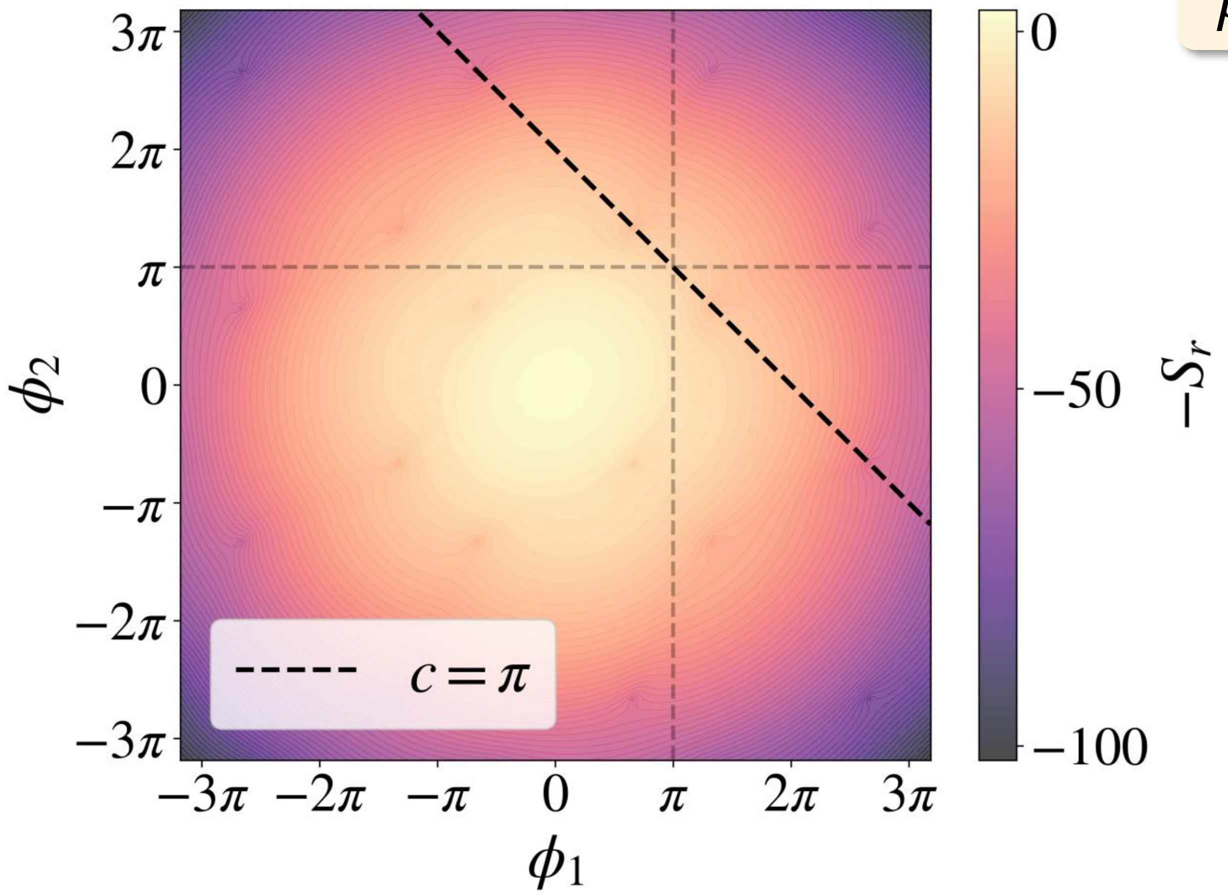
Dominic Schuh

Christian Schmidt-Sonntag

Back-Up Slides

The Hubbard Model

Diagonal discretisation



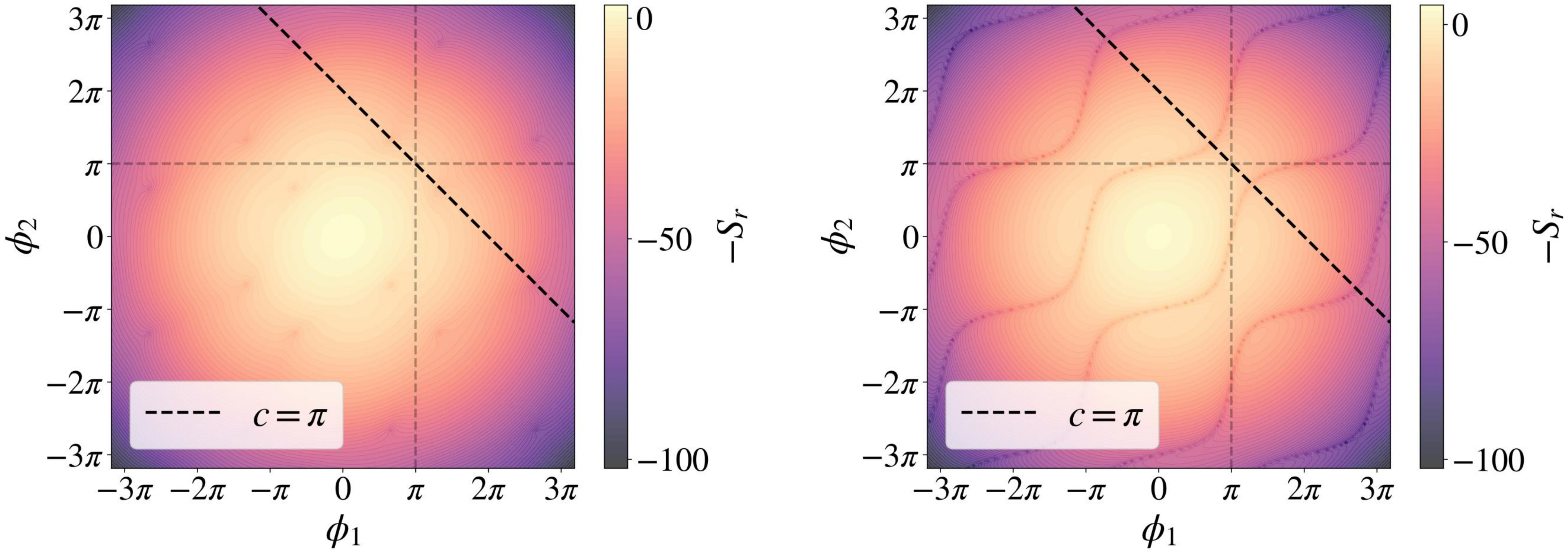
$\beta = 1, N_t = 1$

The Hubbard Model

$\beta = 1, N_t = 1$

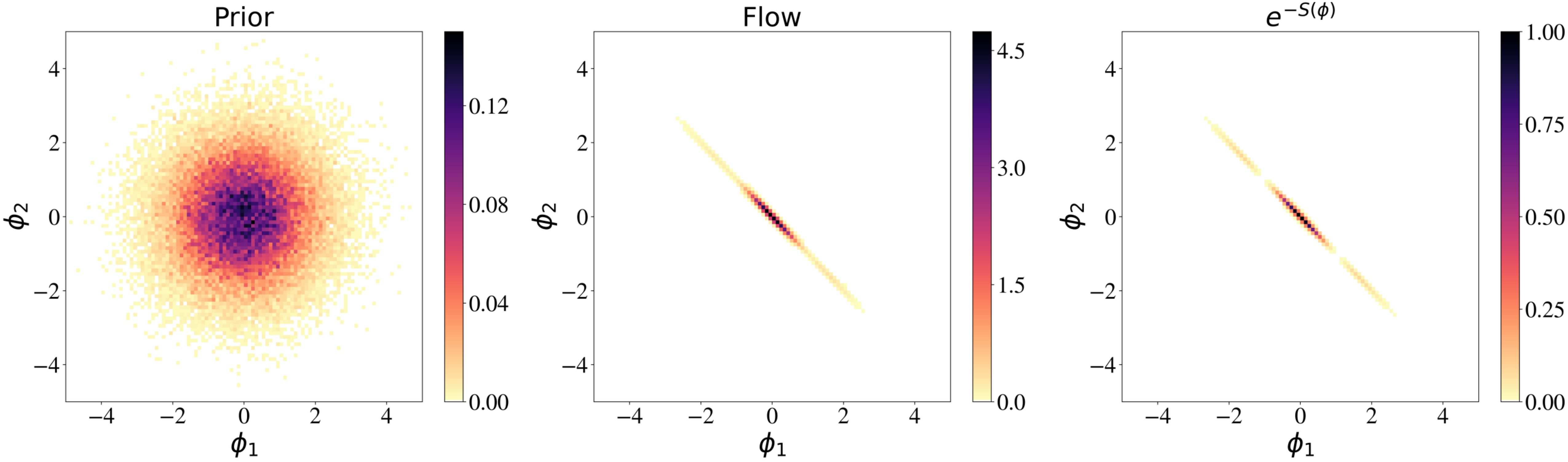
Diagonal discretisation

Exponential discretisation



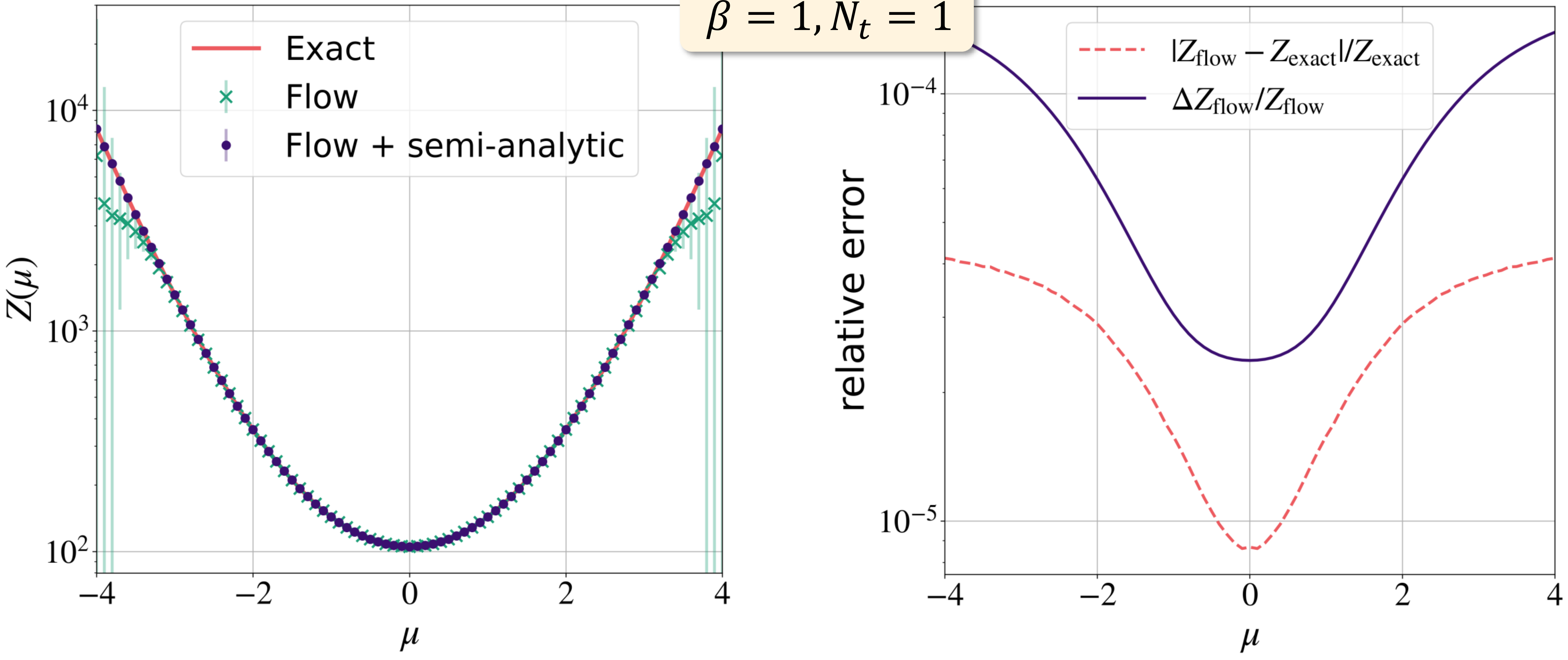
The distribution

$\beta = 1, N_t = 1, c = \pi$



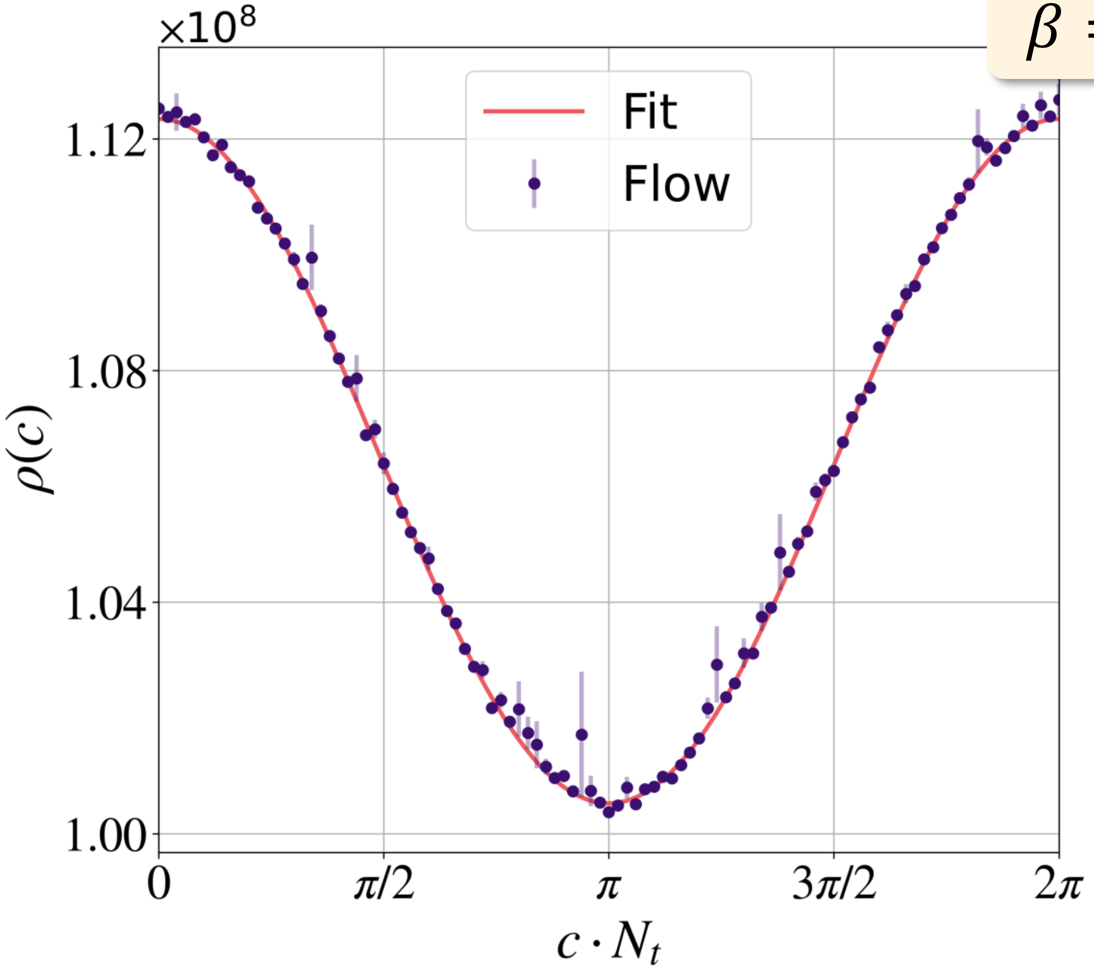
Partition function

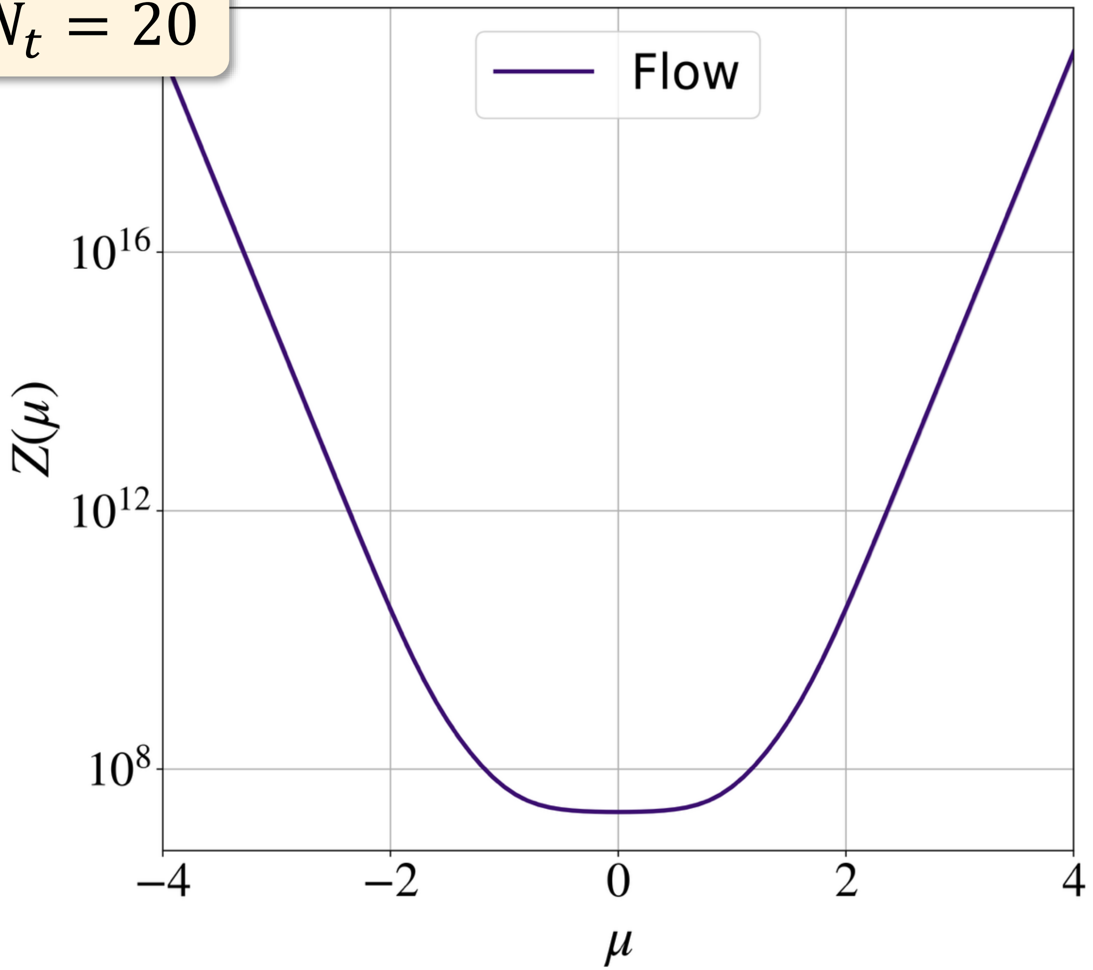
$\beta = 1, N_t = 1$



Results for higher β, N_t

$\beta = 5, N_t = 20$





Charge density

$$Q = \frac{1}{\beta}\frac{d}{d\mu}\ln Z$$

$$= \frac{\sum_{\mathrm{k}=1}^{N_x} \mathrm{a_k} e^{\frac{-k^2 N_t^2}{2\alpha\gamma}} k \sinh(\mu\beta k)}{\sum_{\mathrm{k}=0}^{N_x} \mathrm{a_k} e^{\frac{-k^2 N_t^2}{2\alpha\gamma}} \cosh(\mu\beta k)}$$

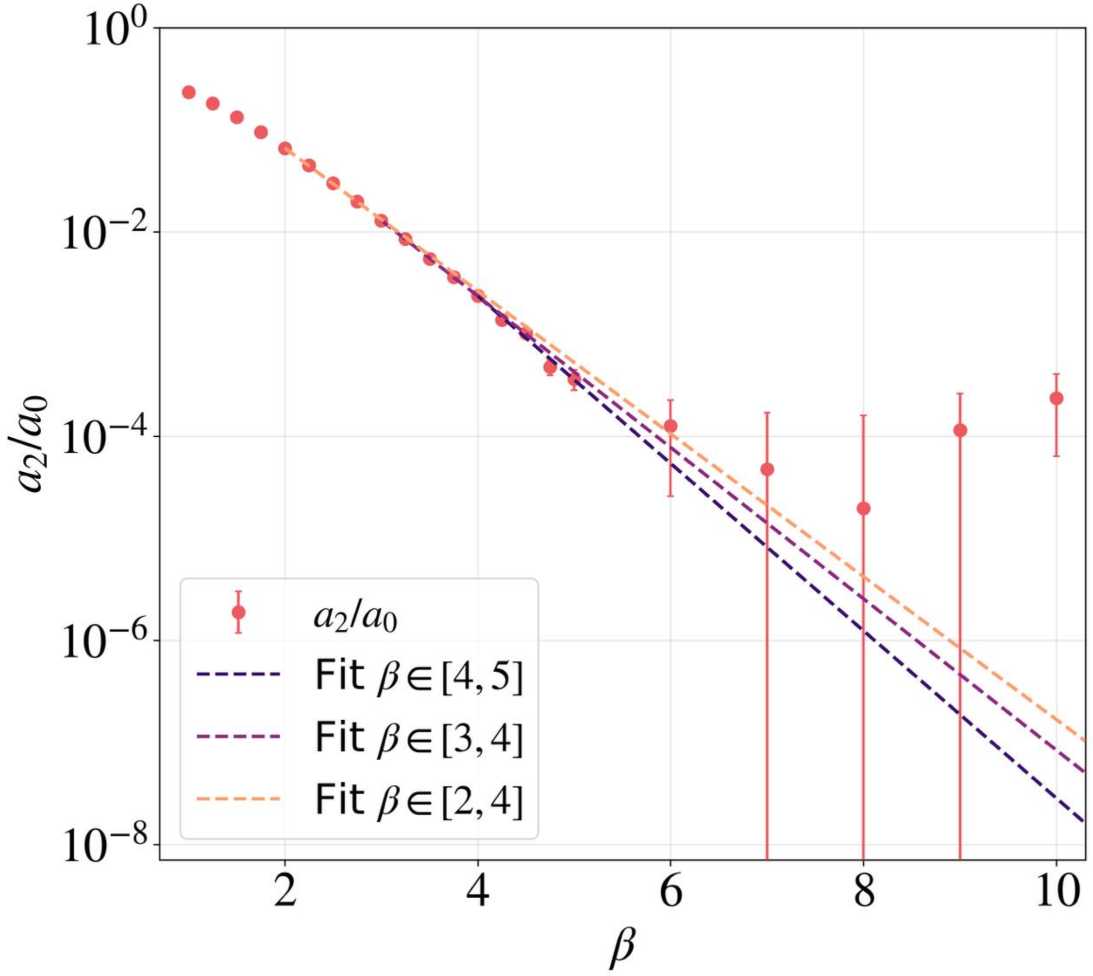
Charge density

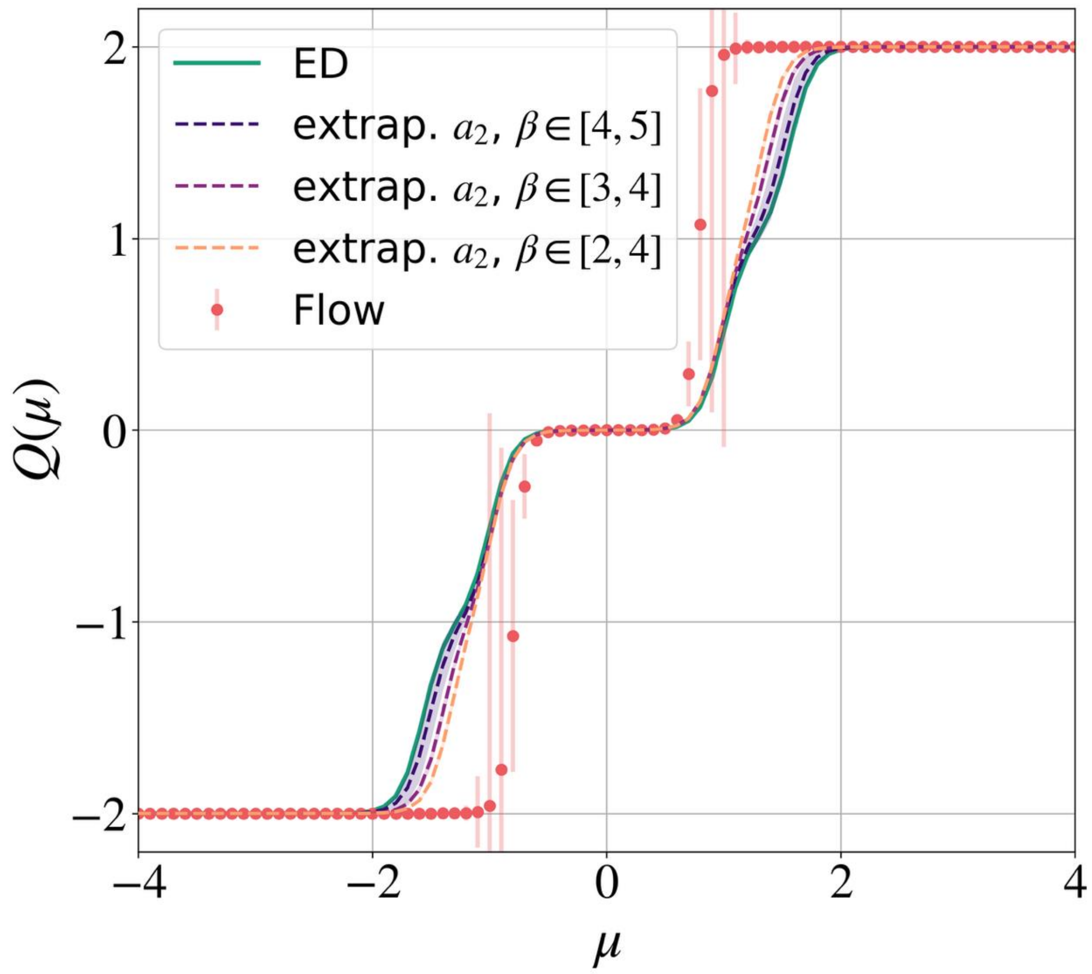
- Grandcanonical partition function: $Z = \sum_{n=-N_x}^{N_x} e^{\mu\beta n} g_n$ with $g_n = \sum_j e^{-\beta E_j^{(n)}} = d_0^{(n)} e^{-\beta E_0^{(n)}} + d_1^{(n)} e^{-\beta E_1^{(n)}} + \cdots$

For $\beta \to \infty$

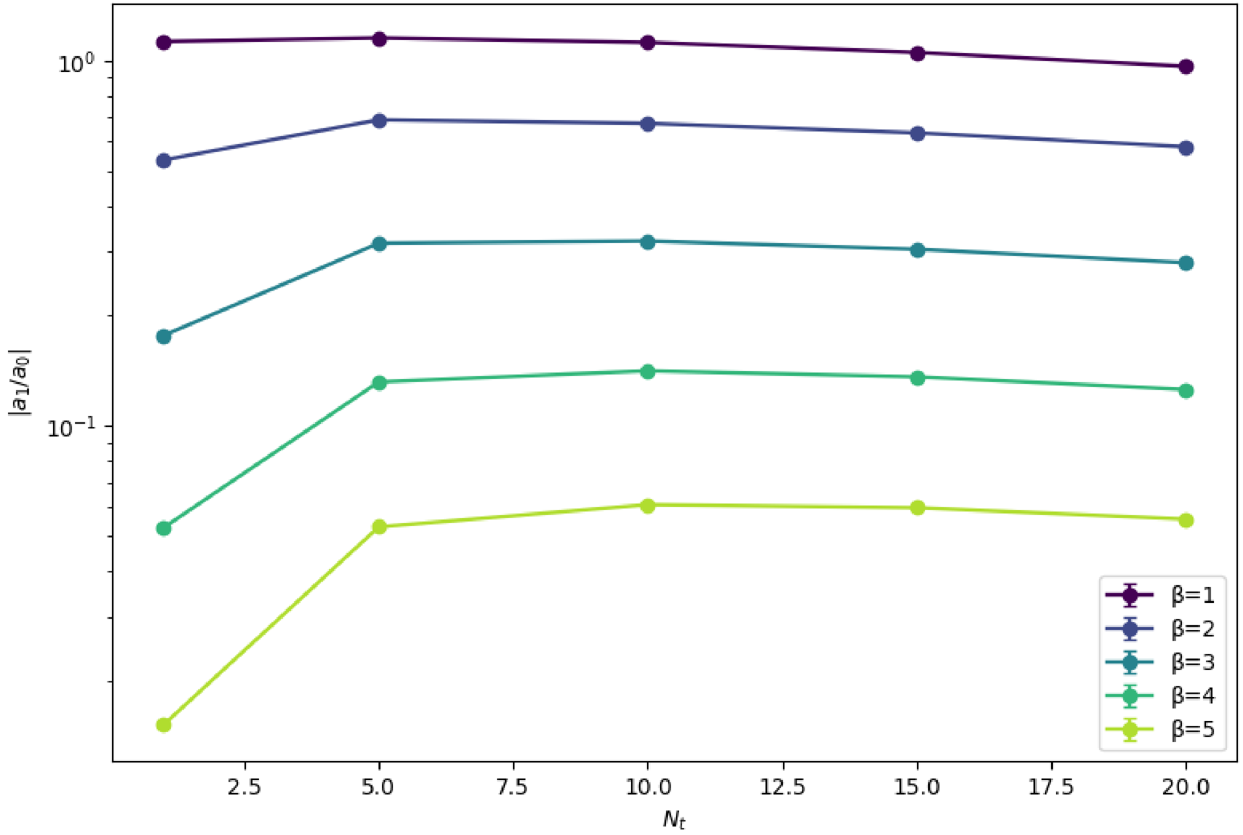
- $\ln(a_k) = -\beta E_0^{(k)} + \frac{k^2 U\beta}{2N_x} + \ln\left(d_0^{(k)}\right) + \ln(2) - \frac{k^2 N_t^2}{2P} = m\beta + n$

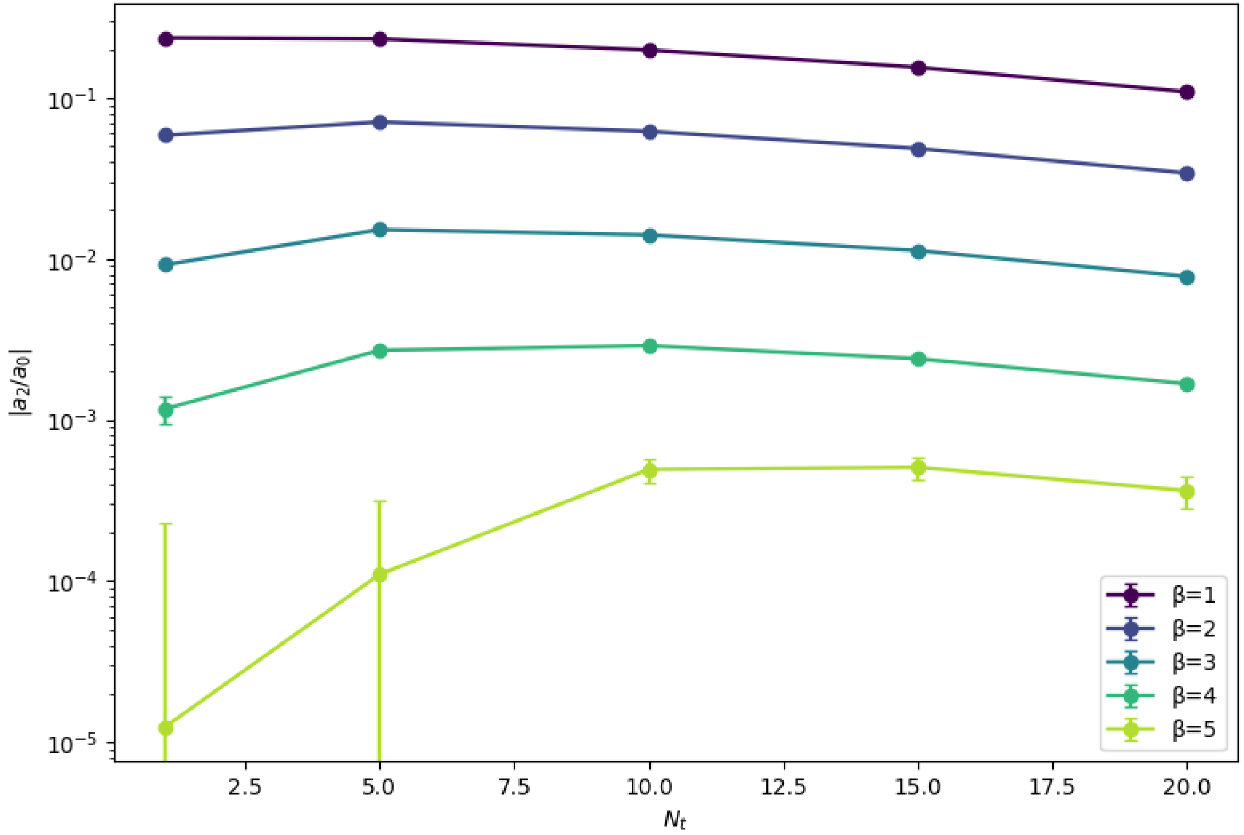
The fitting range





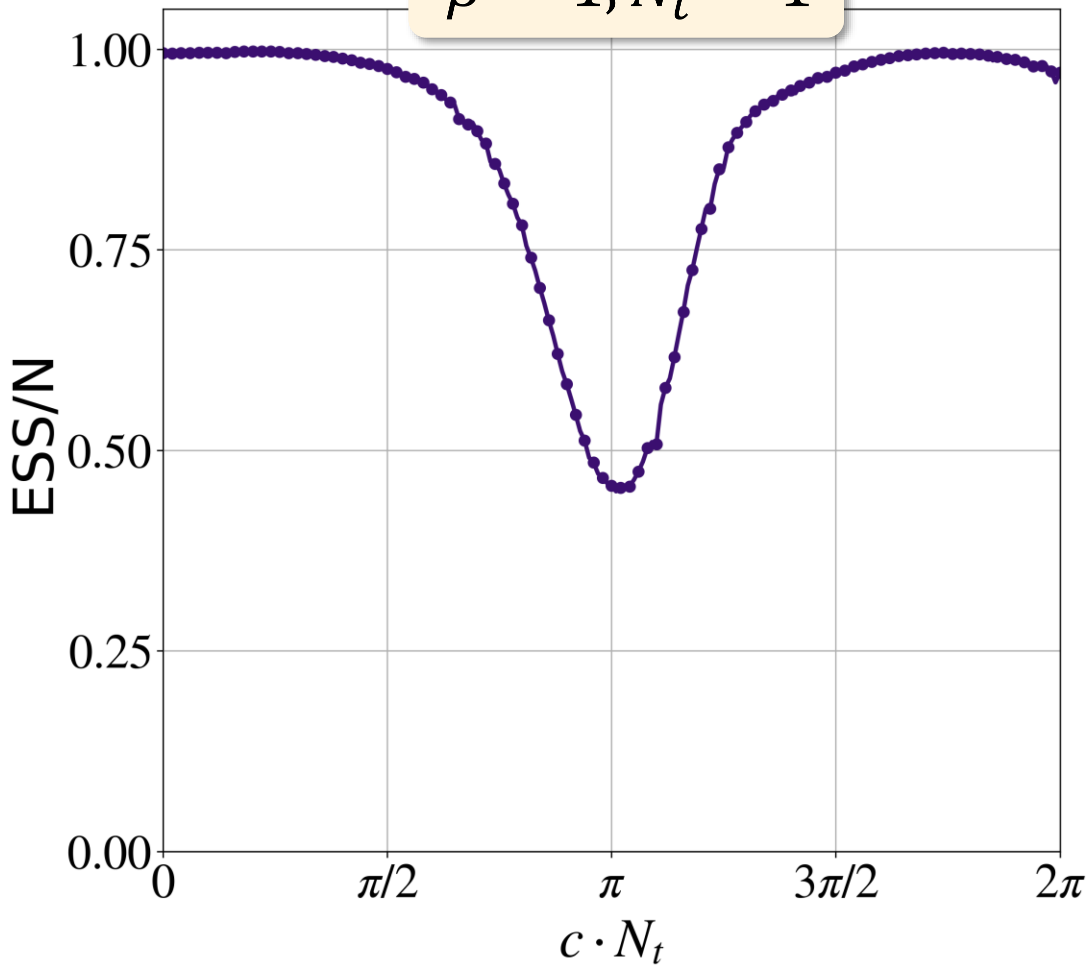
N_t-dependence



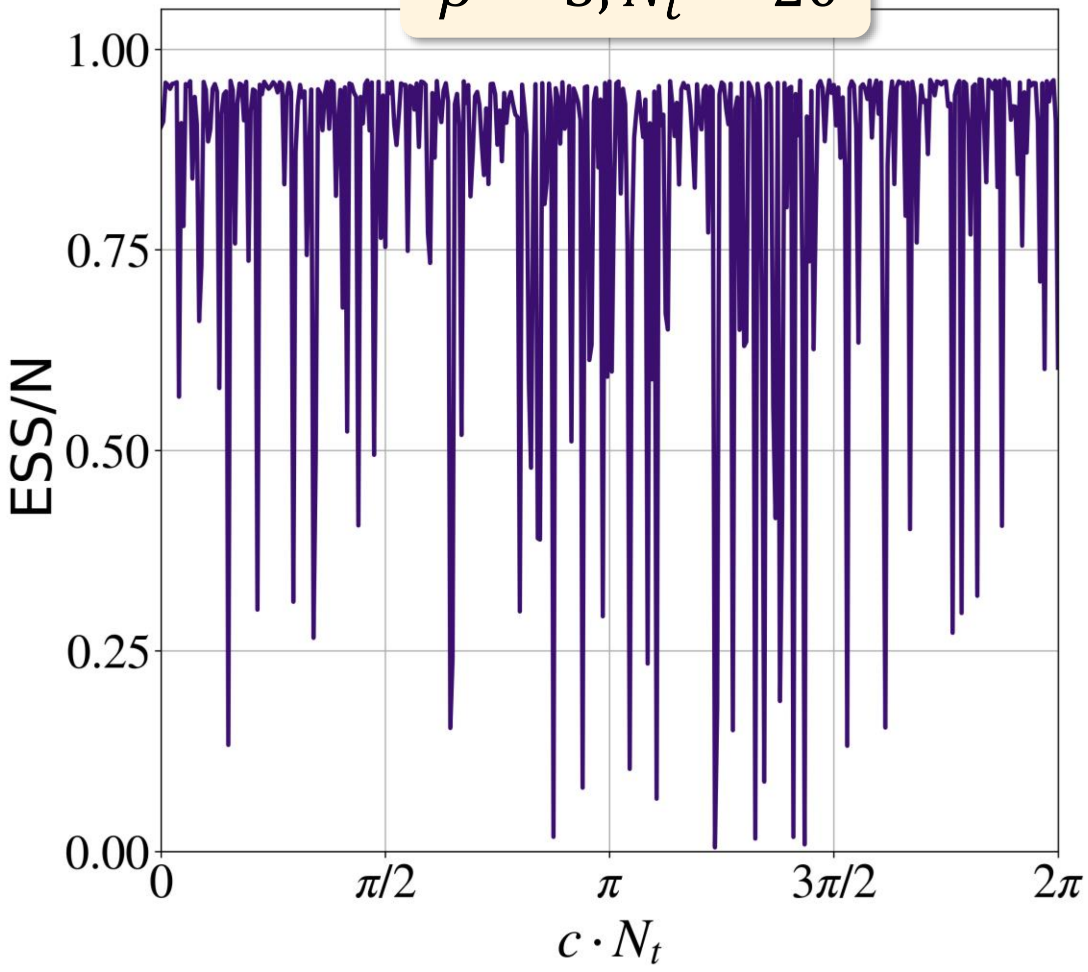


ESS

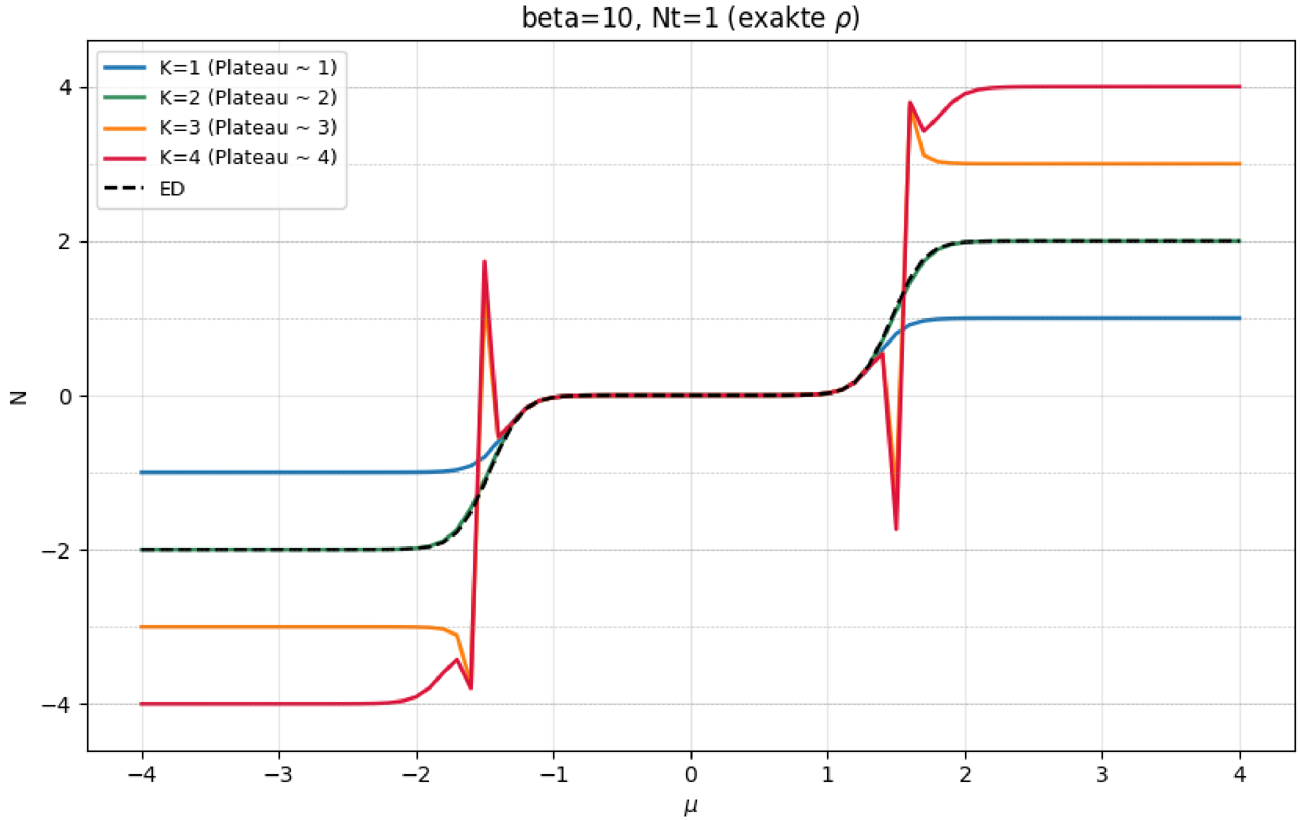
$\beta = 1, N_t = 1$

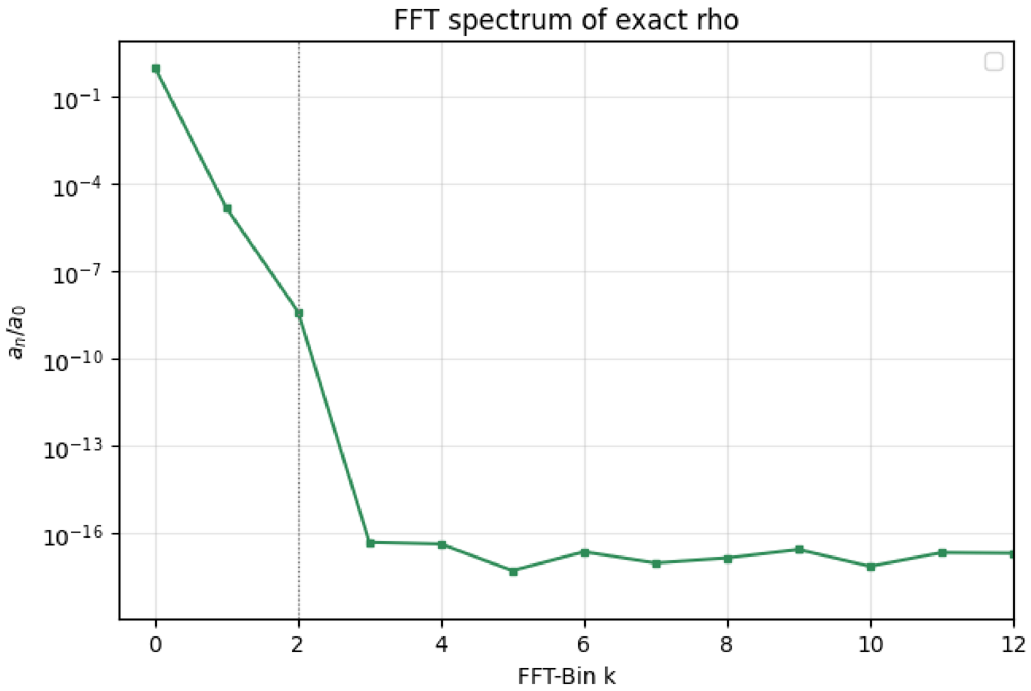


$\beta = 5, N_t = 20$



How to choose K





$\Rightarrow$ $K = 2$

Smekal et al. : $\#\ of\ Fouriermodes = N_x + 1$ $\Rightarrow$ $K = N_x$