Sign Reweighting for finite density QCD

by

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Reference:
https://arxiv.org/abs/2004.10800
https://arxiv.org/abs/2108.09213

Content

Motivation

- Lattice QCD at finite density needed for the phase diagram in the T-μ plane

  - Harmed by the complex action problem

  - Standard Monte Carlo techniques not applicable

- Different approaches to overcome this :

  - Taylor expansion around vanishing chemical potential

  - Simulation at imaginary chemical potential

  - Reweighting from zero chemical potential

- For small μ, these methods give correct results.
- When μ is not small becomes unreliable.

Motivation

- Examples:

  - Taylor expansion method from μ=0 : No extrapolation beyond radius of convergence

  - Extrapolation from imaginary chemical potential : assumptions about the dependence of observables on the functional form of μ^2

  - Reweighting from zero chemical potential : overlap problem

- No sign problem but have systematic uncertainties thus not reliable

- Need a method with purely statistical errors

  - Sign Reweighting

  - sign problem is severe : cannot calculate observables.

  - sign problem mild : results with no uncertainties

  - run simulations directly at real chemical potential

General reweighting strategy

- Desired target theory :

$$Z_t = \int \mathrm{DU}\ w_t(\mathrm{U})$$

- cannot be sampled efficiently.

- Perform simulations in a theory that can be sampled

$$Z_s = \int \mathrm{DU}\ w_s(\mathrm{U})$$

- $$\left\langle \frac{w_t}{w_s} O \right\rangle_s = \frac{1}{Z_s} \int DU\, \frac{w_t}{w_s}\, O\, w_s = \frac{Z_t}{Z_s} \frac{1}{Z_t} \int DU\, w_t\, O = \frac{Z_t}{Z_s} \langle O \rangle_t$$

$$\left\langle \frac{w_t}{w_s} \right\rangle_s = \frac{1}{Z_s} \int DU\, \frac{w_t}{w_s}\, w_s = \frac{Z_t}{Z_s}$$

- Observables in desired target theory:

$$\langle O \rangle_t = \frac{\left\langle \frac{w_t}{w_s} O \right\rangle_s}{\left\langle \frac{w_t}{w_s} \right\rangle_s}$$

Overlap problem

- Reweighting method : Calculate observables in target theory of interest by performing simulations in a theory with weights that can be sampled efficiently.
- Target theory : lattice QCD with finite baryon density; weights : $w_t = det\, M$

  - wildly fluctuating phases

  - infamous sign problem
- Example : Phase reweighting

  - weights : $w_s = |det\, M|$

  - reweighting factor : $\frac{w_t}{w_s} = e^{i\theta}$

  - Probability distribution of reweighting factor has a long tail
- Overlap problem :

  - Sampling the tail of the histogram is prohibitively expensive

  - No reliable error estimate at finite statistics

  - no sharply defined condition to know if overlap problem is present or not

Sign Reweighting

- Overlap problem - immediate bottleneck in QCD when we try to extend reweighting results to finer lattices

  - Overcome this by Sign Reweighting.

- At finite chemical potential :

$$Z(\mu) = \int dU \det D(U,\mu) e^{-S_g(U)}$$

$$\langle \mathcal{O} \rangle_\mu = \frac{1}{Z(\mu)} \int dU\, \mathcal{O}(U) \det D(U,\mu) e^{-S_g(U)}$$

- *Det D(U,μ)* is complex but the partition function is real :

$$Z(\mu) = \int dU\, \mathrm{Re} \det D(U,\mu) e^{-S_g(U)}$$

$$\langle \mathcal{O} \rangle_\mu = \frac{1}{Z(\mu)} \int dU\, \mathcal{O}(U)\, \mathrm{Re} \det D(U,\mu) e^{-S_g(U)}$$

- Note : Replacing the determinant by its real part is not permitted for arbitrary expectation value but it is allowed for observables obtained as derivatives of Z with respect to real parameters like m_q.

- Target theory with weight : $w_t = Re\, det\, D(U,\mu) e^{-S_g(U)}$

Sign Reweighting

- Idea : the sign of the weights is split from the absolute value

$$\epsilon(U,\mu) \; = \; sign[Re\,Det\,D(U,\mu)]$$

- Simulated theory :

$$Z_{SQ}(\mu) \; = \; \int dU \, |Re\,Det\,D(U,\mu)| e^{-S_g(U)}$$

$$\langle O \rangle_{SQ} \; = \; \frac{1}{Z_{SQ}(\mu)} \int dU \, O \, |Re\,Det\,D(U,\mu)| e^{-S_g(U)}$$

- weights : $w_s \; = \; |Re\,Det\,D(U,\mu)| e^{-S_g(U)}$

- reweighting factor:

$$\frac{w_t}{w_s} \; = \; \frac{\epsilon(U,\mu)\,|Re\,Det\,D(U,\mu)|e^{-S_g(U)}}{|Re\,Det\,D(U,\mu)|e^{-S_g(U)}} \; = \; \epsilon(U,\mu)$$

- reweighting factors have values +1 or -1 - discrete sectors

- no probability distribution over continuous variables

- no tails by construction; no inaccurate sampling

Sign reweighting

- No overlap problem
- Sign problem ?

  - positive and real weights

  - Observable in target theory :

$$\langle O \rangle_\mu = \frac{\langle \epsilon \, O \rangle_{SQ}}{\langle \epsilon \rangle_{SQ}}$$

  - only meaningful if the denominator is non-zero

  - The denominator becoming zero is due to the sign problem.

- Only problem is the sign problem which is under control as long as $<\varepsilon>_{SQ}$ is not zero (within errors).
- Sufficient and necessary condition for the correctness of the results:

  - If $<\varepsilon>_{SQ}$ is zero within errors : no result.

  - Otherwise, the result has only statistical errors without any systematic uncertainties.

Simulation setup

- Wilson plaquette action; 2+1 flavors of rooted staggered fermions
- $N_t = 4$; $N_\sigma = 8,10,12$
- Fermion masses set to physical values
- Chemical potential for light quarks only
- Monte Carlo runs with μ>0 :

  - configurations generated with weight $|Re\,Det\,D(U,\mu)|e^{-S_g(U)}$

  - non-trivial problem

  - can be written as
  $$\frac{|Re\,Det\,D(U,\mu)|}{|Re\,Det\,D(U,0)|}\,Det\,D(U,0)|e^{-S_g(U)}$$

  - standard HMC algorithm at μ=0

  - include μ-dependent ratio in the metropolis accept/reject step at the end of the trajectory

  - calculate observables by calculating the reweighting factor ε.

Numerical results

- Expensive algorithm

  - full determinant calculated

- Measure whether the results are reliable:

  - <ε>$_{SQ}$: strength of the sign problem

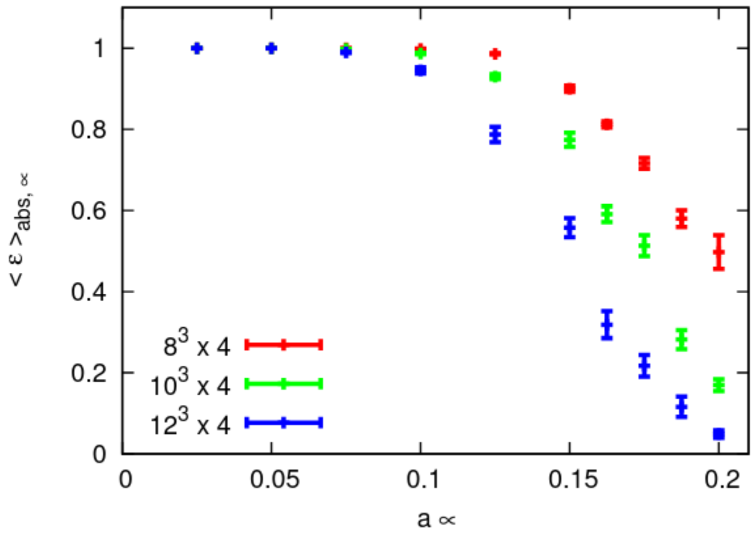
  - <ε>$_{SQ}$ away from zero: sign problem is mild, perform sign reweighting

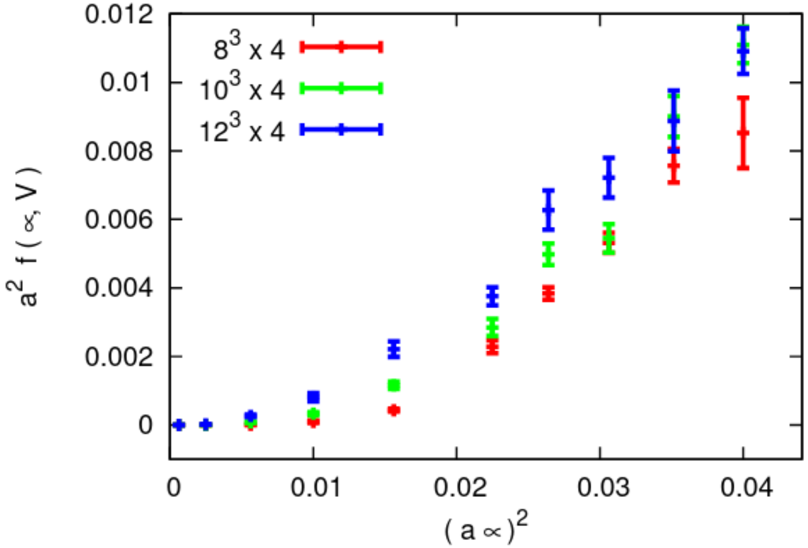
- Since $\langle \epsilon \rangle_{SQ} \to 1\,;\ \mu \to 0$

  - parametrize it as

$$\langle \epsilon \rangle_{SQ} = e^{-V\mu^2 f(\mu, V)}$$

  - f(μ,V) depends mildly on V but non-trivially on μ



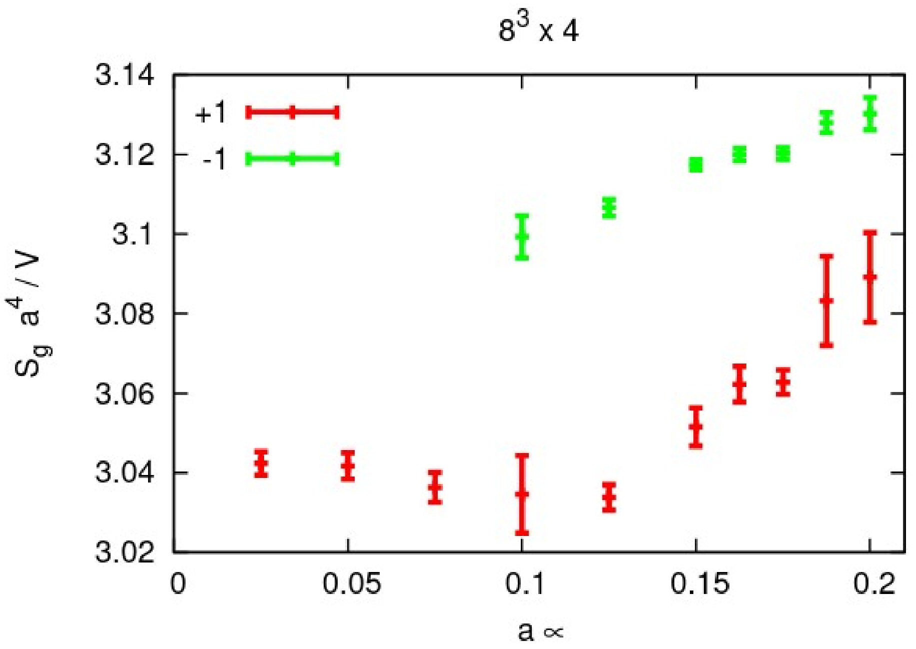


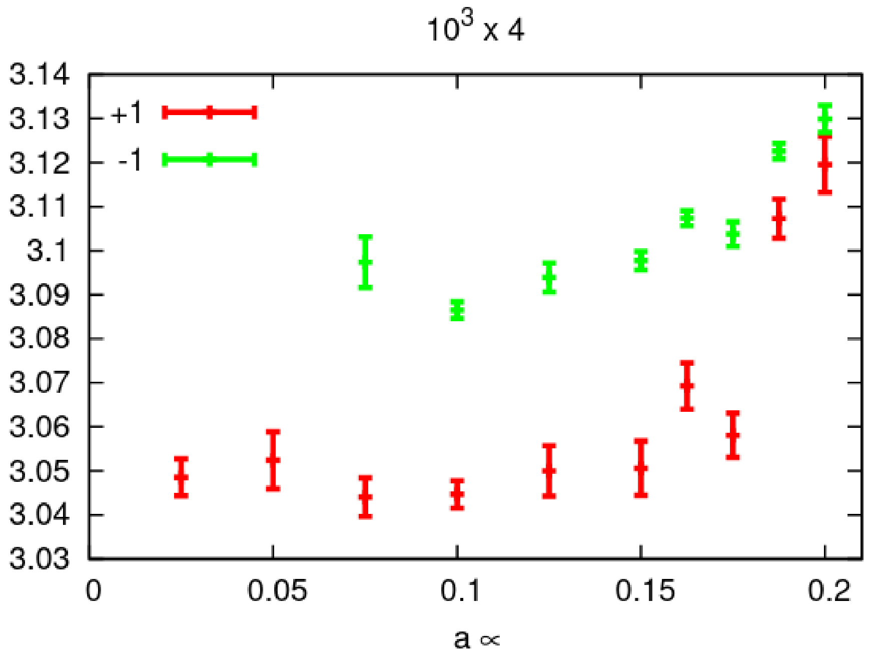
Numerical results

- Effect of sign reweighting on some observables

  - Difference in ε=+1 and ε=-1 sectors

- Gauge action per unit space-time volume :





- For low chemical potentials no configurations in the -1 sector which is the case when $\mu=0$

Fisher zeros

- Determined volume and chemical potentials for sign reweighting

  - Calculate observables in this regime

- Goal : know order of the phase transition

  - calculate Fisher zeros in β : roots of Z

  - find complex β such that $Z(\mu, \beta) = 0$

  - Z(μ,β) has several zeros as a function of complex β

  - need closest to real axis : coincide to (β_c,0) at infinite volume (leading zero)

- Volume scaling of Im(β) determines the order of the transition :

  - Im(β) = constant : crossover

  - Im(β) = a^3/L^3 : first order

  - Im(β) = $(a/L)^\alpha$: second order

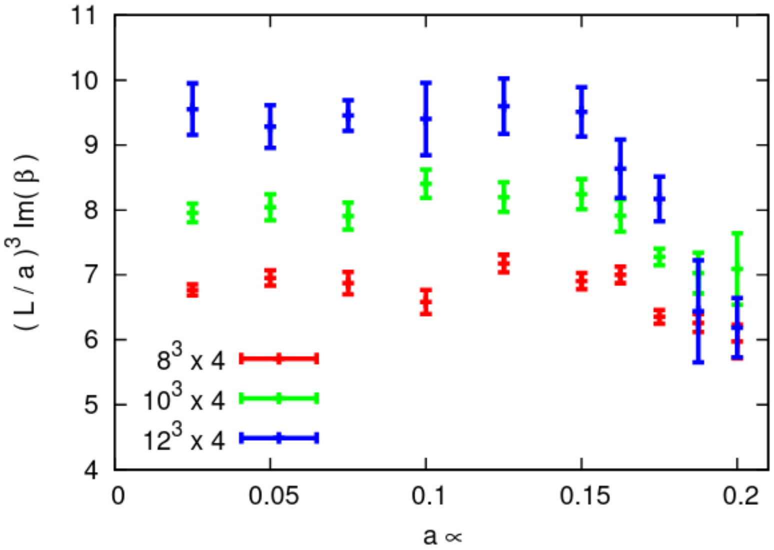
Fisher zeros

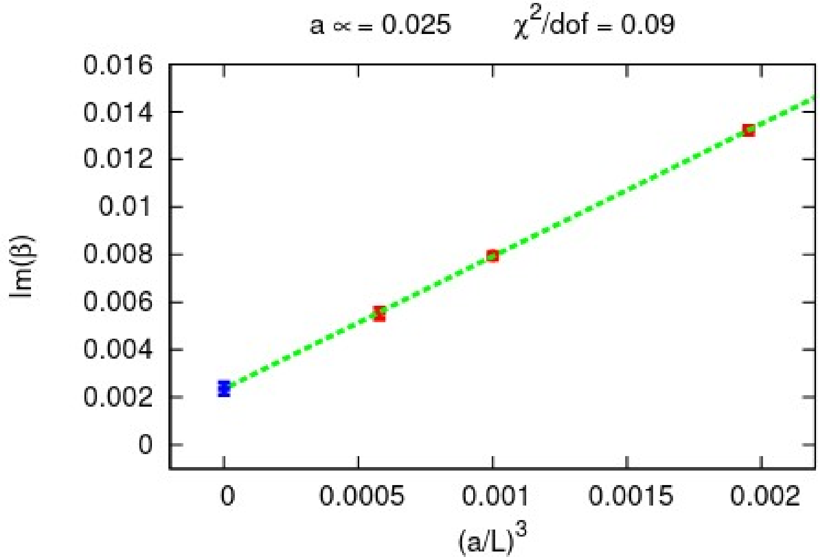
- Im(β) decreases when μ is sufficiently large
- Im(β) extrapolated to infinite volume by the ansatz.

$$Im\,\beta = A + B(a/L)^3$$

- fit function has acceptable statistical fits

- for a true phase transition, A~0 for infinite volume





Fisher zeros

- μ=0.2 ~ μ_B/T=2.4 plot :

  - Infinite volume extrapolation of Im(β) consistent with zero.

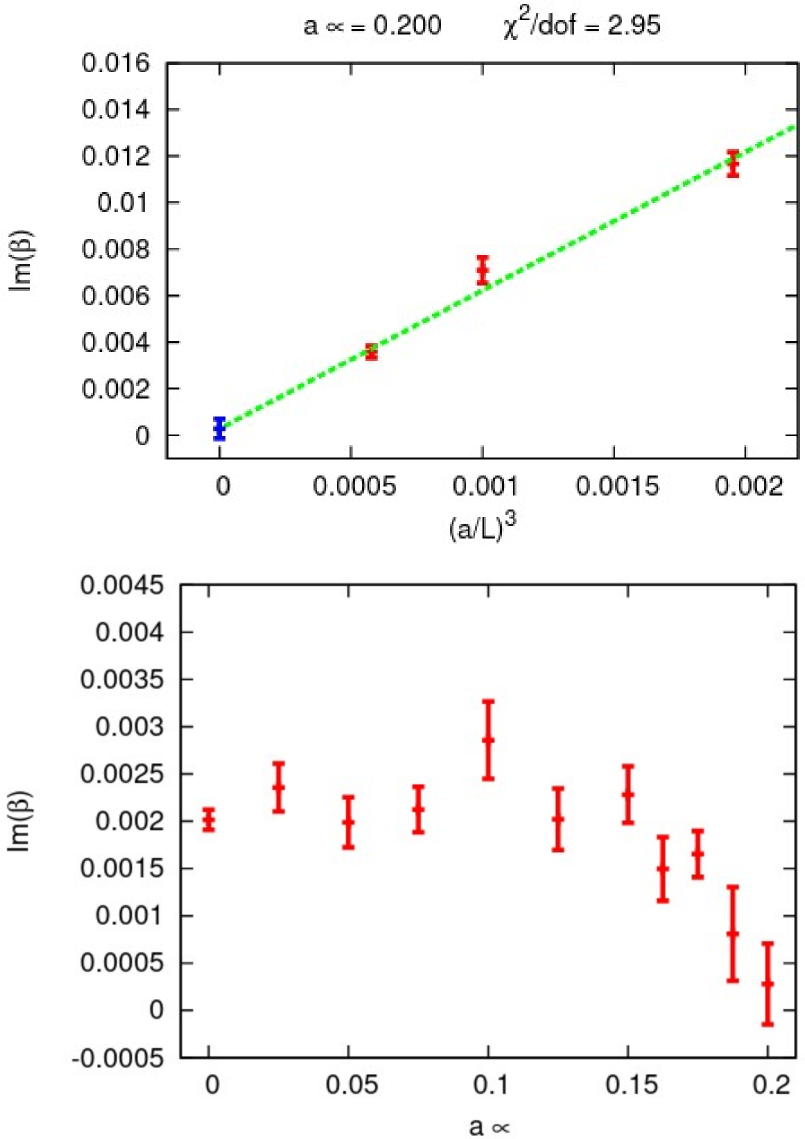
- Existence of a critical end point would suggest that Im(β) at infinite volume is a decreasing function of μ and as $\mu=\mu_c$ it is zero

  - Infinite volume extrapolation of Im(β) is flat upto μ=0.15 and then there is a sharp decrease for 0.15<μ<0.2.

  - Singularity of lnZ is moving closer to the real axis

  - Strength of the transition is increasing

  - Suggests a true phase transition around μ=0.2



Severity of the sign problem

- Weakest sign problem :

  - compare with phase reweighting

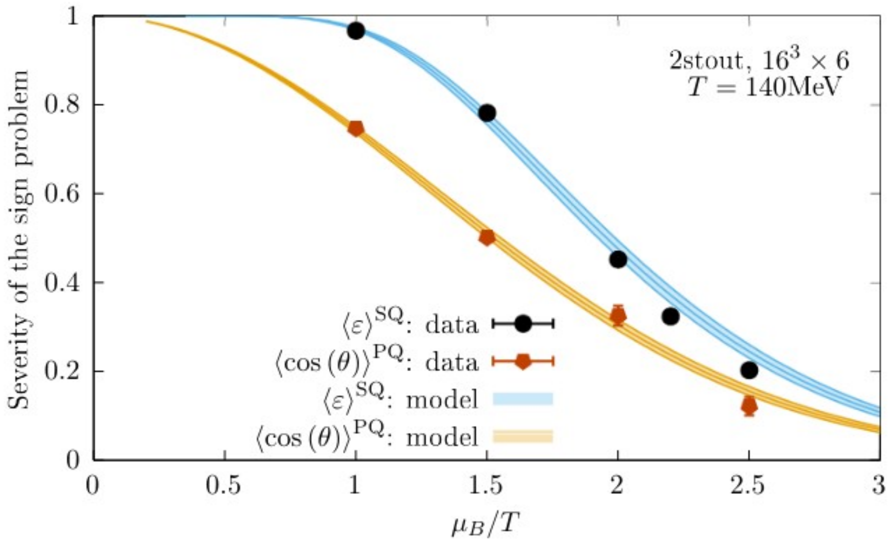
  - severity of sign factor measured by average reweighting factor

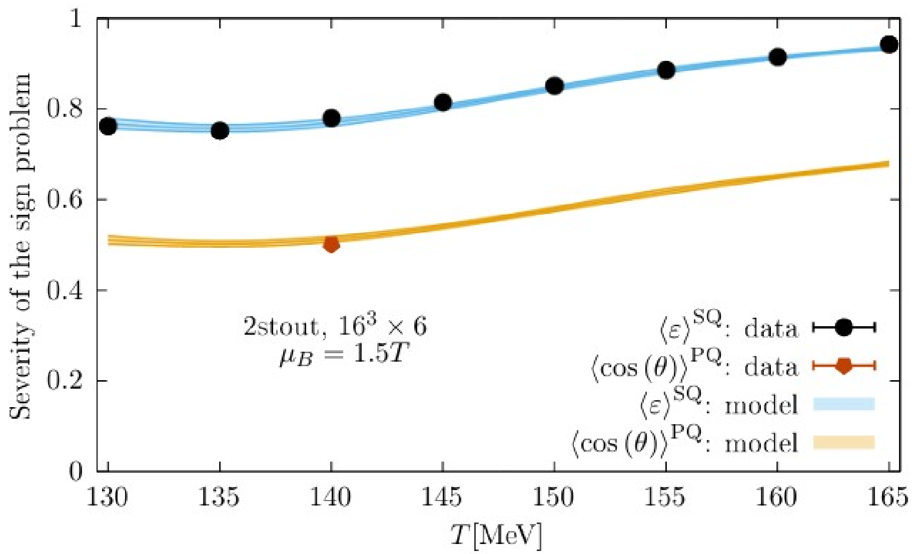
  - phase factor for phase reweighting

$$\langle cos(\theta)\rangle_{PQ}$$

  - sign reweighting : $\langle\varepsilon\rangle_{SQ}$.

  - Sign problem is more severe in phase reweighting than sign reweighting





Conclusion

- Sign reweighting is a new technique for evaluating path integral at finite baryon chemical potential.
- It generates configurations by the absolute value of the real part of the fermionic determinant and takes the sign into account by a discrete reweighting.
- The results do not have an overlap problem and are perfectly reliable when the sign problem is not too severe.
- The sign problem is the least severe with this method compared to other reweighting strategies.
- $\mathrm{Im}(\beta)$ stays flat within $0<\mu<0.15$ and decreases sharply for $0.15<\mu<0.2$. This tells us that the strength of the phase transition increases as chemical potential increases.
- The infinite volume extrapolation of $\mathrm{Im}(\beta)$ at $\mu\sim0.2$ corresponding to $\mu_B/T\sim2.4$ is zero which is consistent with a true phase transition.

Thank You