Results from combining ensembles at several values of chemical potential

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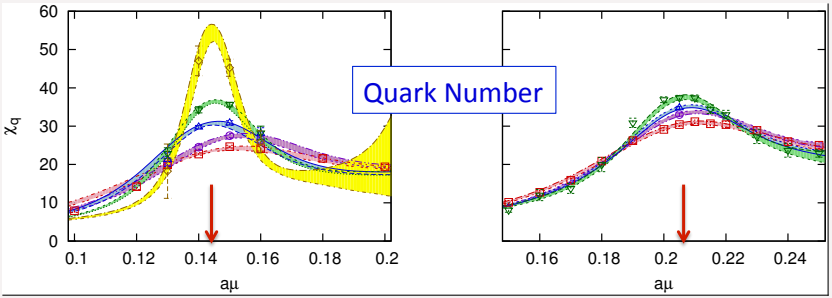
Introduction

- Simulations with 4 flavors [arXiv:1307.7205] described in S. Takeda's talk
- Phase quenched simulations of grand canonical ensembles

$$Z_{||}(\mu) = \int [\mathrm{d}U]\, e^{-S_g(U)+N_f \ln|\det D(\mu;U)|}$$

- $(\beta,\ \kappa)$= $(1.58, 0.1385)$ and $(1.60, 0.1371)$.
- $N_t = 4$ with spatial volumes from 6^3 to 10^3.
- $50,000$ up to $\sim 300,000$ trajectories with $1/10$ measured.
- μ-reweighting using Taylor expansion of $\ln\det D$ works well.



First order at $\beta = 1.58$ Weak at $\beta = 1.60$

Contents of this talk

Multi-ensemble reweighting and probability density.

Pitfalls and how to avoid them.

Zeros of the partition function with a complex μ.

Reweighting

- Probability density

$$\text{Prob}(U) = \frac{1}{\mathcal{Z}} \exp[-S(U)] \xrightarrow{\text{MC}} \frac{1}{N} \sum_{l=1}^{N} \delta(U - U_l)$$

- Reweight from simulation S_s to target S_t using weight $w_\text{t}(U)$

$$\text{Prob}_\text{t}(U) = \text{Prob}_\text{s}(U) \exp[S_\text{s}(U) - S_\text{t}(U)] \frac{\mathcal{Z}_\text{s}}{\mathcal{Z}_\text{t}}$$

- From multiple simulations of S_1, S_2, ...

$$\text{Prob}_\text{t}(U) = \sum_s p_s(U) \, \text{Prob}_s(U) \exp[S_s(U) - S_\text{t}(U)] \frac{\mathcal{Z}_s}{\mathcal{Z}_\text{t}}$$

- F.–W. (1989) $\Rightarrow$ Choose $p_s(U)$ to minimize $\sigma^2[\text{Prob}_\text{t}(U)]$ ($\mathcal{Z}_1$ chosen arbitrary)

$$\text{Prob}_\text{t}(U) = \left(\sum_{s'} N_{s'} \, \text{Prob}_{s'}(U) \right) \left(\sum_s N_s \exp[S_\text{t}(U) - S_s(U)] \frac{\mathcal{Z}_1}{\mathcal{Z}_s} \right)^{-1} \frac{\mathcal{Z}_1}{\mathcal{Z}_\text{t}}$$

- In general (ratio of $\mathcal{Z}$ determined by $\int \mathcal{D}[U] \, \text{Prob}(U) = 1$)

$$\text{Prob}_\text{t}(U) = \frac{1}{\mathcal{Z}_\text{t}} \exp[-S_\text{t}(U)] \xrightarrow{\text{MC-RW}} w_\text{t}(U) \sum_\text{conf} \delta(U - U_\text{conf})$$

Reweighted probability distribution

- Any quantity $f(U)$ with real valued $\langle f \rangle_t$ for real actions

$$\langle f \rangle_t = \int \mathcal{D}[U] f(U) \operatorname{Prob}_t(U) = \int \mathcal{D}[U] f(U) w_t(U) \sum_{\text{conf}} \delta(U - U_{\text{conf}})$$

- Its probability density is

$$\begin{aligned} \operatorname{Prob}_t^f(X) &= \int \mathcal{D}[U] \delta(X - f(U)) \operatorname{Prob}_t(U) \\ &= \int \mathcal{D}[U] \delta(X - f(U)) w_t(U) \sum_{\text{conf}} \delta(U - U_{\text{conf}}) \end{aligned}$$

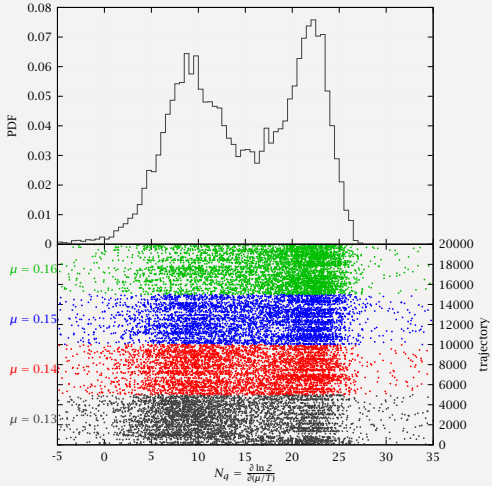
- With complex actions, for real partition functions, keep the real probability

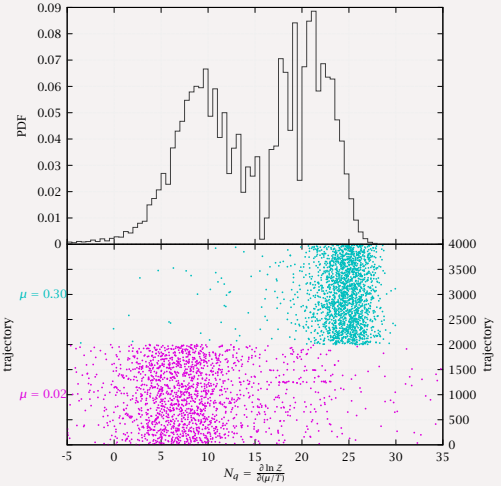
$$\begin{aligned} \langle f \rangle_t &= \int \mathcal{D}[U] f(U) \operatorname{Prob}_t(U) \\ &= \int \mathcal{D}[U] \left(\operatorname{Re} f(U) - \operatorname{Im} f(U) \frac{\operatorname{Im} w_t(U)}{\operatorname{Re} w_t(U)} \right) \operatorname{Re} w_t(U) \sum_{\text{conf}} \delta(U - U_{\text{conf}}) \end{aligned}$$

- Define the probability density with real probability

$$\operatorname{Prob}_t^{\tilde{f}}(X) = \int \mathcal{D}[U] \delta(X - \tilde{f}(U)) \operatorname{Re} \operatorname{Prob}_t(U)$$

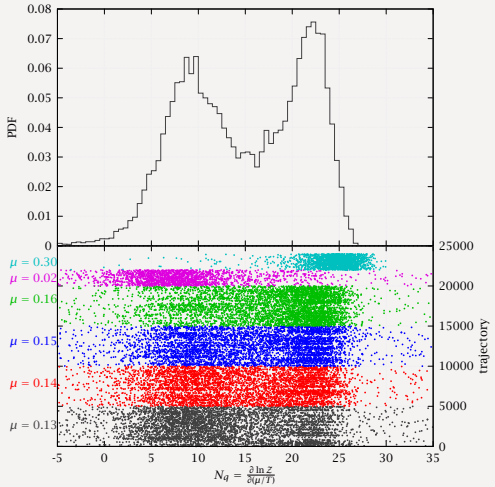
Quark number using different ensembles

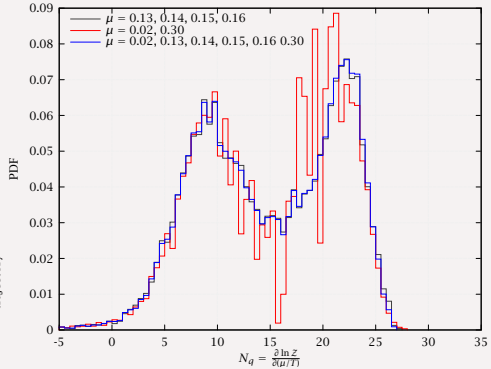




- Reweighted to $\mu = 0.139$
- Quite visible defect if reweighted from too far

Quark number—Compare



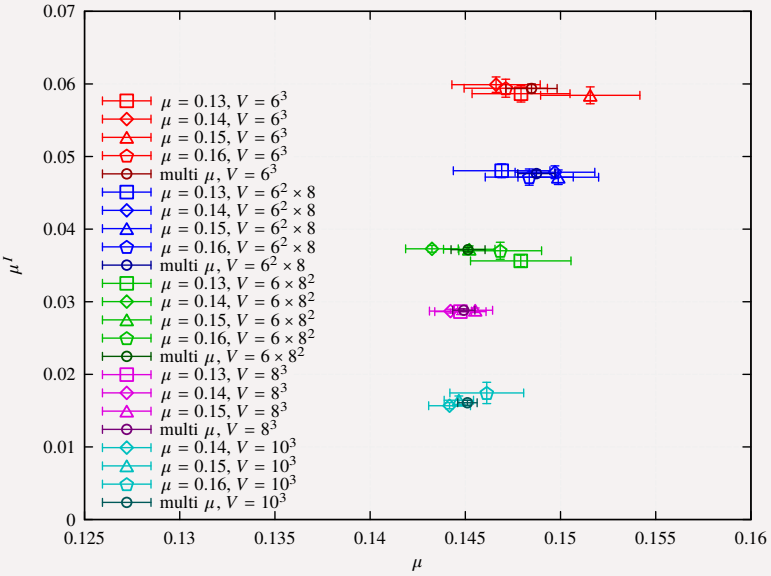


- Very slight change from remote ensembles
- More noise than signal
- We only use ensembles near the transition

Partition function zeros with complex μ

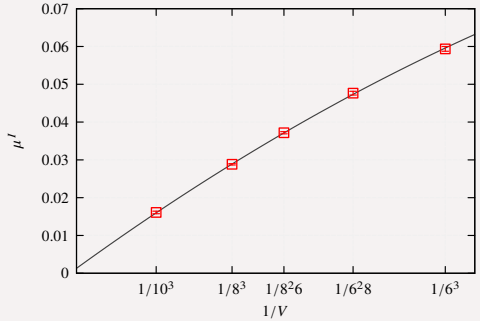
- Ratios of partition functions can be determined
$$\frac{\mathcal{Z}_a}{\mathcal{Z}_b} = \frac{\sum_{\text{conf}} w_a(U_{\text{conf}})}{\sum_{\text{conf}} w_b(U_{\text{conf}})}$$
- Define normalized partition function at $\mu + i\mu^I$
$$\mathcal{Z}_{\text{norm}} = \frac{\mathcal{Z}(\mu + i\mu^I)}{\mathcal{Z}(\mu)}$$
- Use the symmetry to reduce the noise
$$\mathcal{Z}_{\text{norm}} = \frac{\mathcal{Z}(\mu + i\mu^I) + \mathcal{Z}^*(\mu - i\mu^I)}{2\,\text{Re}\,\mathcal{Z}(\mu)}$$
- Additionally remove a factor $\exp\langle \ln w \rangle$, which includes a large real factor and an oscillating complex phase

Locations of the first zero, $\beta = 1.58$, $\kappa = 0.1385$



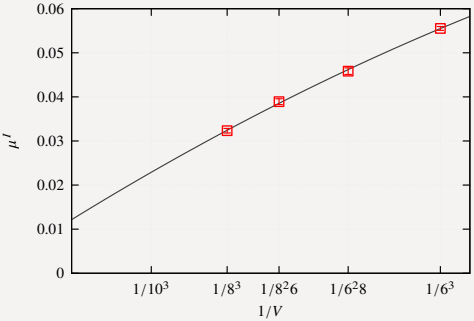
Better statistics after combining multiple ensembles.

Volume scaling of μ^I of first zeros



$\beta = 1.58, \kappa = 0.1385$

Consistent with first order PT



$\beta = 1.60, \kappa = 0.1371$

Inconsistent with first order

Estimate the confidence region in μ-reweighting

- How far can we reweight in μ? Zeros of $\mathcal{Z}(\mu + i\mu^I)$ with larger μ^I?
- Complex β studied by Alves, Berg, and Sanielevici (1992)
- Introduce imaginary parameter by Fourier transform probability density

$$\tilde{\mathcal{Z}}(\mu, \mu^I) = \int dX \exp[iX\frac{\mu^I}{T}] \mathrm{Prob}^f(X) = \frac{1}{\mathcal{Z}(\mu)} \int \mathcal{D}[U] \exp[if(U)\frac{\mu^I}{T}] \exp[-S(\mu; U)]$$

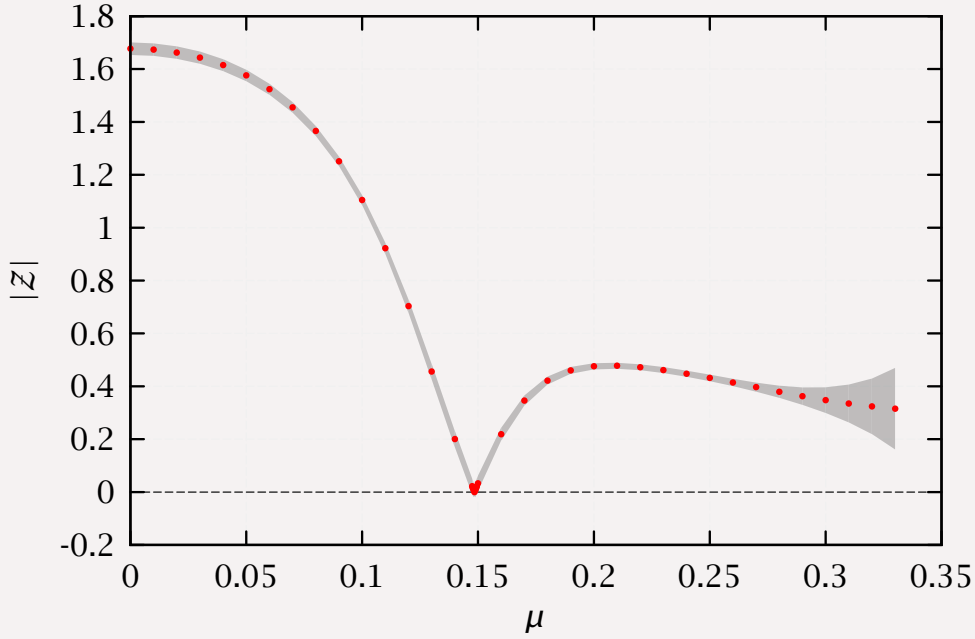
- Taking $f(U)$ to be the quark number, $\tilde{\mathcal{Z}}(\mu, \mu^I)$ approximates $\mathcal{Z}_{\mathrm{norm}}$ up to the first derivative of μ/T
- Approximate N_q distribution with Gaussian peaks, k stdev away from zero with L i.i.d. samples, and consider one Gaussian (note: variance is additive)

$$\left| \langle \exp[N_q(\Delta\mu + i\Delta\mu^I)/T] \rangle \right| \geq k \sqrt{\frac{\sigma^2(|\exp[N_q(\Delta\mu + i\Delta\mu^I)/T]|)}{L}}$$

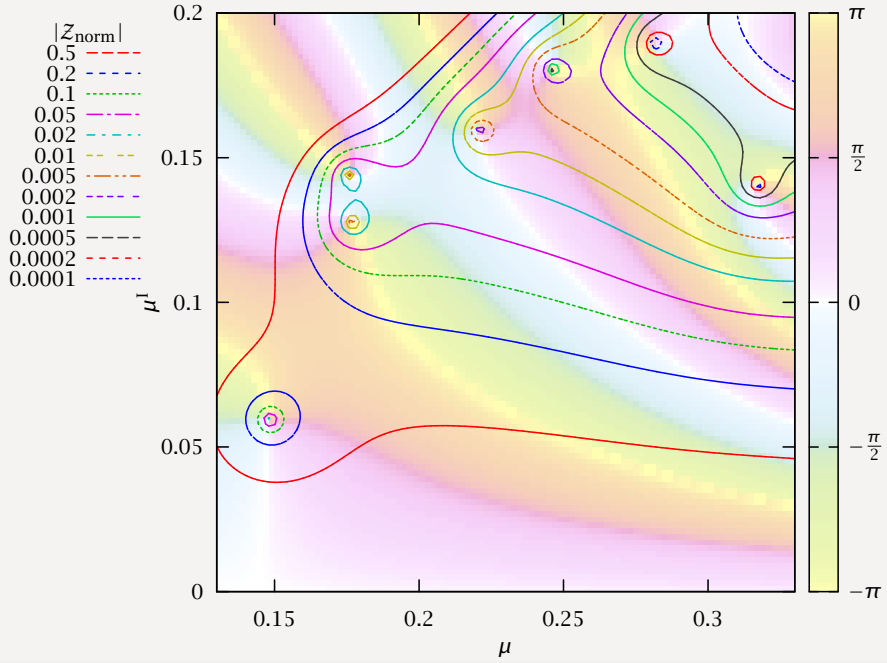
$$\sqrt{\Delta\mu^2 + (\Delta\mu^I)^2} \leq \sqrt{\frac{\ln\left(\frac{L}{k^2} + 1\right)}{\sigma^2(N_q)/T^2}} \xrightarrow{k=1, N_l=6^3} 0.2$$

- Circle around the simulation, volume factor hidden in the width of N_q
- Effects of cancellations between two peaks not included

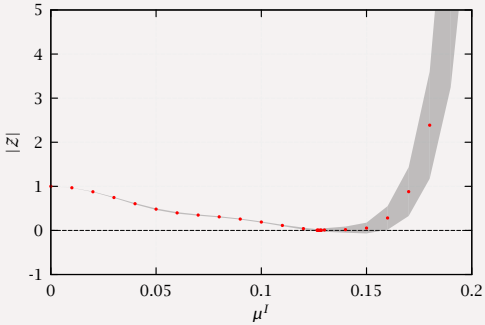
$|\mathcal{Z}_{\text{norm}}|$ vs. μ, fixing μ^I at the first zero

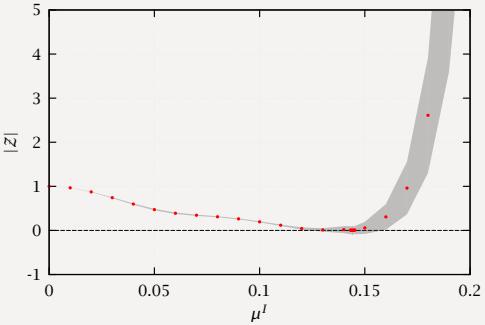


$\mathcal{Z}$ with complex μ, 6^3 ($\beta = 1.58$, $\kappa = 0.1385$)



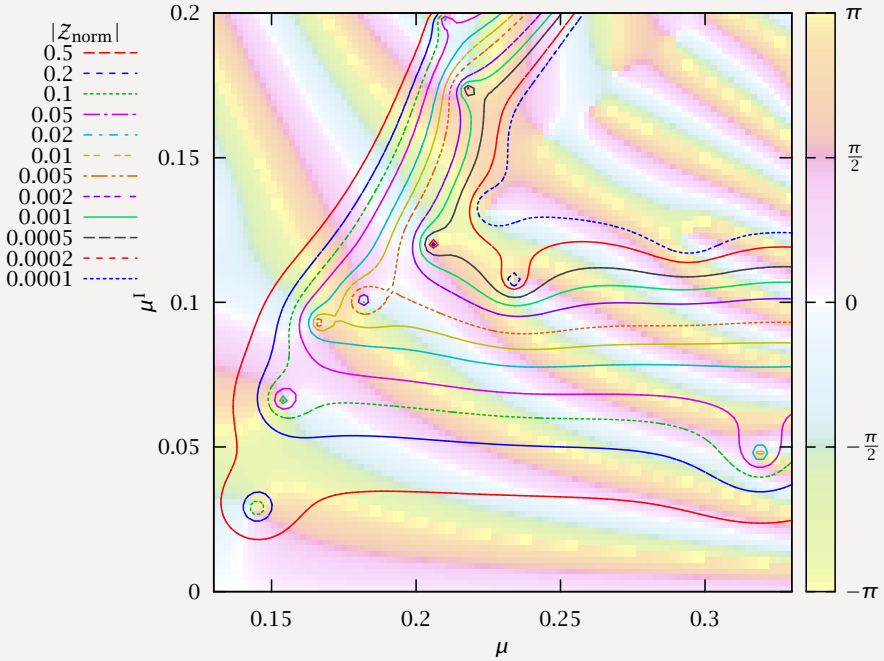
Spurious zeros within the confidence region



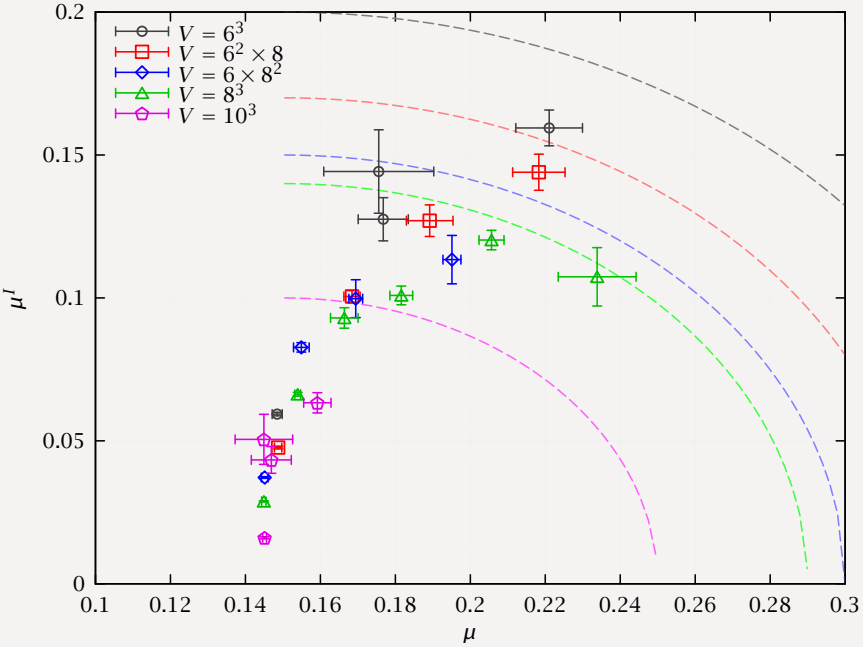


- Plot $|\mathcal{Z}_{\text{norm}}|$ vs. μ^I, at the two second lowest zeros
- Statistically they are the same zero

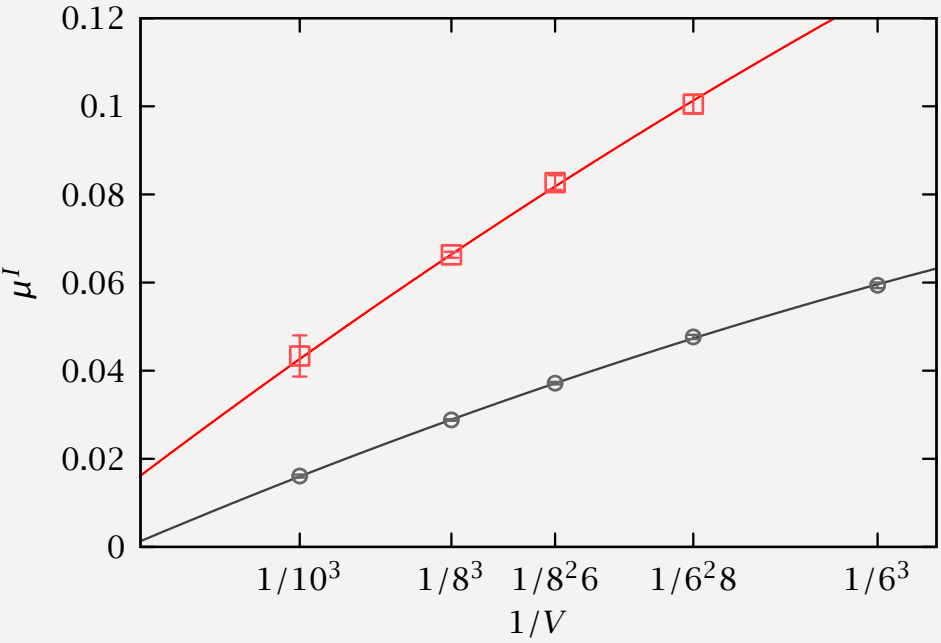
$\mathcal{Z}$ with complex μ, 8^3, ($\beta = 1.58$, $\kappa = 0.1385$)



Zeros of the partition function with complex μ



Volume scaling of μ^I for the first two zeros



Summary

- Taylor expansions of the logarithm of the fermion determinant enables us to do μ-reweighting accurately and efficiently.
- μ-reweighting is excellent in the range of parameters we are interested in.
- Carefully combining ensembles at multiple μ gives better statistics.
- Locations of partition function zeros with complex chemical potential form a curve starting from a finite real μ and extending to larger values of both real and imaginary parts of the chemical potential.
- Volume dependence of the locations of zeros is interesting.