Finite density lattice QCD: multiple fronts against the sign problem

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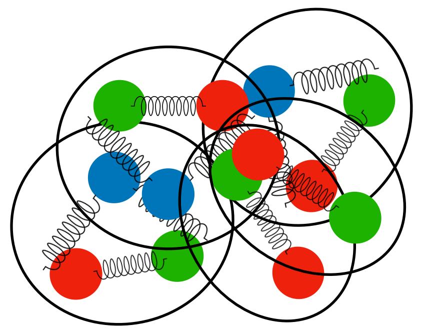
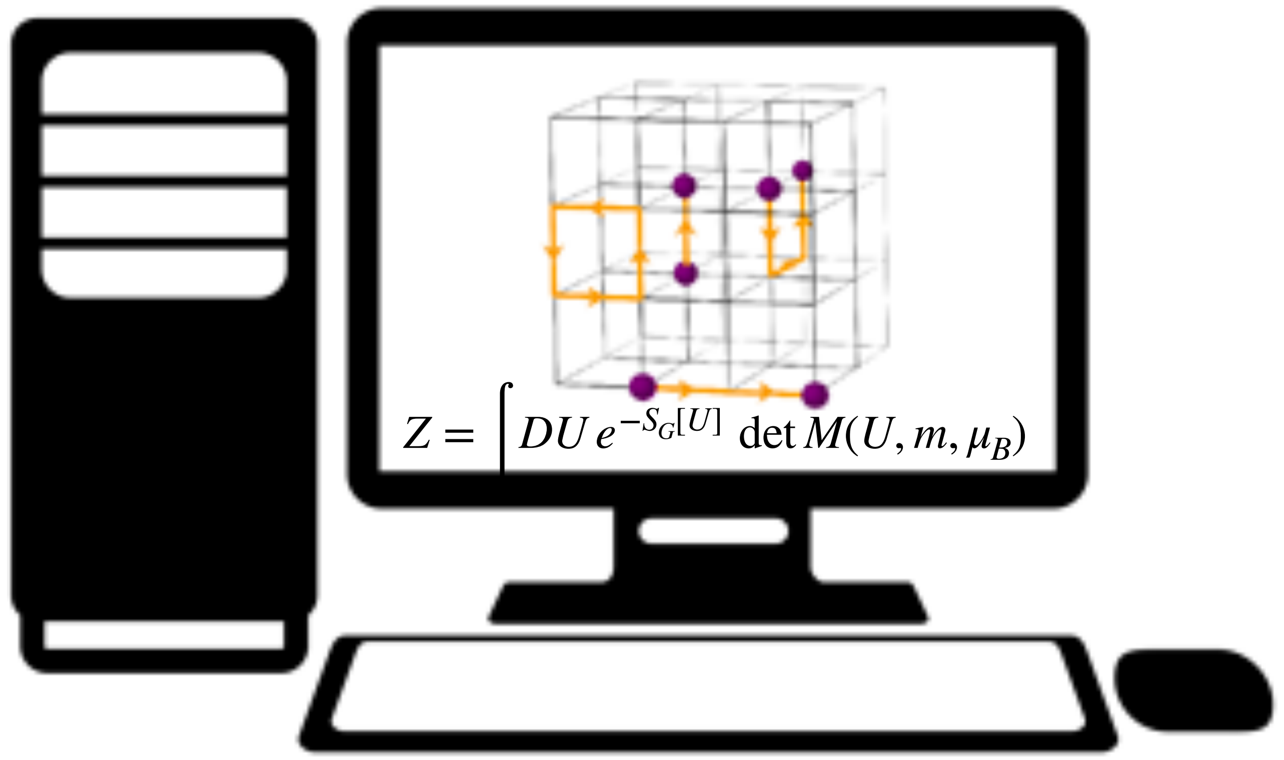
What is exactly the sign problem?

- Finite density $\leftrightarrow$ Finite μ_B



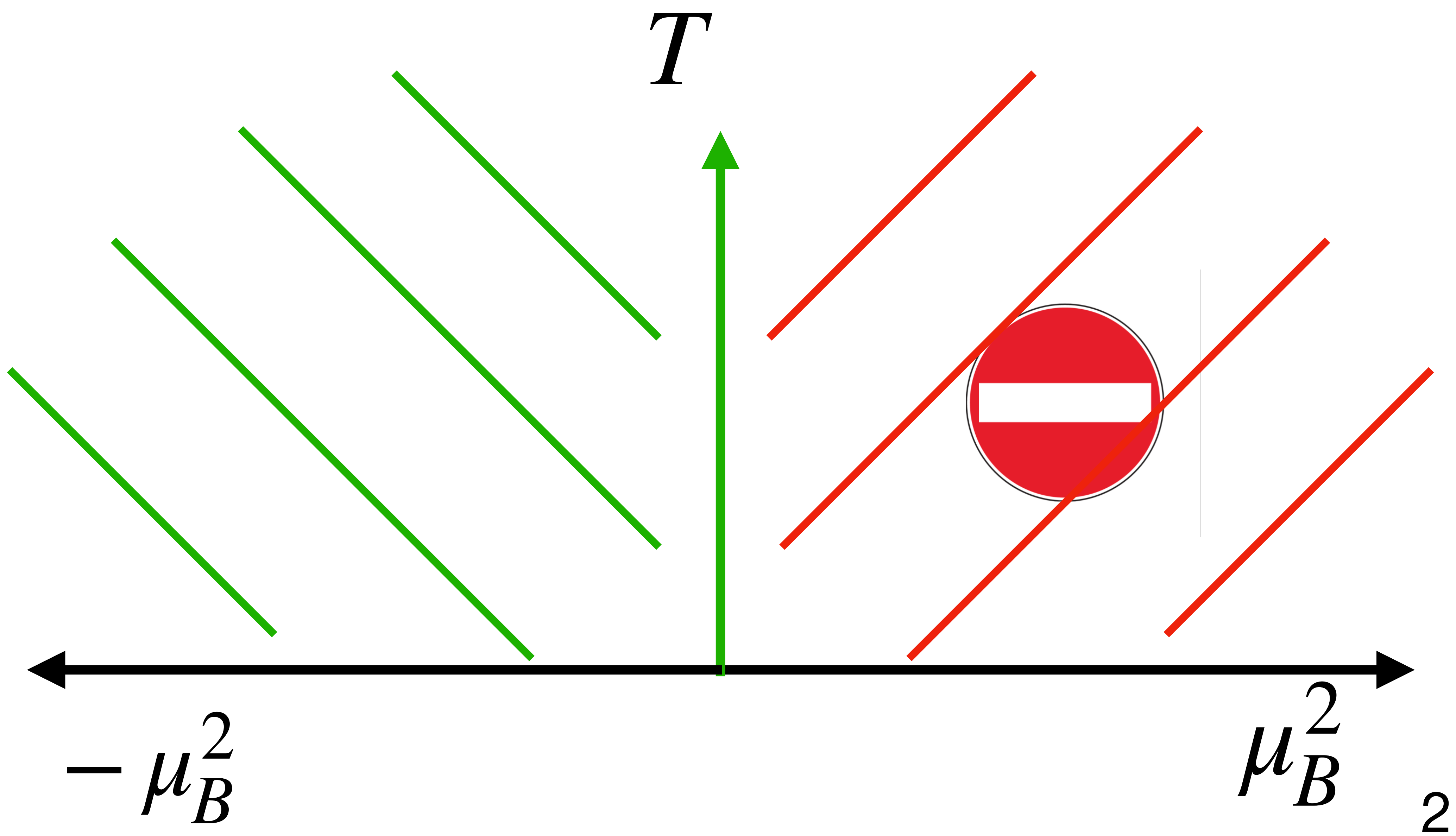


- $$Z = \int DU\, e^{-S_G[U]}\, \det M(U, m, \mu_B)$$

- $\det M(U, m, \mu_B)$ is real and positive only for $\mu_B^2 \leq 0$

- we can't measure directly any observable with Monte Carlo methods for $\mu_B^2 > 0$

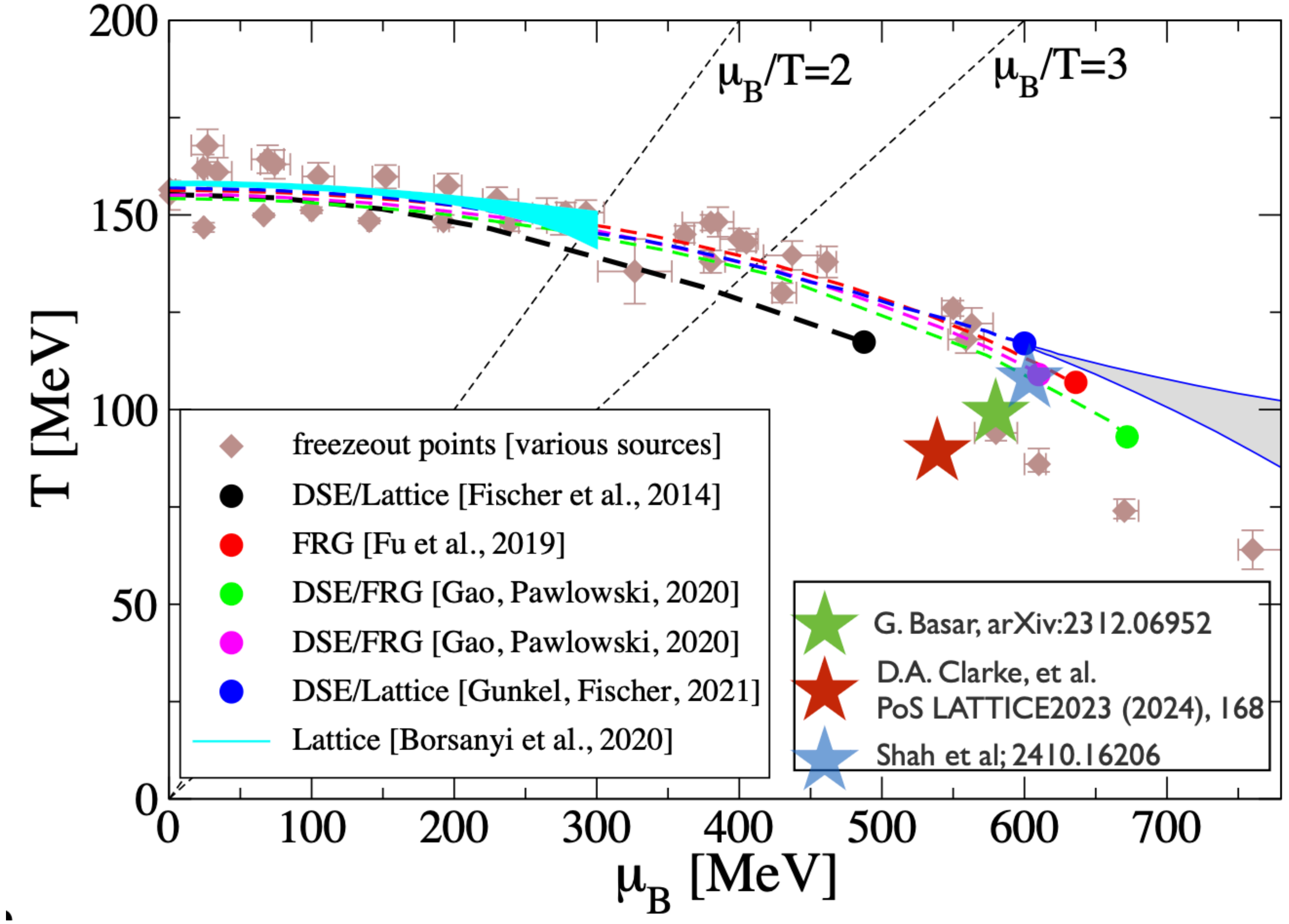
- $$< O > = \frac{1}{N_{\text{conf}}} \sum_{U_i \text{ with prob} \sim \mathrm{e}^{-S_{\text{eff}}}} O[U_i]$$



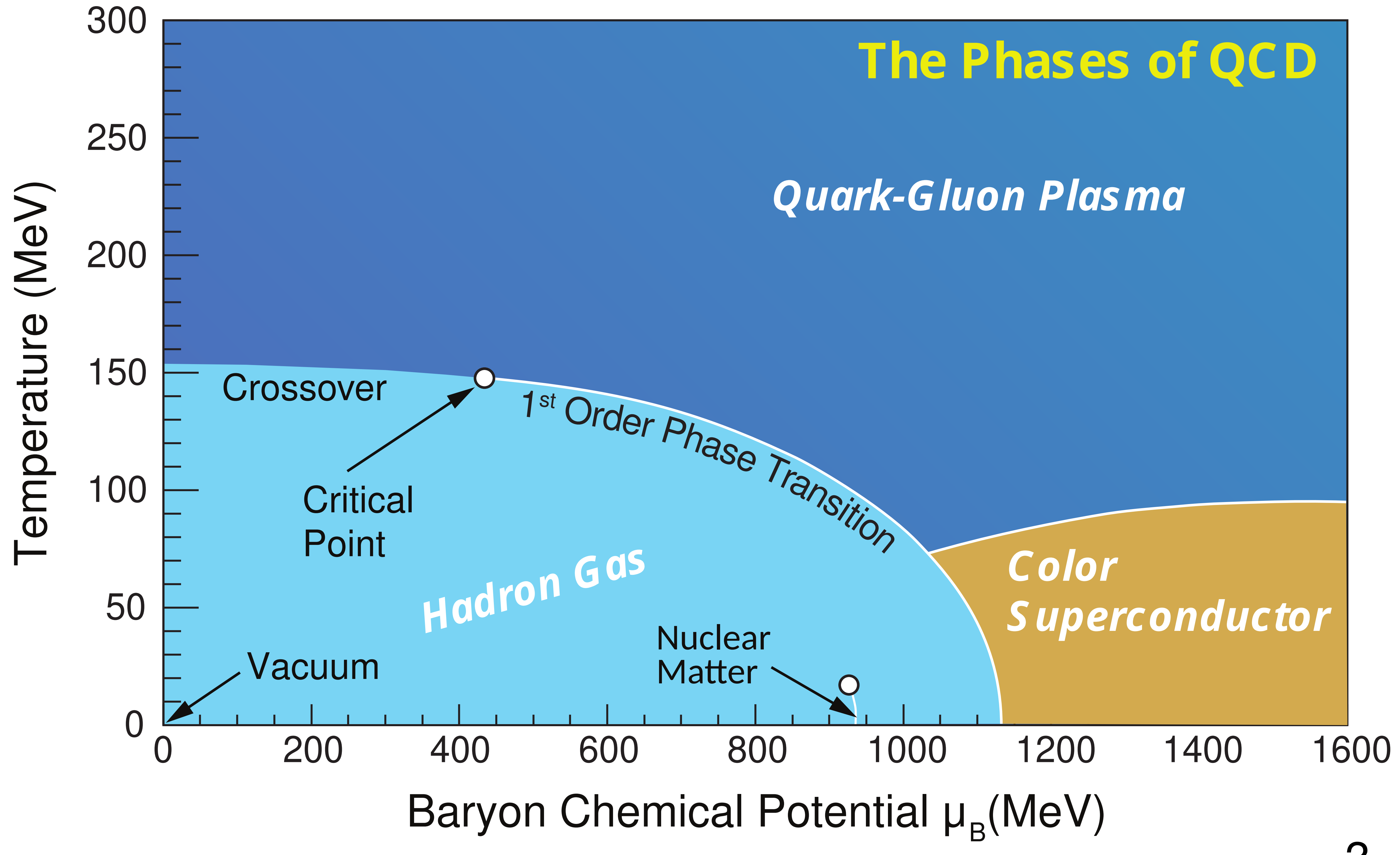
Why do we actually wish to reach **high** μ_B?

- Active area of research: search for Critical End Point in (T, μ_B) plane
- CEP excluded for low μ_B/high T corner of the phase diagram (arXiv:2507.13254) NEW!

Plot from Christian Fischer's talk at XQCD 2025

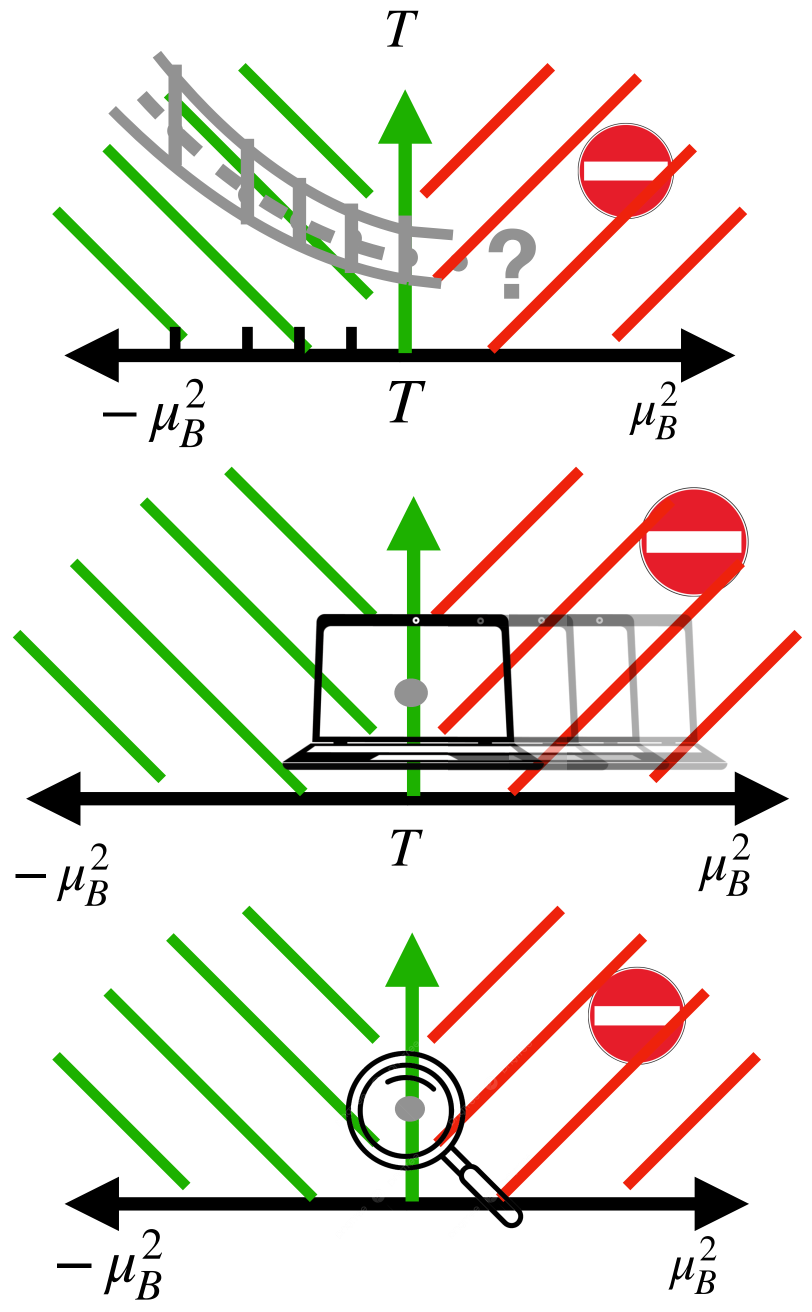


Plot from arXiv:1906.00936



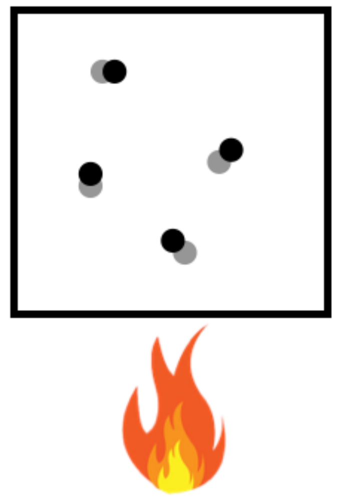
Circumventing the sign problem: multiple fronts

- Analytical continuation arXiv:2002.02821
- Reweighting in μ_B arXiv:2108.09213
- Taylor / T' methods arXiv:2410.06216



Some "classical" methods

- Canonical lattice QCD



something unusual (not completely new)

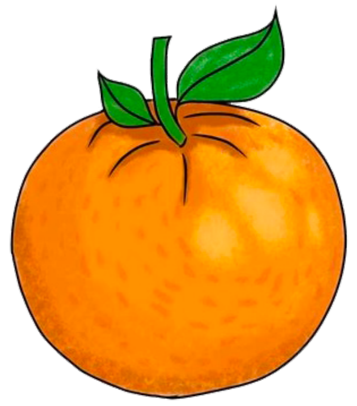
We won't discuss all these methods in detail.

~~Multiple~~ fronts → "a couple of" fronts

Plan of the talk

- Analytical continuation
- Reweighting in μ_B

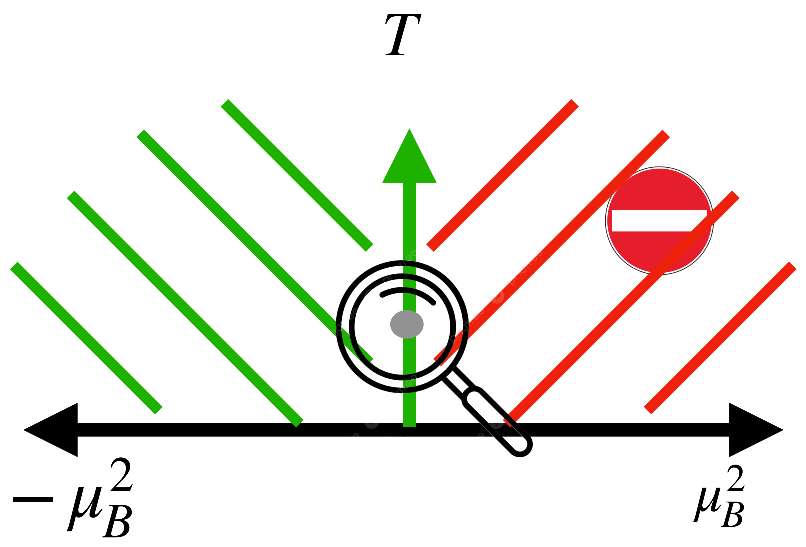
- Description
- Drawbacks

Then, an “apples”  versus “oranges”  comparison

We will show two sets of results. They are *not* the same results in both cases.
We are more interested in the possible advantages/problems that we have in producing them

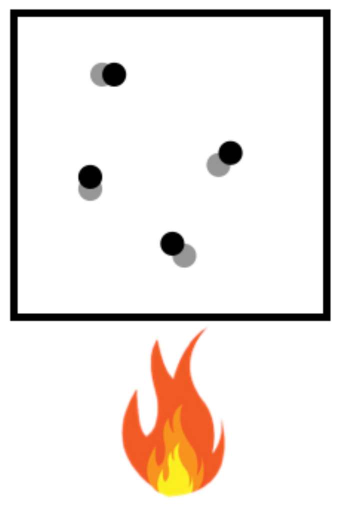
“We just want to see how well the apples/oranges grow in the 2 cases”

- Taylor methods



arXiv:2410.06216

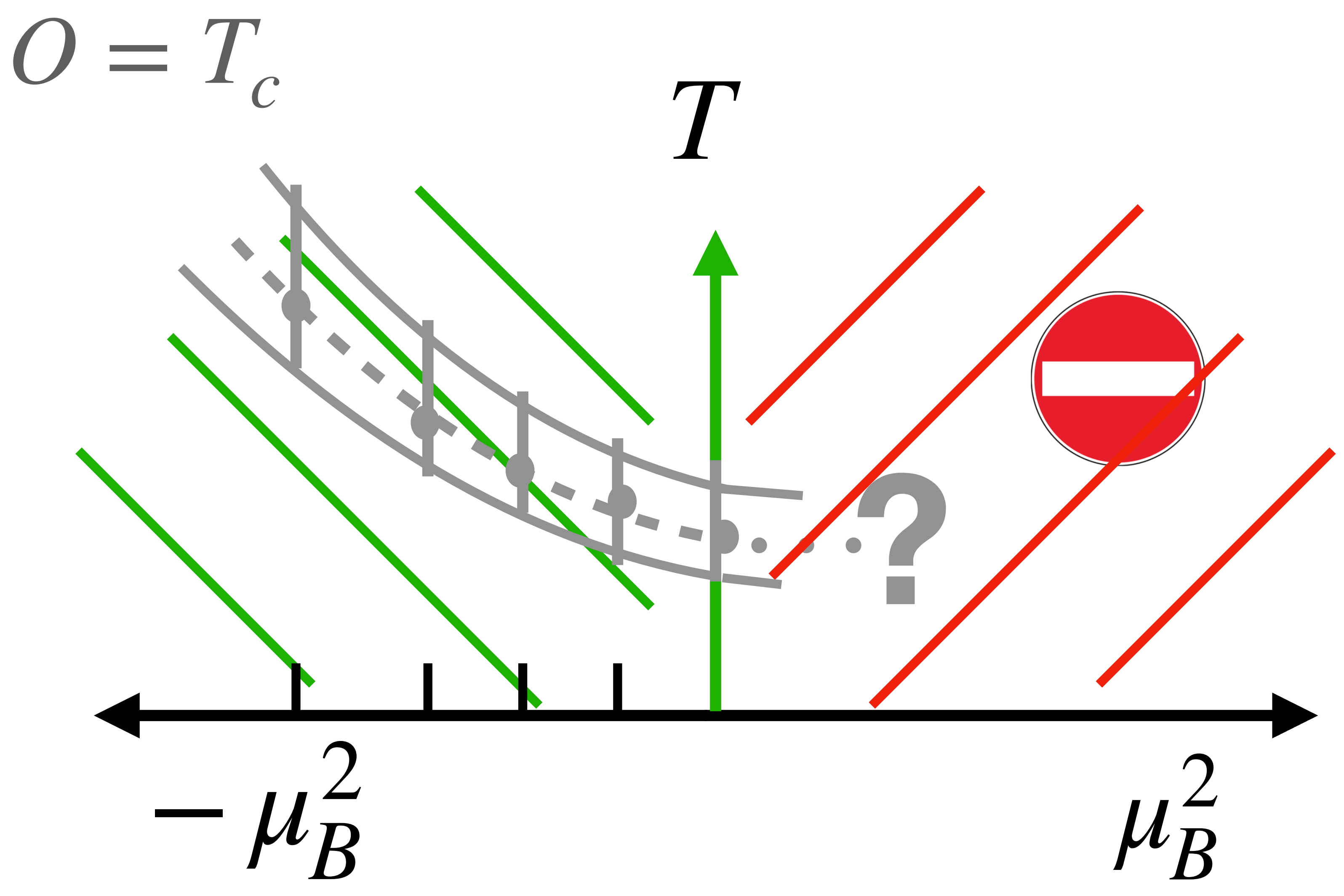
- Canonical lattice QCD

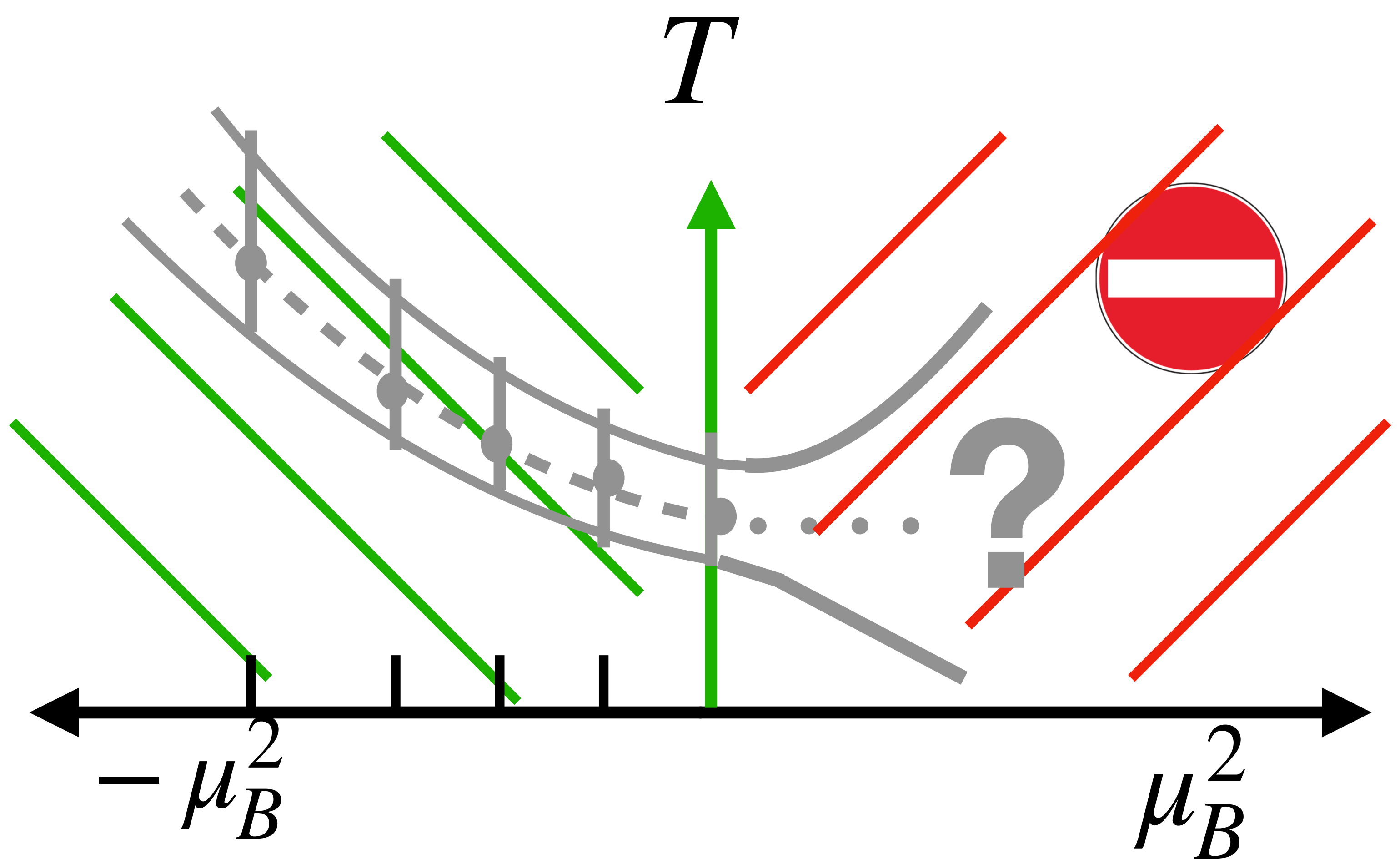


arXiv 25xx.xxxx

Analytical continuation

- simulate at $\mu_B^2 < 0$ and extrapolate to $\mu_B^2 > 0$
- conceptually very simple





- Problem: lots of systematics

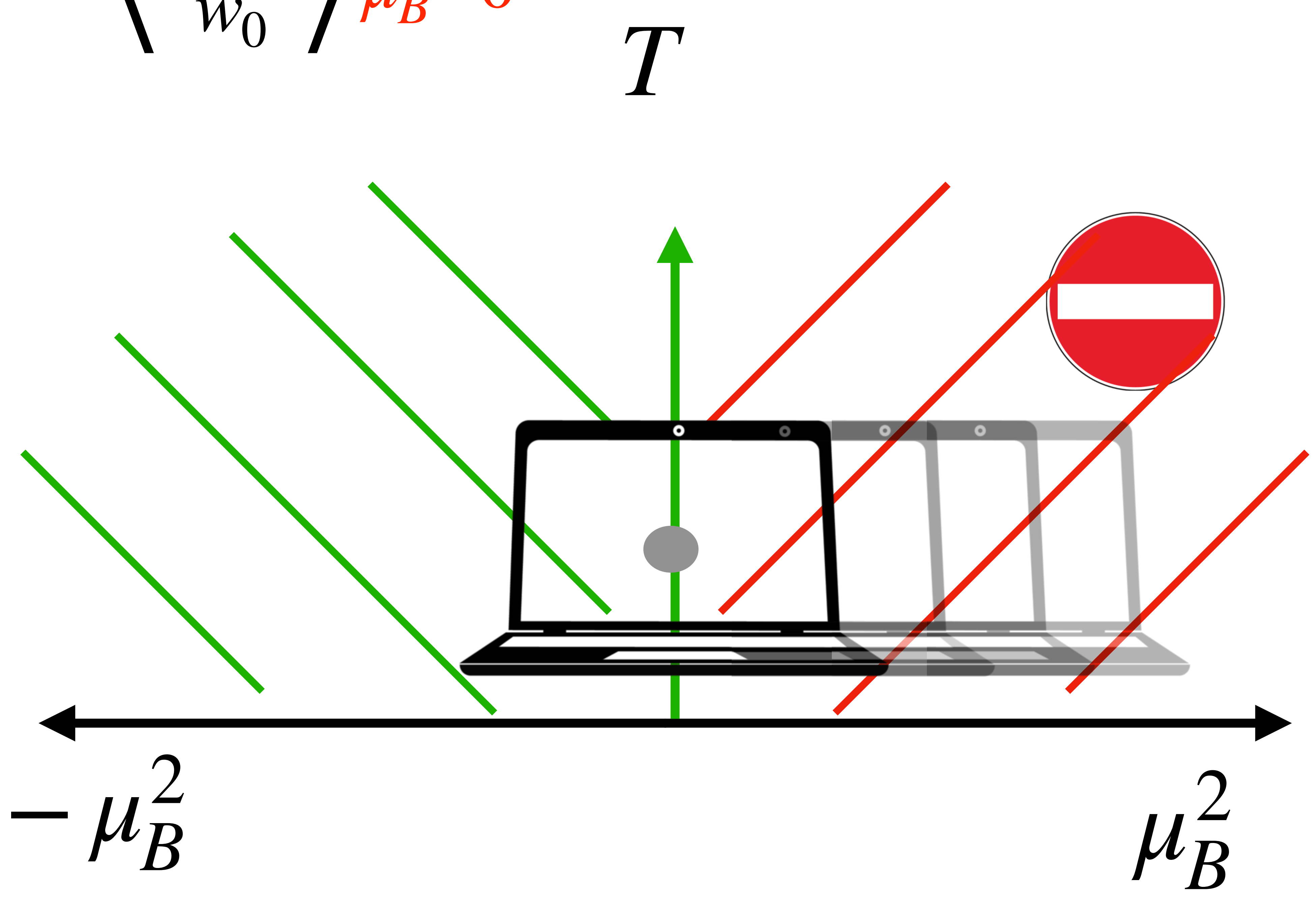
Reweighting in μ_B

- make the simulations at $\mu_B = 0$ and correct the weights in the observable measure

- $$< O >_{\mu_B} = \frac{\int DU\, e^{-S_G[U]}\, O(U) \frac{w_{\mu_B}(U)}{w_0(U)}\, w_0(U)}{\int DU\, e^{-S_G[U]}\, \frac{w_{\mu_B}(U)}{w_0(U)}\, w_0(U)} = \frac{\left\langle O \ \frac{w_{\mu_B}}{w_0} \right\rangle_{\mu_B=0}}{\left\langle \frac{w_{\mu_B}}{w_0} \right\rangle_{\mu_B=0}}$$

- $$\frac{Z(\mu_B)}{Z(0)} = \left\langle \frac{w_{\mu_B}}{w_0} \right\rangle_{\mu_B=0} = \left\langle \frac{\det M(\mu_B)}{\det M(0)} \right\rangle_{\mu_B=0}$$

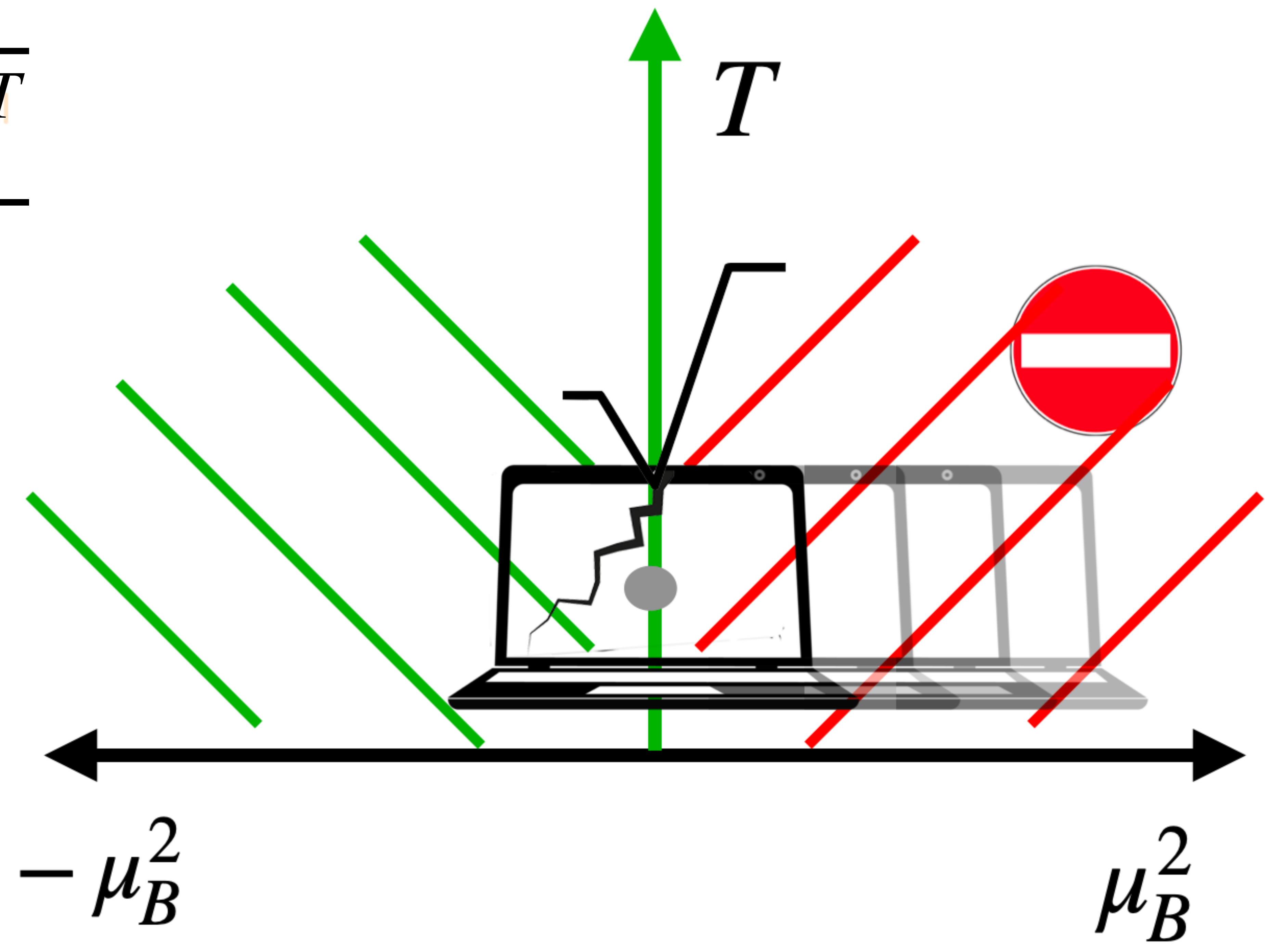
- No extrapolations systematics, but…



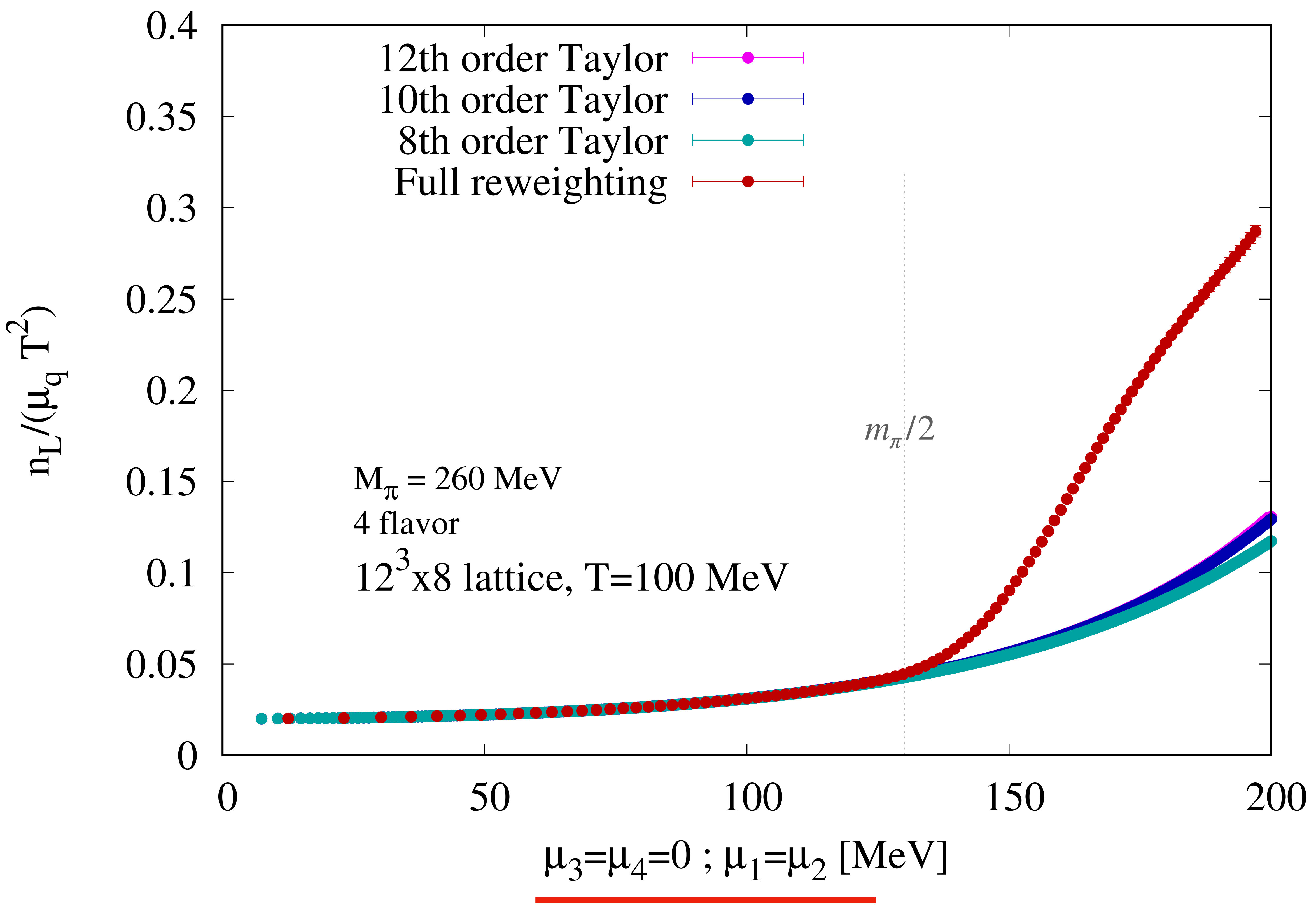
- …there is a technical problem associated with staggered fermions
- Let's look at the 2+1 flavours theory with $\mu_u = \mu_d = \mu_q, \mu_s = 0$
- $$Z_{2+1}(T, \mu_q) = \int DU\, e^{-S_G[U]} \det M(U, m_q, \mu_q)^{\frac{1}{2}} \det M(U, m_s, 0)^{\frac{1}{4}}$$
- $$\frac{\det M(U, m_q, \mu_q)^{\frac{1}{2}}}{\det M(U, m_q, 0)^{\frac{1}{2}}} = e^{-3N_s^3 \mu_q/T} \prod_{k=1}^{6N_s^3} \sqrt{\frac{\lambda_k[m, U] - e^{\mu_q/T}}{\lambda_k[m, U] - 1}}$$

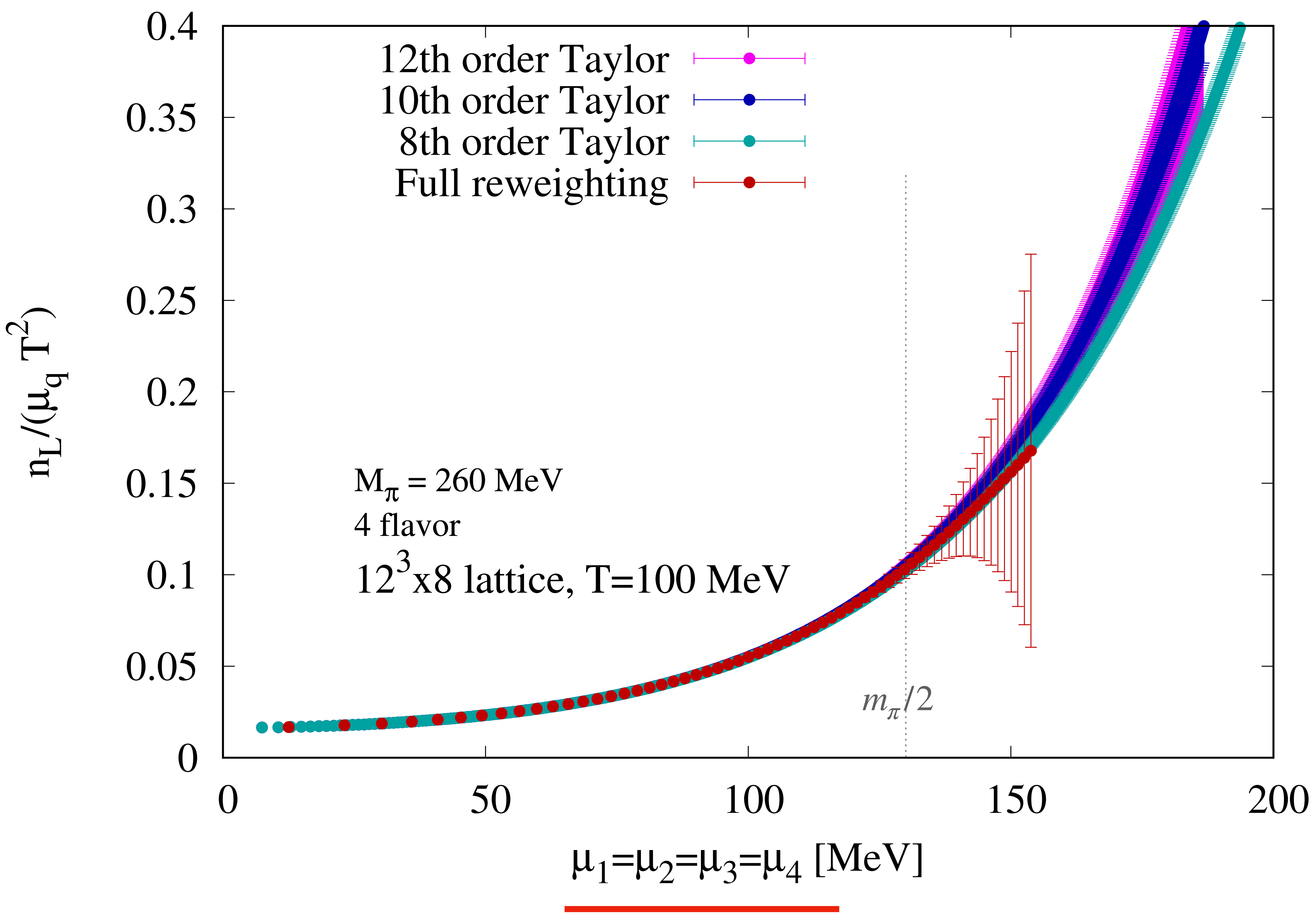
  in a reduced matrix formalism
- $\frac{w_{\mu_B}}{w_0}$: the ambiguity in the root can be solved,

  but have we ruled all the non-analicities out?



[arXiv:2308.06105](), results for the light quark density n_L





- rise at $m_\pi/2$ for the reweighted case

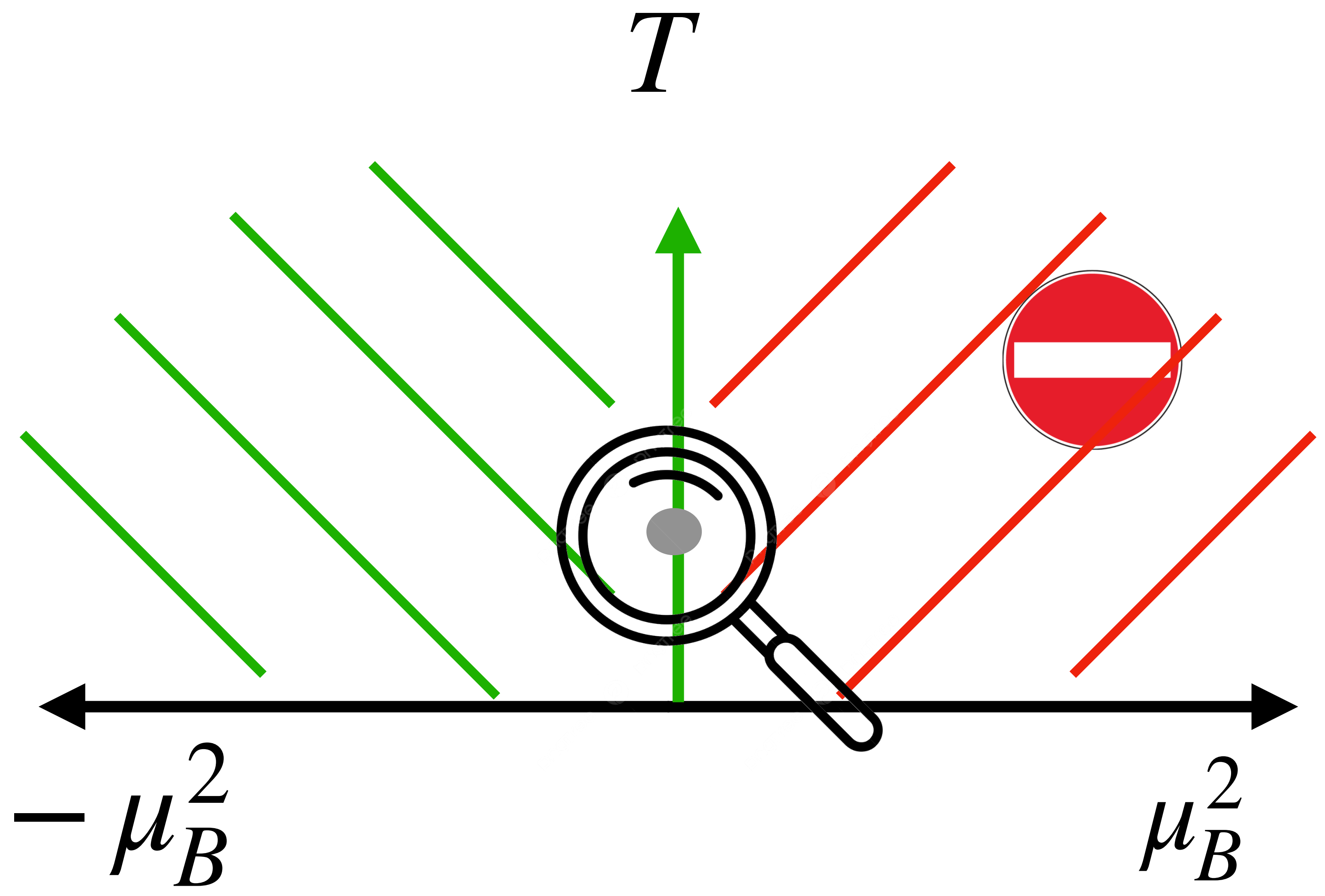
- $\rightarrow$ no rooting
- reweighting and Taylor (up to 12th order) agree

we have a problem with rooting for staggered fermions

Taylor expansion

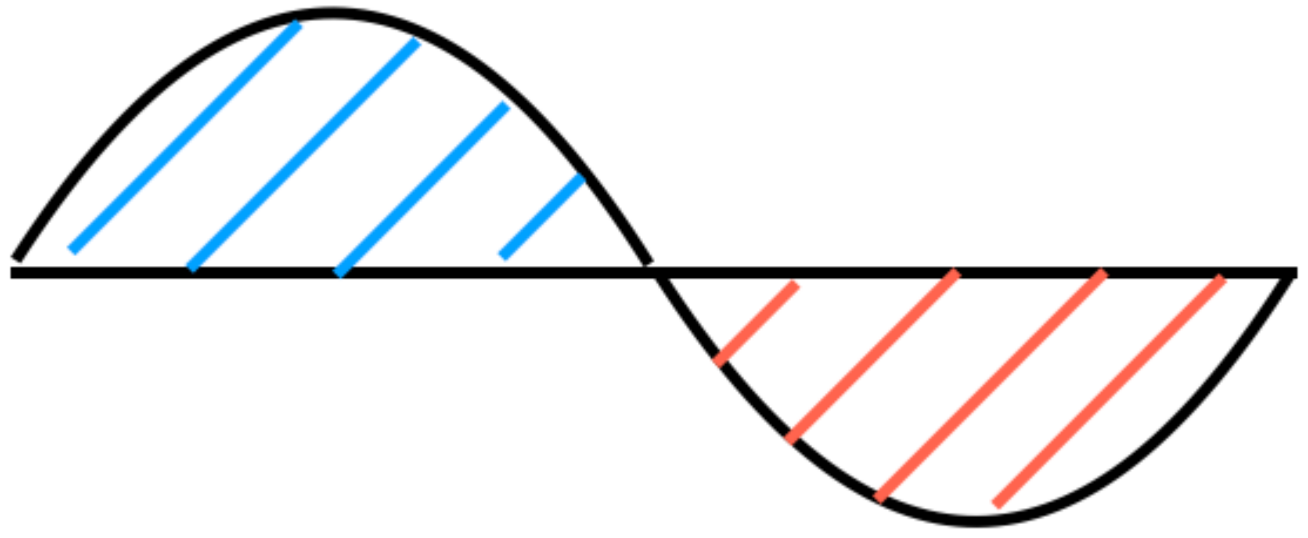
- compute the derivatives at $\mu_B = 0$

$$O(\mu_B) = O(0) + \frac{1}{2!}\mu_B^2 \frac{\partial^2 O}{\partial \mu_B^2}(0) + \frac{1}{4!}\mu_B^4 \frac{\partial^4 O}{\partial \mu_B^4}(0) + \dots$$



- Truncation in μ_B is uncontrolled: the error is determined by the next term in the expansion

- Sign problem is not really away
- it still manifests itself in the cancellations of the terms inside the Taylor coefficients



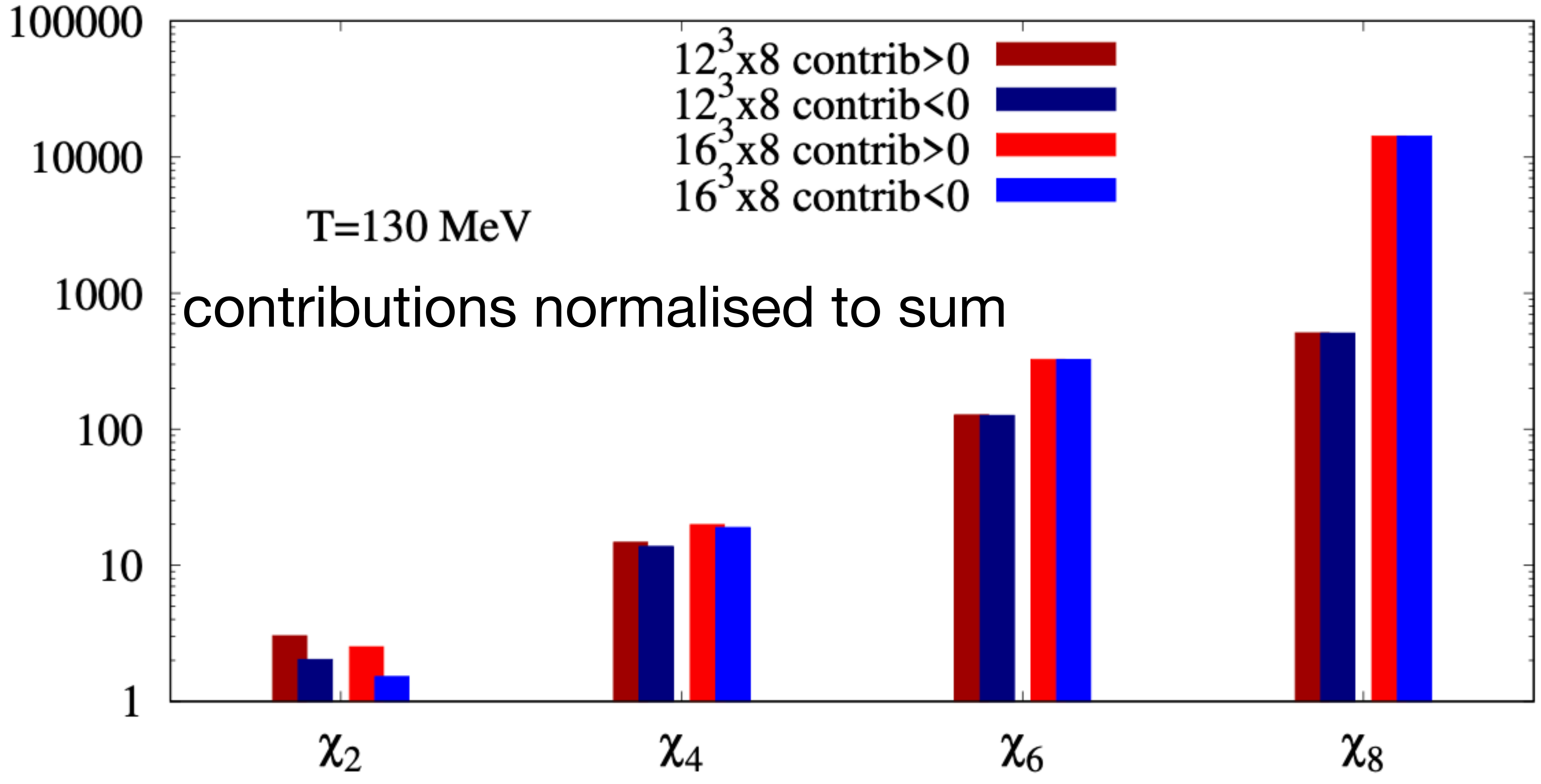
- We look at the derivatives of $\log Z$, that are related to quark number susceptibilities

$$\chi^{uds}_{ijk}(T, \mu_u, \mu_d, \mu_s) = \frac{T}{V} \frac{\partial^{i+j+k} \log Z}{(\partial_u)^i (\partial_d)^j (\partial_s)^k}$$

- then for any O

$$\partial_i < O > = < O \, \partial_i \log(\det M)^{\frac{1}{4}} > - < O > (\partial_i \log Z) + < \partial_i O >$$

- χ_{2n}: cancellation is $O(V^{n-1})$
- we need small volumes!!



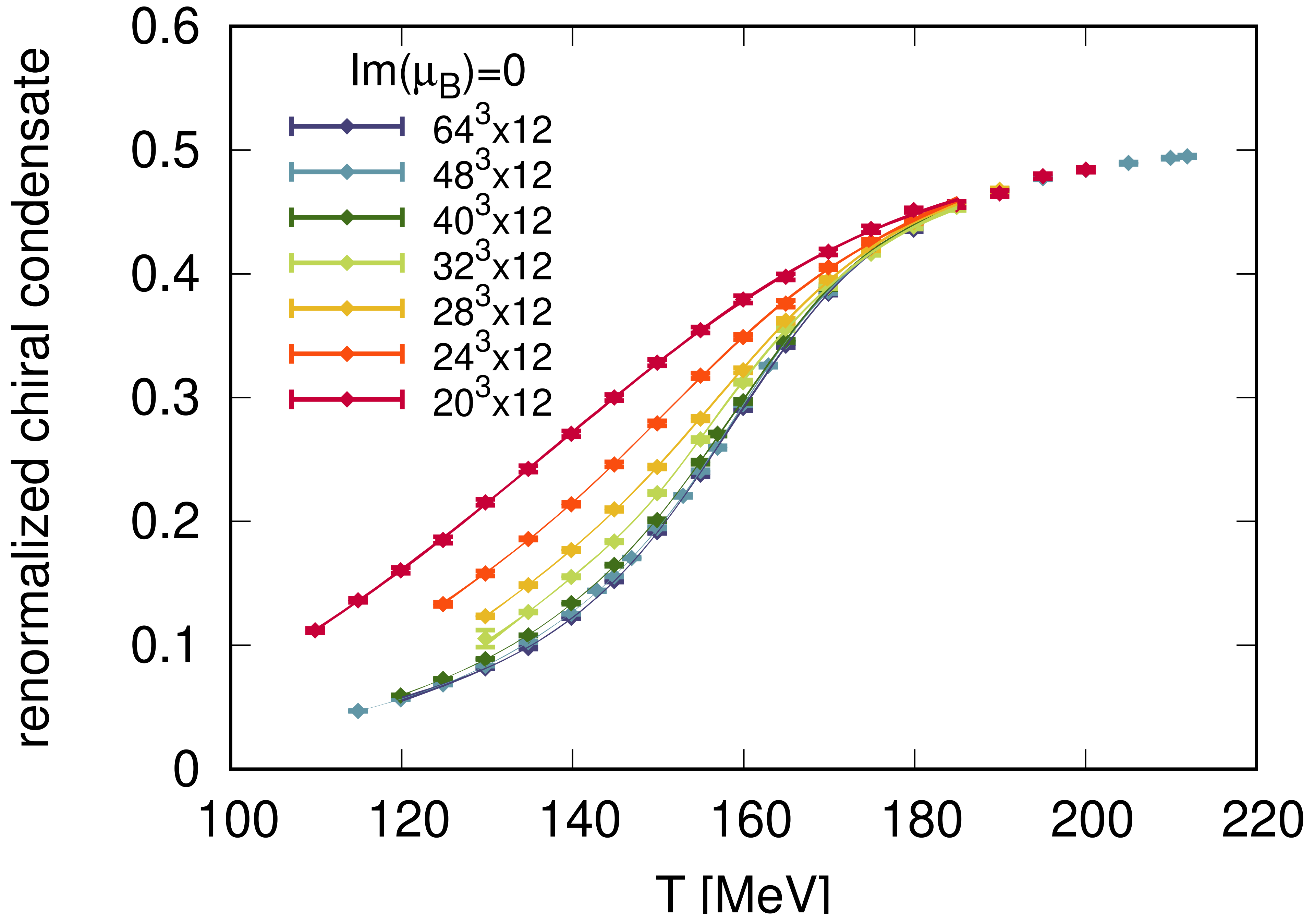
Chiral observables

- Chiral symmetry restoration in limit $m_q \to 0$
- **order parameter:** chiral condensate

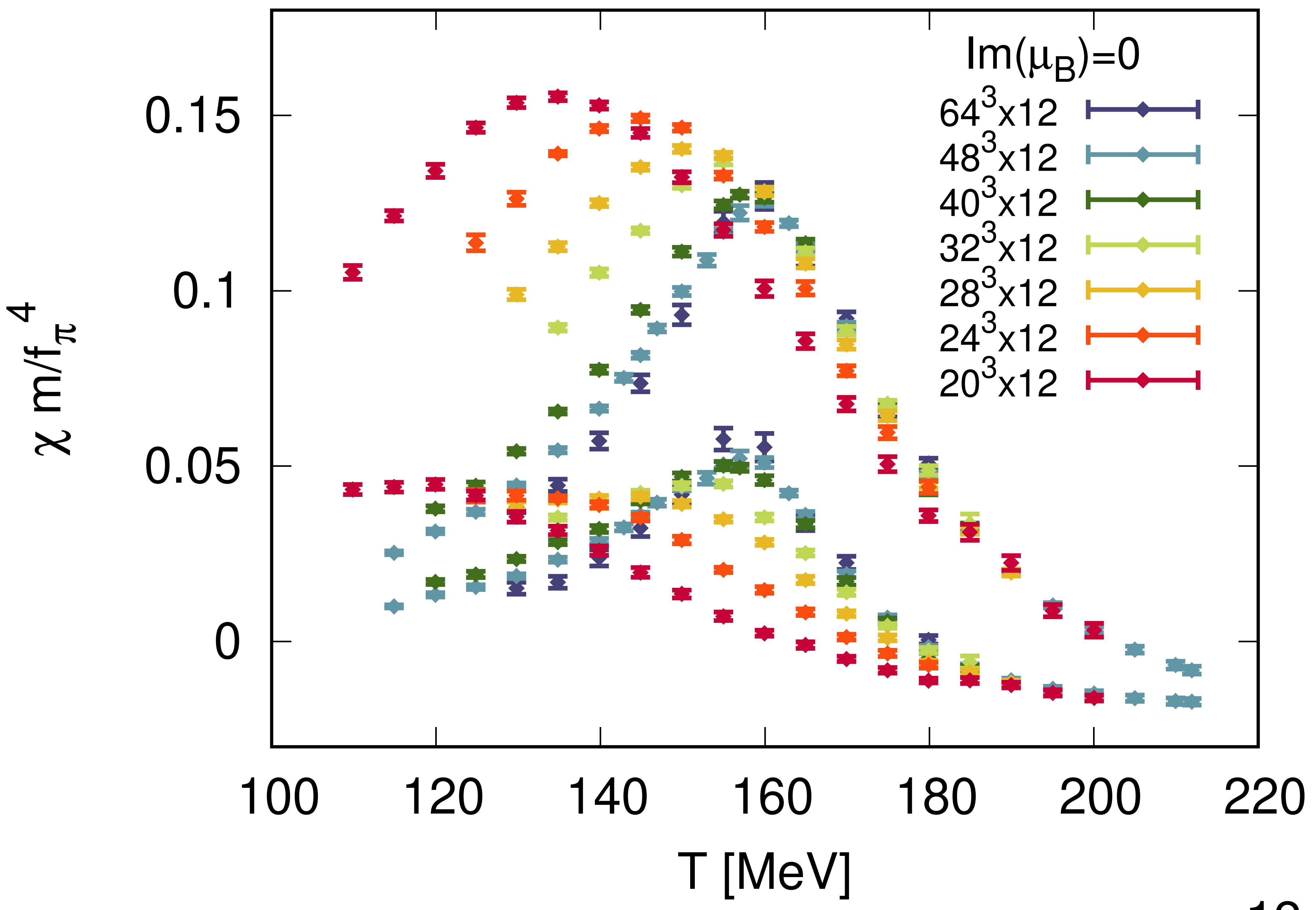
$$< \bar{\psi}\psi > = \frac{T}{V}\frac{\partial \log Z}{\partial m_{ud}}$$

- **chiral susceptibility** $\chi = \frac{T}{V}\frac{\partial^2 \log Z}{\partial m_{ud}^2}$
- disconnected chiral susceptibility

$$\chi_{\text{disc}} = \frac{T}{V}\left(\frac{\partial^2 \log Z}{\partial m_u \partial m_d}\right)_{m_u=m_d}$$



Quite **sensitive to volume!!**

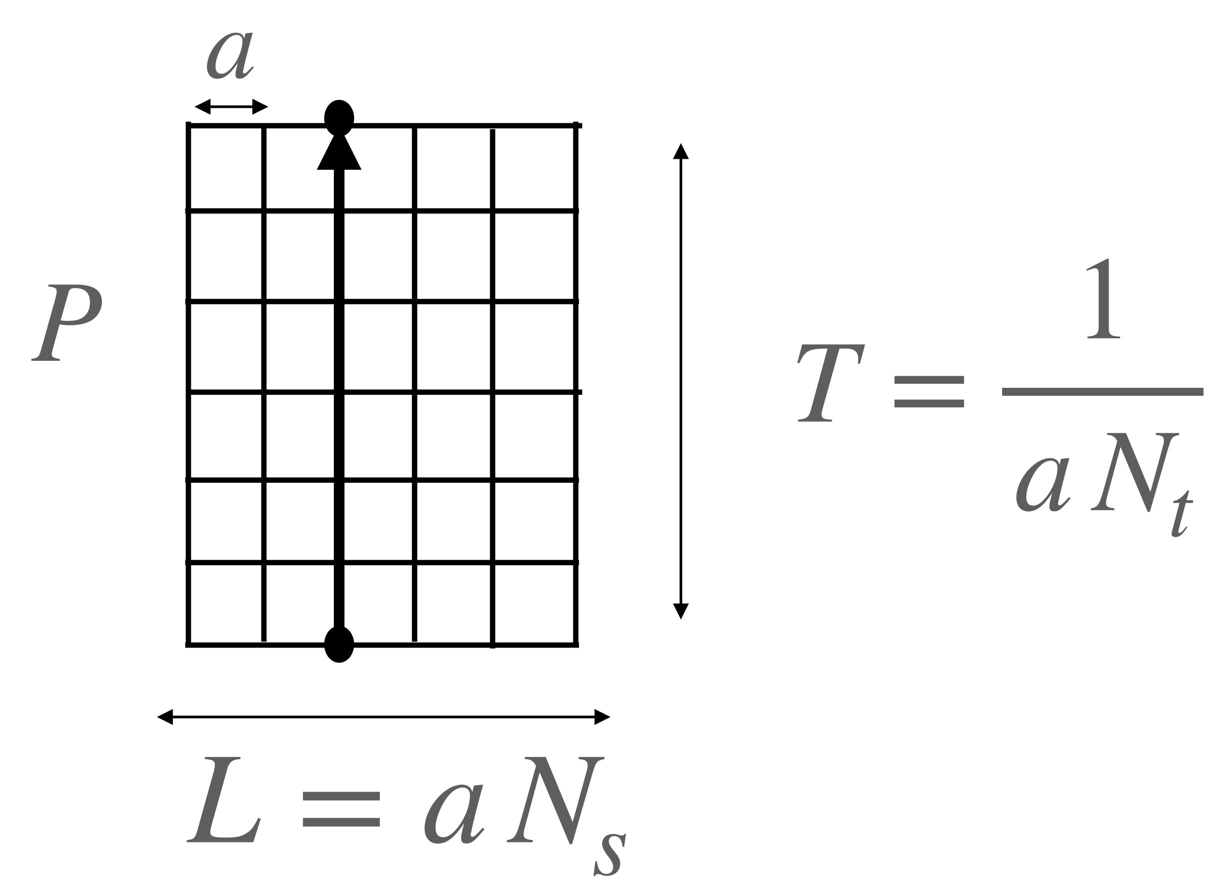


arXiv 2405.12320

Other observables?

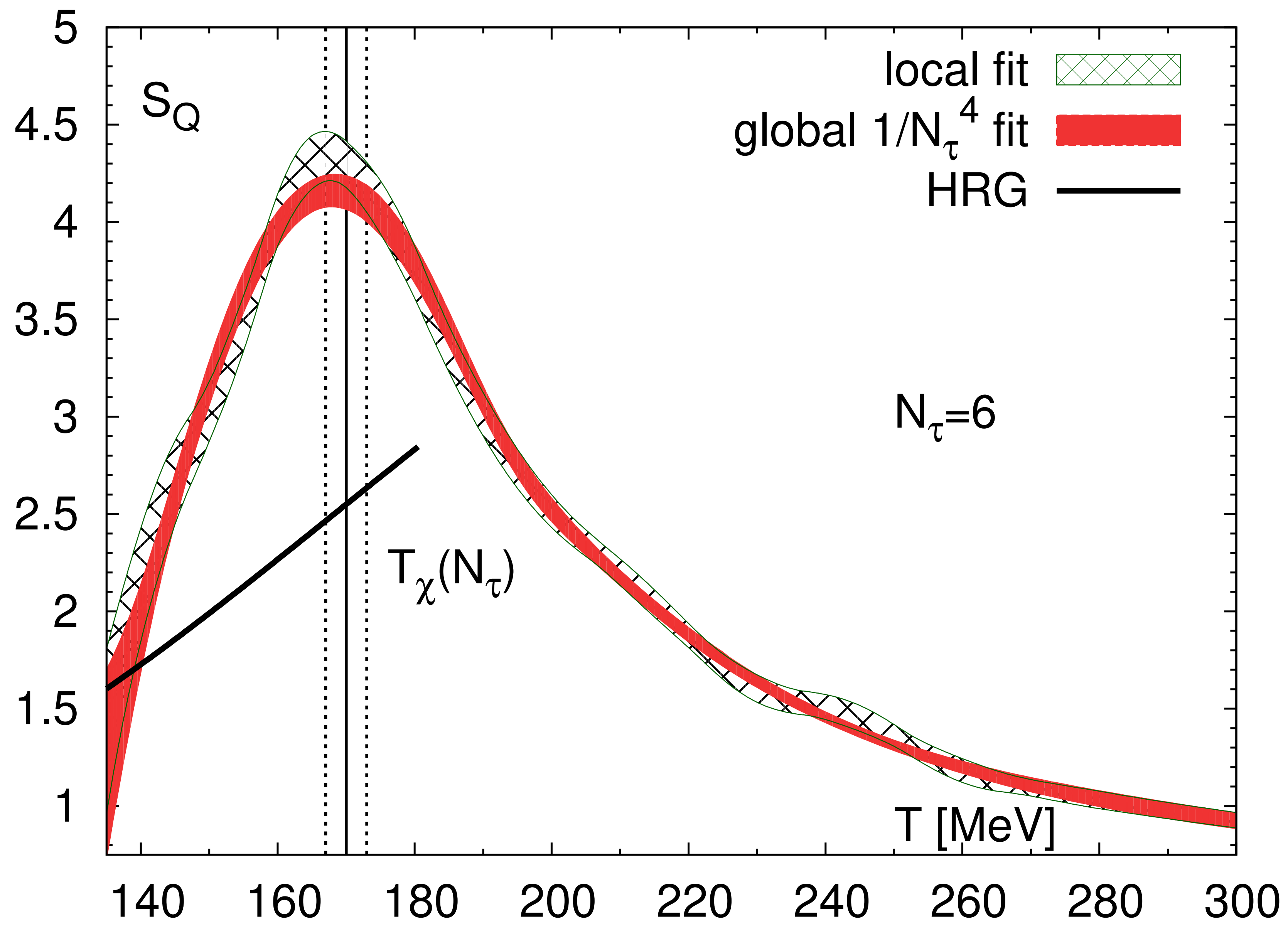
arXiv 1603.06637 (TUMQCD Collaboration):

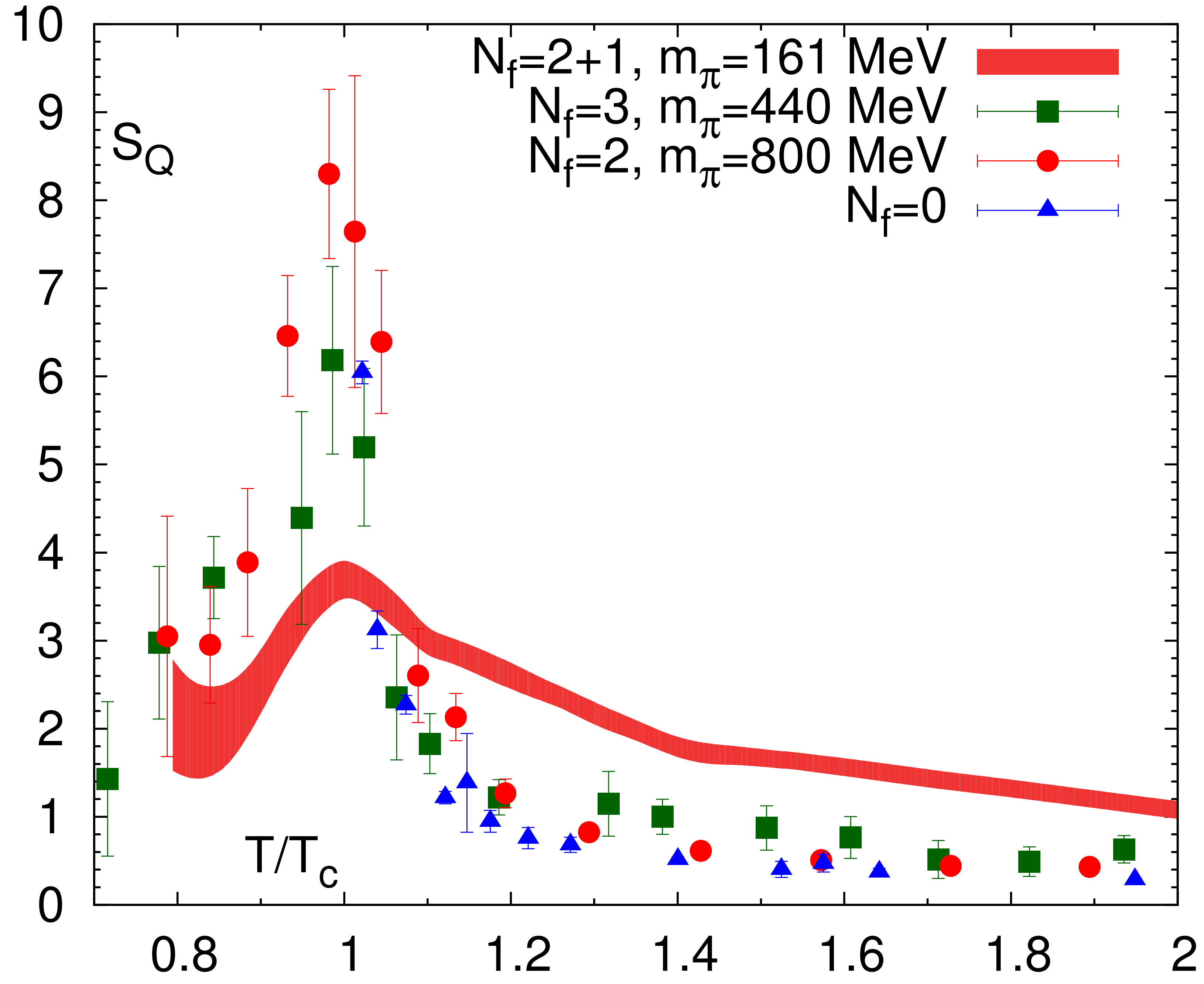
look at **Polyakov loop**



for **infinite** quark masses it is a probe of **deconfinement** $P \sim e^{-F_Q/T}$

static quark entropy $S_Q = -\frac{\partial F_Q(T)}{\partial T}$**:** it has a peak near chiral crossover temperature

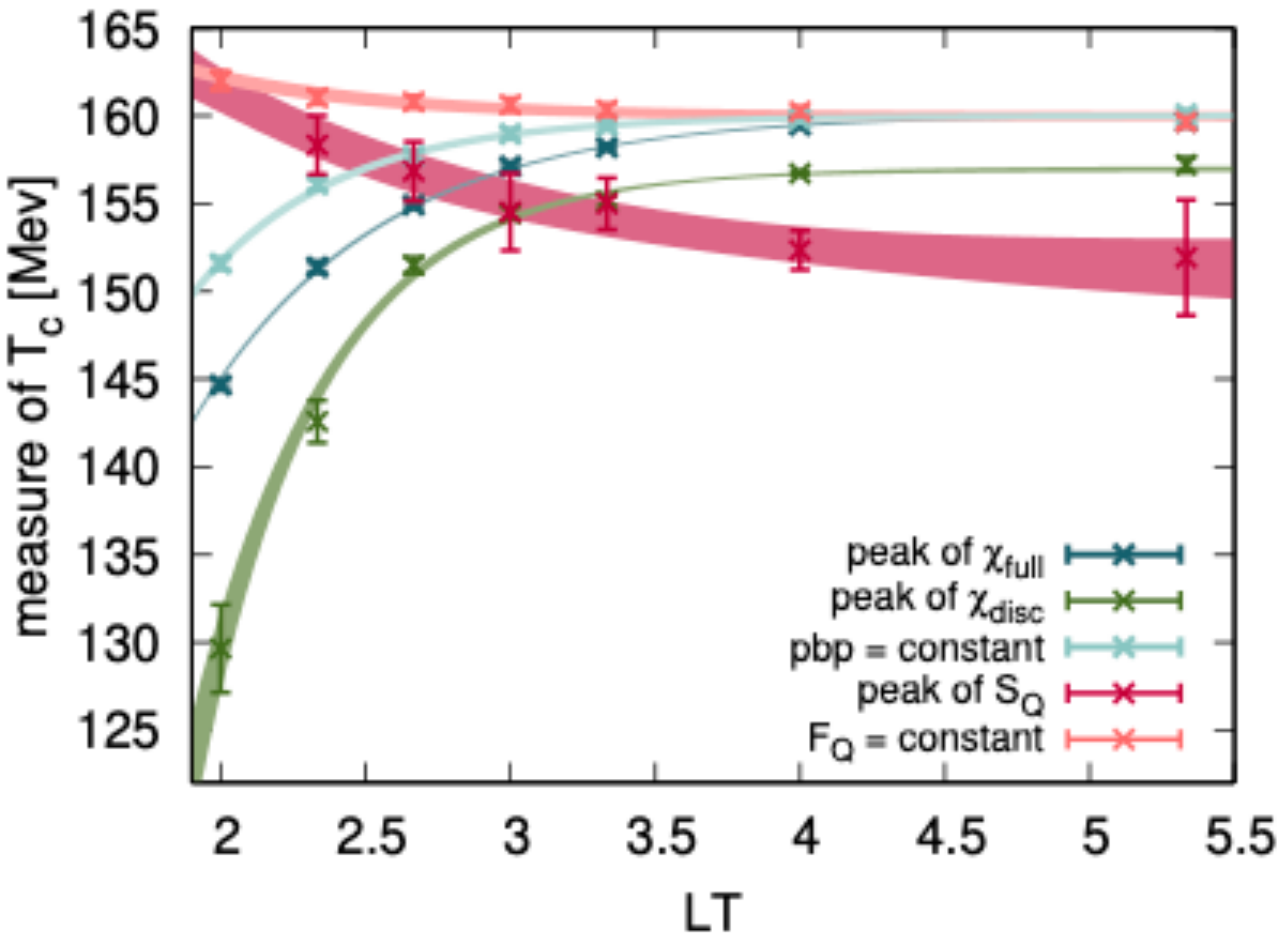


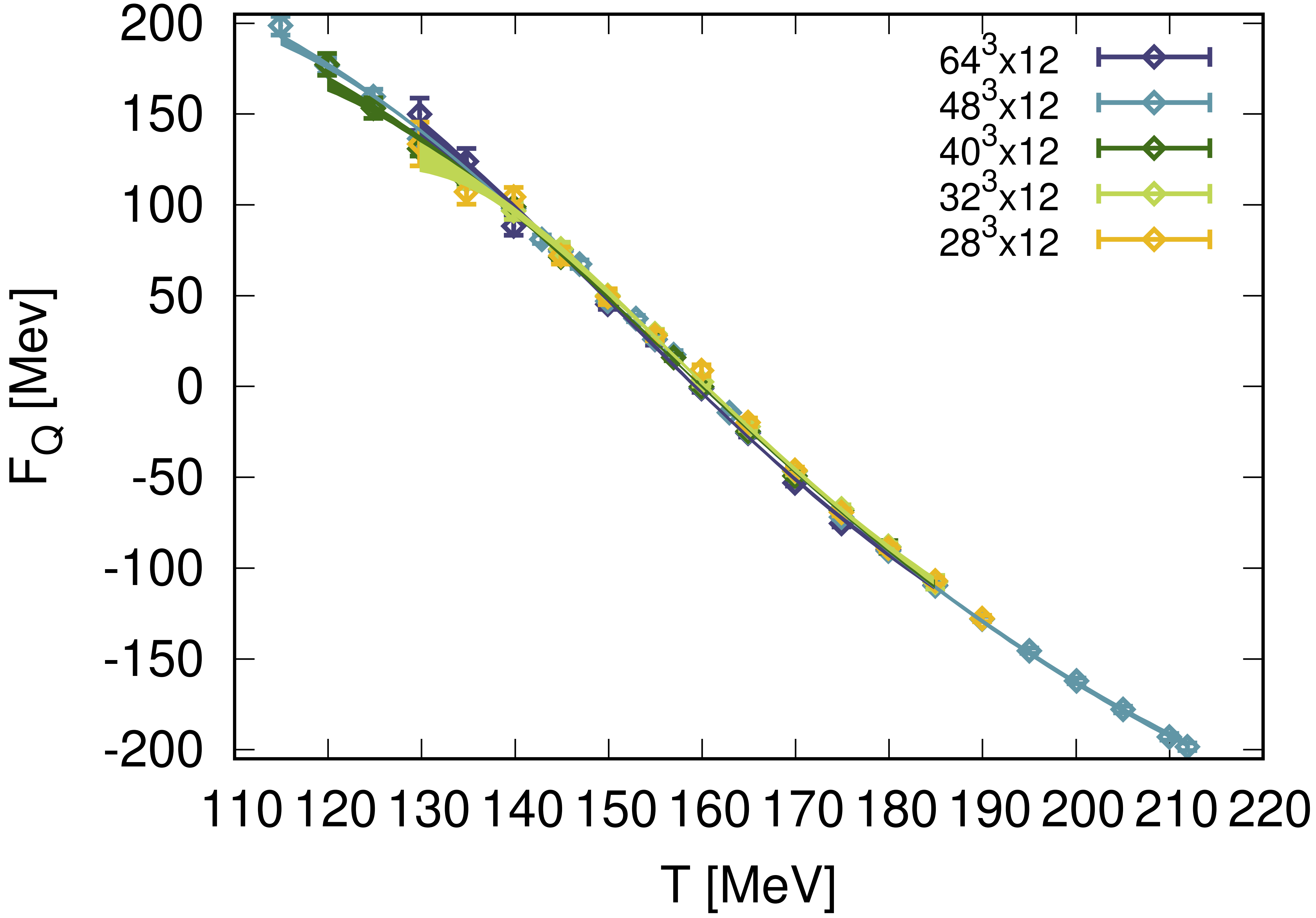


If S_Q is not very sensible to volume, that's exactly what we need!

Is $T_c^{(S_Q)}$ anyway similar to $T_c^{(\mathrm{chiral})}$? arXiv:2405.12320

$\mu_B = 0$





- $T_c^{(S_Q)}$ < $T_c^{(\chi^R_{\mathrm{disc}})}$ < $T_c^{(\chi^R)}$ **for** $LT \geq 3$

- **small** volume effects!

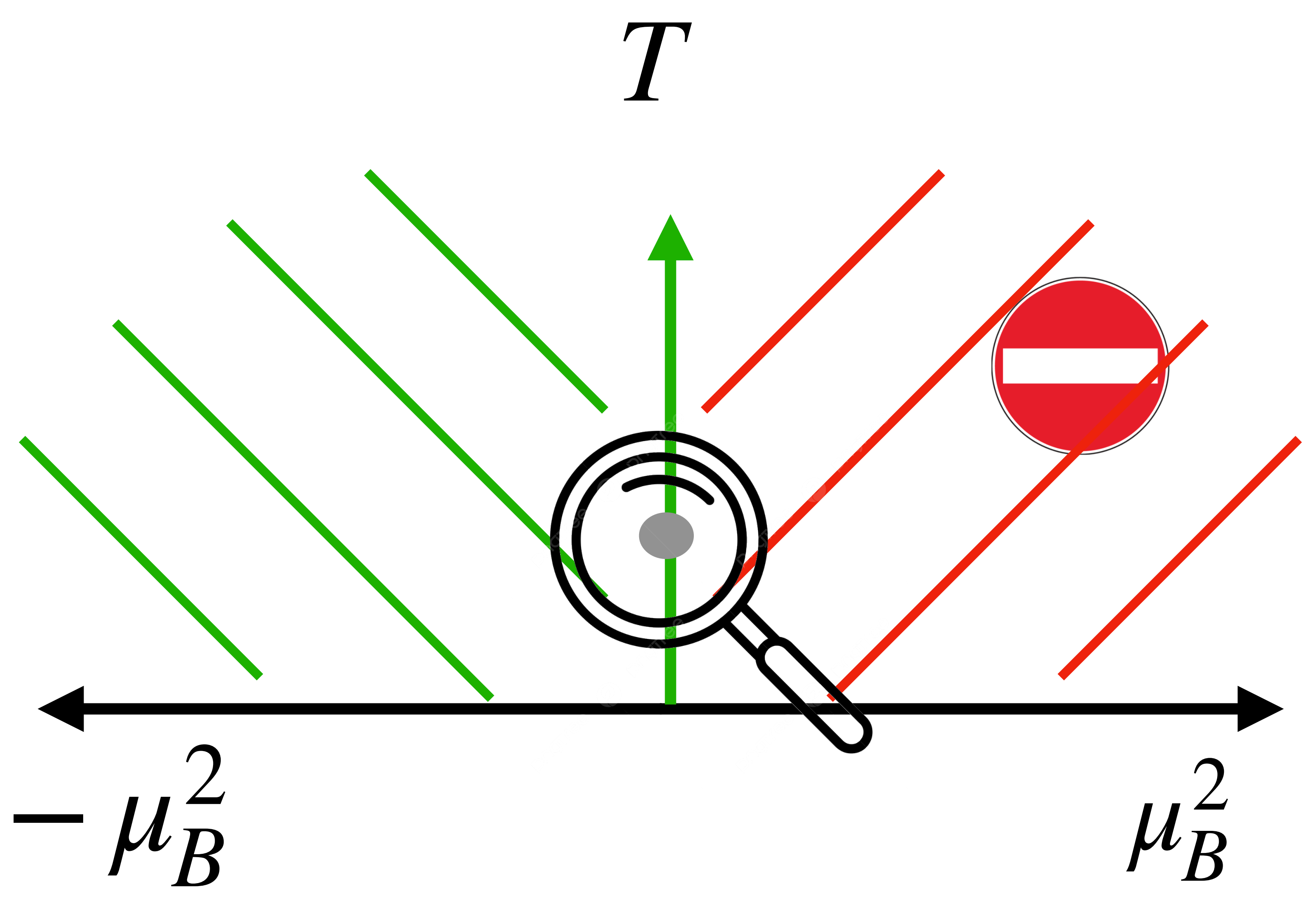
Sketch of the method in 2410.06216

- Goal: QCD transition line from the peak position of S_Q
- We use Taylor methods to circumvent the sign problem
- What we compute: the derivatives $Q^{(n)} = \partial^n Q / \partial \mu_B^n$, with $Q = |<P>|^2$, with $n = 2,..,8$

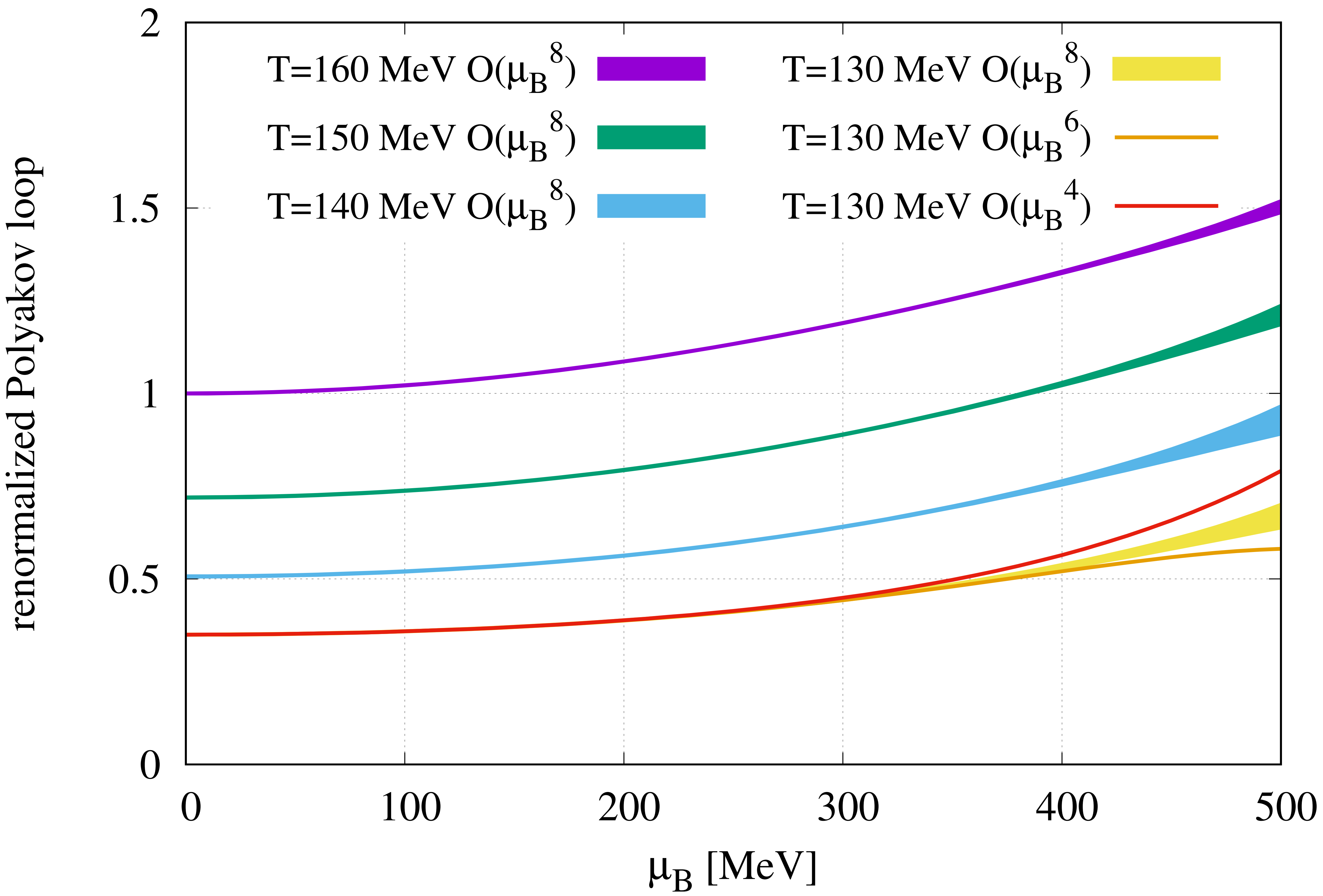
(previous ref. D'Elia, arXiv 1907.09461: up to n=2)

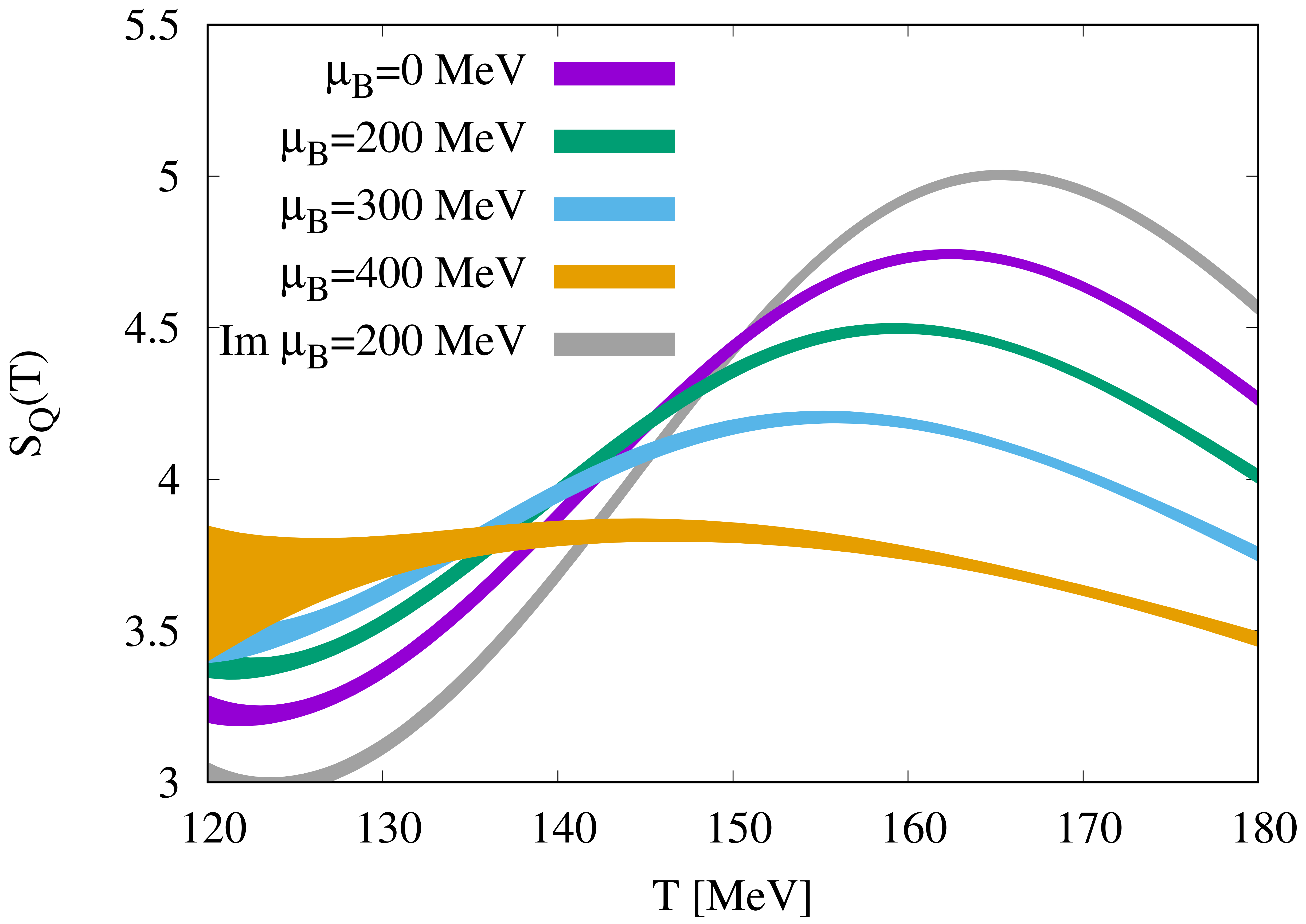
- The steps in a nutshell:

1. $Q^{(n)} \rightarrow F_Q^{(n)}$
2. $F_Q^{(n)} \rightarrow F_Q(\mu_B, T)$
3. $F_Q(\mu_B, T) \rightarrow S_Q(\mu_B, T)$



Results in 2410.06216





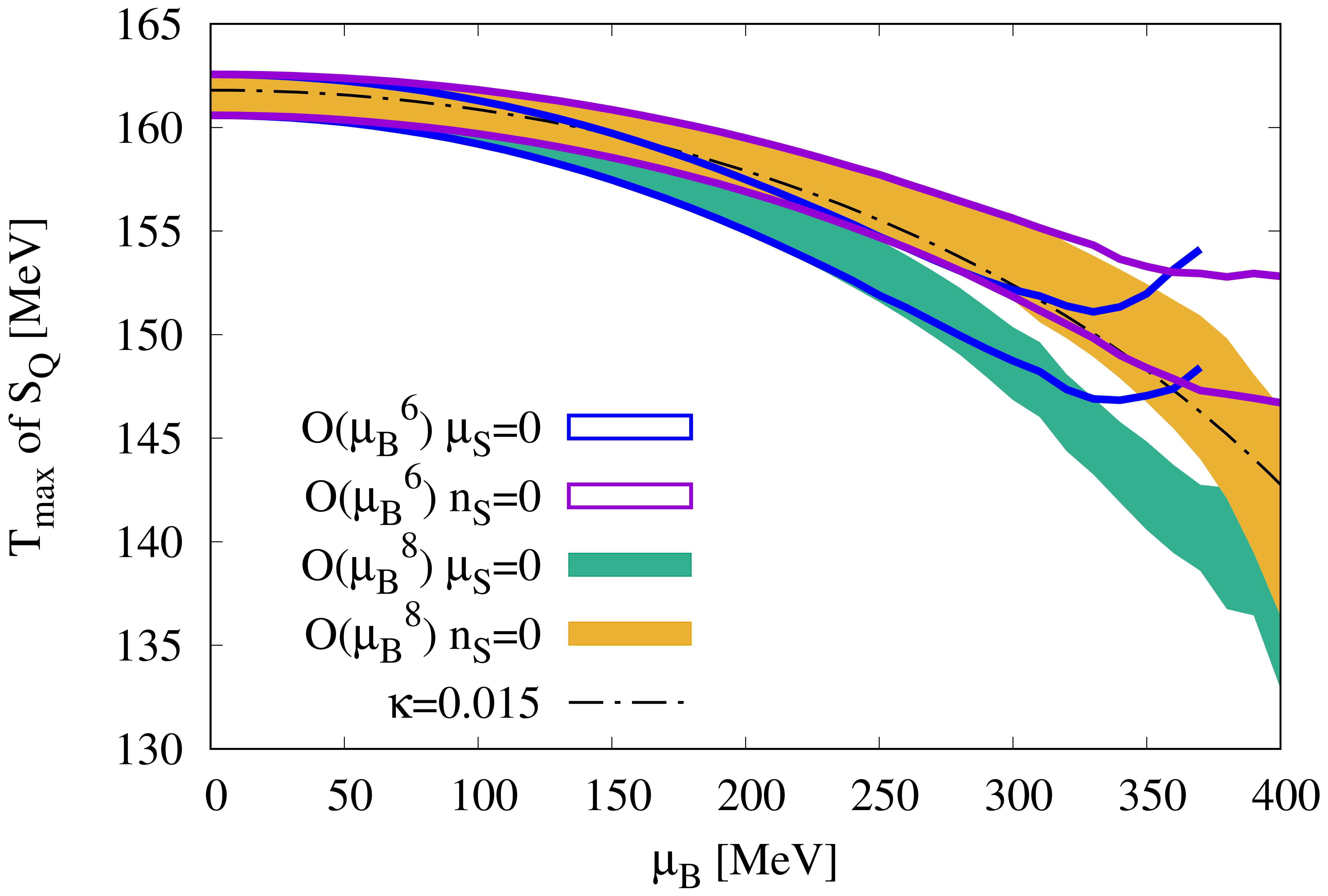
until 400 MeV:

- we can extract a peak of S_Q (after: it is too broad!)
- Taylor orders converge

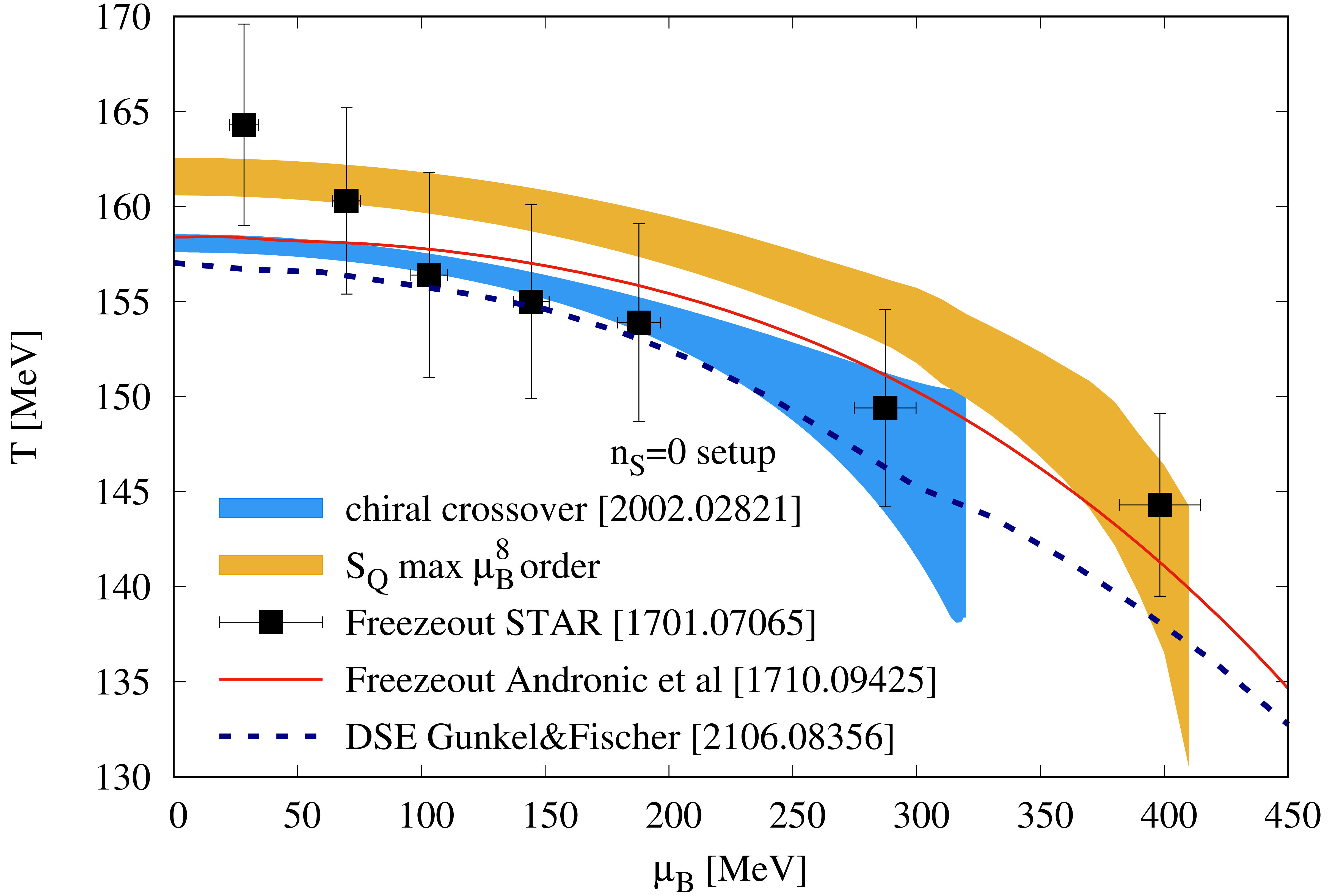
Phase diagrams to different orders in Taylor expansion

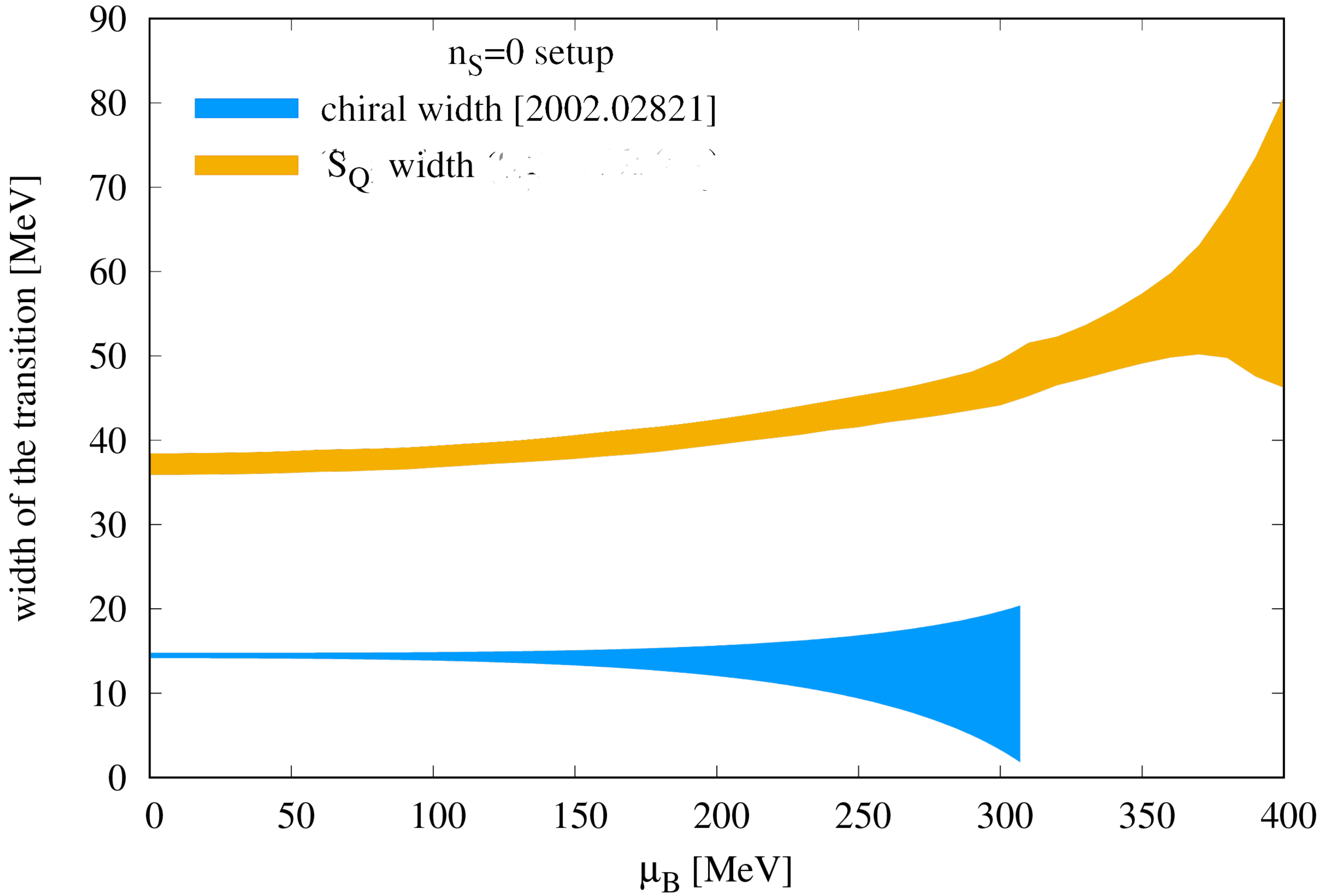
Until when do we trust our Taylor expansion?

- 8th order negligible up to $T \leq 300$ MeV for $n_S = 0$
- 1 sigma errorbars of 8th and 6th order touch at $T \sim 400$ MeV for $n_S = 0$



Some conclusions from 2410.06216





- deconfinement width increases in μ_B
- no sign of CEP up to these μ_B values

What next?

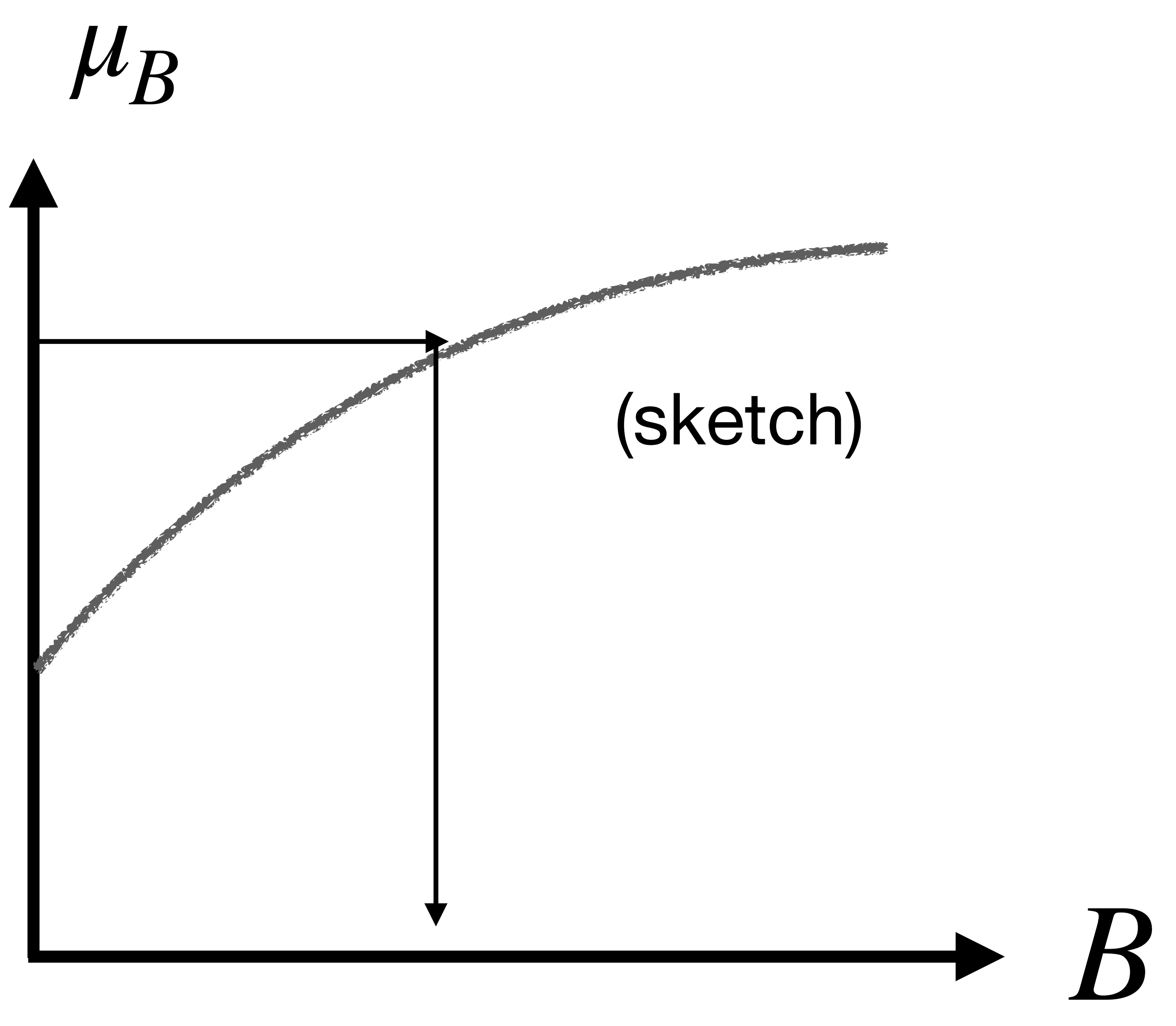
- Go on with Taylor up to order…? Which order?

- The truncation error in μ_B is uncontrolled. We can't really know if at $\mu_B = 400$ MeV we should stop at 8th order, or at 10th, or 12th: it depends only on the available statistics

  - In a canonical formulation that would be controlled

  - Baryon number B is fixed, μ_B is computed

  - Several attempts in the past by various collaborations: arXiv:0507020, 0602024, 0906.1088,…

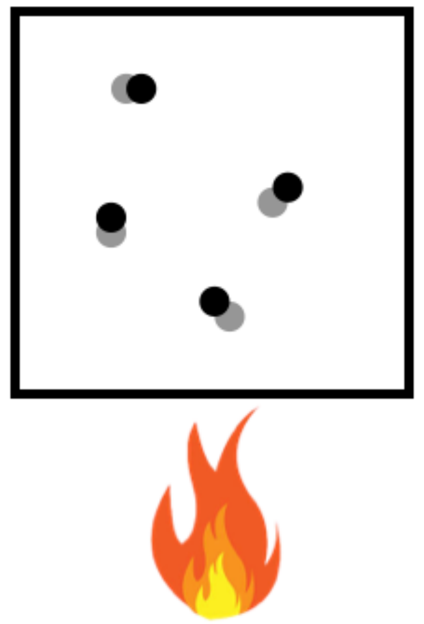


Canonical approach

- In a canonical approach we get rid of the "critical" variable of the sign problem, μ_B
- We change $(T, V, \mu_B) \rightarrow (T, V, N)$
- We do not need to extrapolate in μ_B anymore. We have **results at fixed N**
- For $V \rightarrow \infty$ we obtain the same results in the Grand Canonical and in the Canonical ensemble

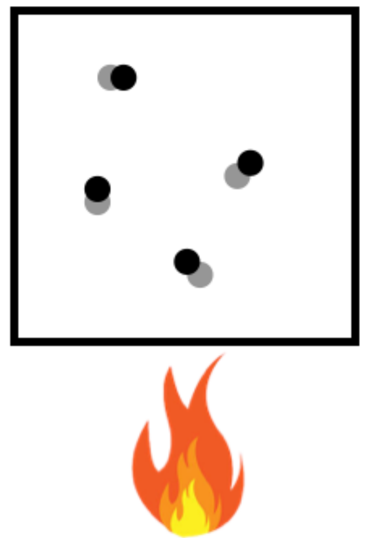
- The steps in a nutshell:

1. $Z_{GC}(T, V_0, \mu_B) \rightarrow Z_C(T, V, N)$
2. $\partial Z_C(T, V, N)/\partial N \rightarrow \mu_B$
3. $\partial Z_C(T, V, N)/\partial V \rightarrow p$



Canonical and Grand Canonical ensemble

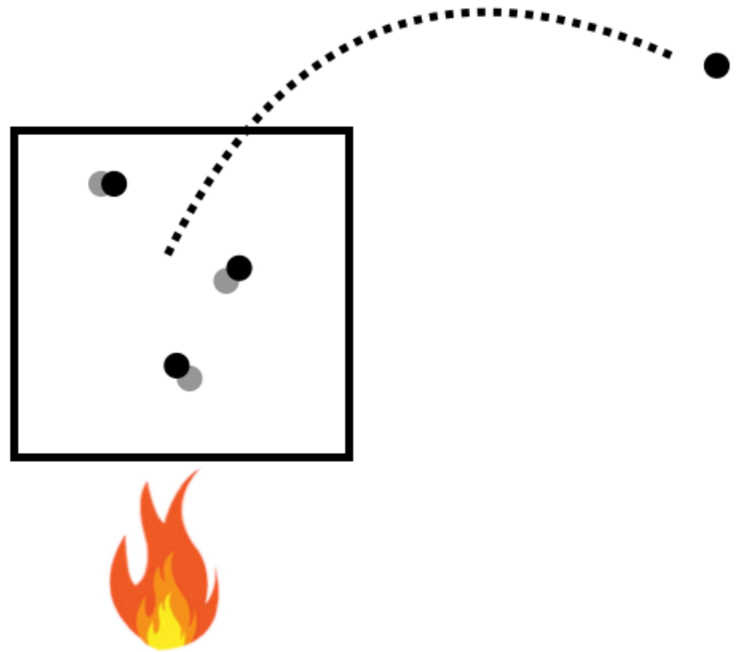
- Canonical
- $(T, V, {\color{red}N})$



- $F(T,V,N) = -\frac{1}{(LT)^3}\log Z_C(T,V,N)$

  CE potential

- Grand Canonical
- $(T, V, {\color{red}\mu_B})$



- $\Omega(T,V,\mu_B) = \frac{V}{V_0}\log Z_{GC}(T,V_0,\mu_B)$

  GCE potential

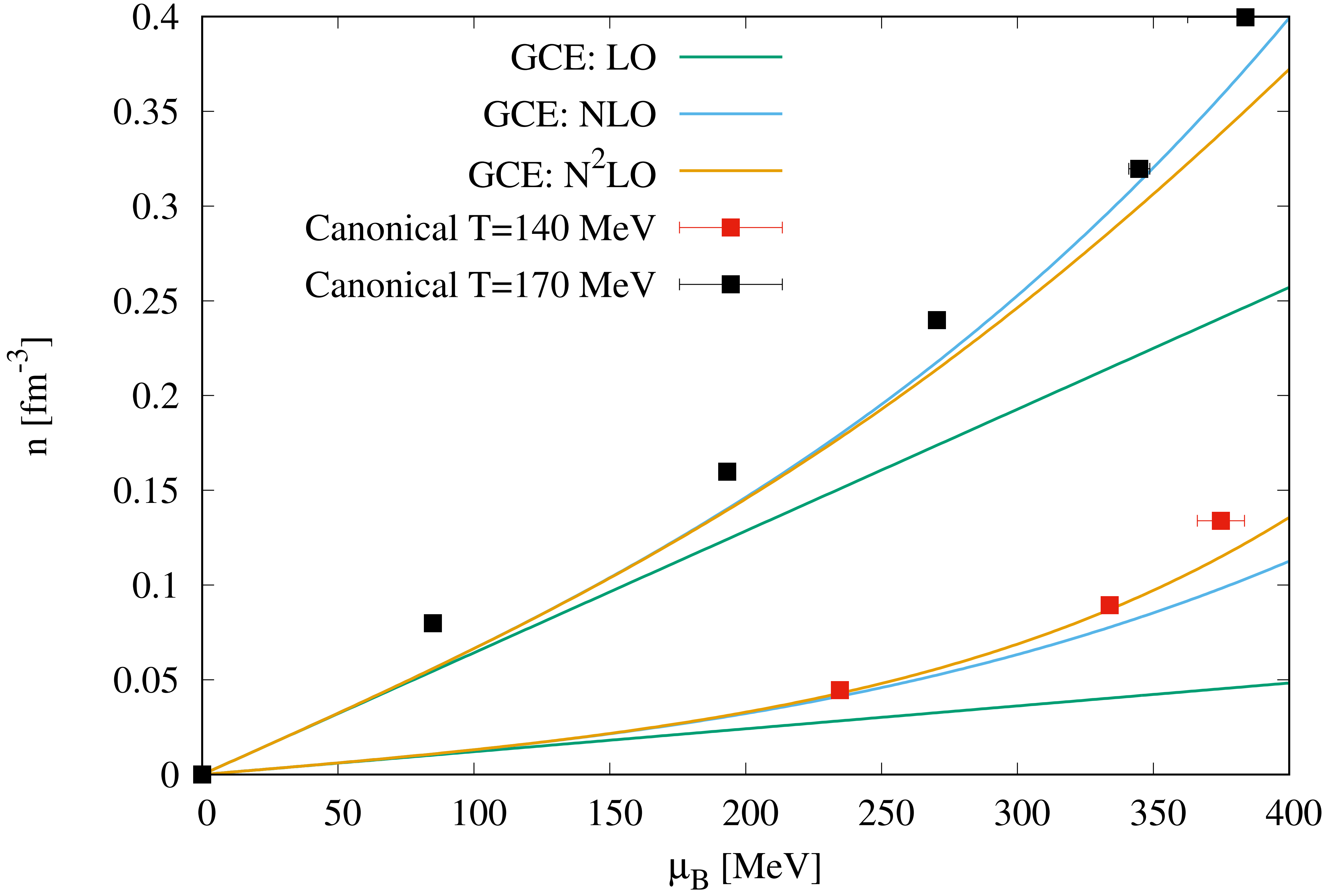
Fourier transform

$$\longleftarrow$$

$${\color{red}Z_C(T,V,N)} = \frac{1}{2\pi}\int_0^{2\pi} {\color{red}Z_{GC}}(T, V_0, \underbrace{\mu_B}_{i\phi_B T}) \cos(N\phi_B)\, d\phi_B =$$

$$= \frac{1}{2\pi}\int_0^{2\pi} \exp\left[{\color{red}\frac{V}{V_0}}\log Z_{GC}(T,V_0,\mu_B)\right]\cos(N\phi_B)\, d\phi_B$$

Results in GCE and CE



nuclear saturation density at T=0:

0.15 $\pm$ 0.01 nucleons/fm^3

(Horowitz et al.) [2007.07117]

- $T = 140$ MeV: corresponds to V $\sim$ 22 fm^3
- $T = 170$ MeV: corresponds to V $\sim$ 13 fm^3

GCE

$$N = \left(\frac{\partial \Omega(T, V, \mu)}{\partial \mu} \right)_{T,V}$$

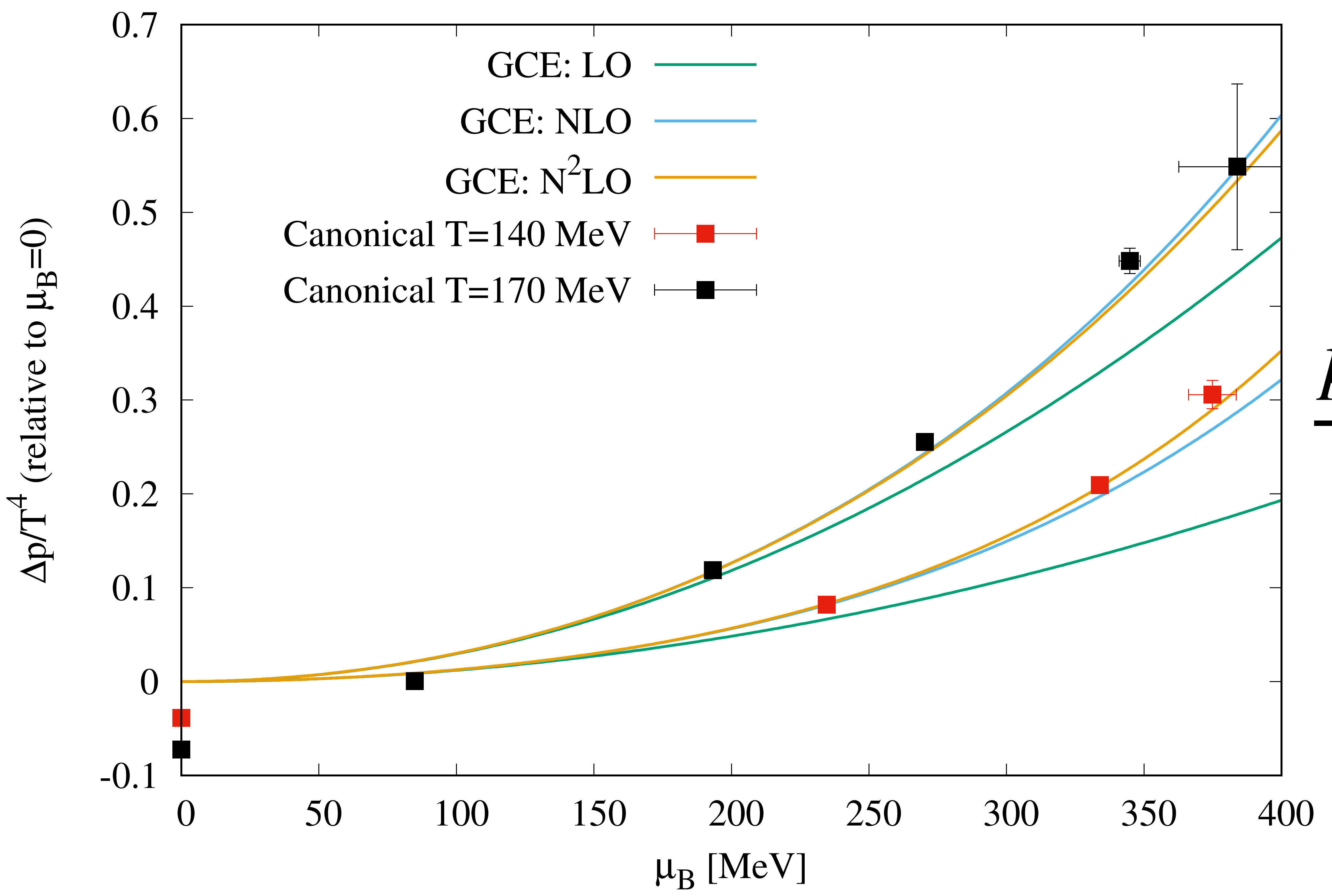
It comes from a **Taylor expansion in $\mu = 0$**

CE

$$\mu = F(T, V, N) - F(T, V, N-1)$$

It comes from a **Fourier transformation**

of the simulated partition function



$$Z_C(T,V,N) = \frac{1}{2\pi}\int_0^{2\pi} \exp\left[\frac{V}{V_0}\log Z_{GC}(T,V_0,\mu_B)\right]\cos(N\phi_B)\,d\phi_B$$

$$\frac{p_C(T,V,N)}{T^4} - \frac{p_{GC}(\mu=0)}{T^4} = \frac{1}{T^3}\frac{1}{Z_C(T,V,N)}\frac{\partial Z_C(T,V,N)}{\partial V} =$$

$$= \frac{1}{VT^3}\frac{\frac{1}{\pi}\int_0^{\pi} Z_{GC}(i\phi)\,\log\left(\frac{Z_{GC}(i\phi)}{Z_{GC}(0)}\right)\cos(N\phi)d\phi}{\frac{1}{\pi}\int_0^{\pi} Z_{GC}(i\phi)\cos(N\phi)d\phi}$$

$$\phi = i\mu/T$$

- $T = 140$ MeV: corresponds to V ~ 22 fm^3
- $T = 170$ MeV: corresponds to V ~ 13 fm^3

- stressing again the differences in the approaches, looking at the above plot:

GCE

at $\mu_B \sim 350$ MeV, T=140 MeV the Taylor expansion need at least NNLO ($O(\mu_B^6)$)

CE

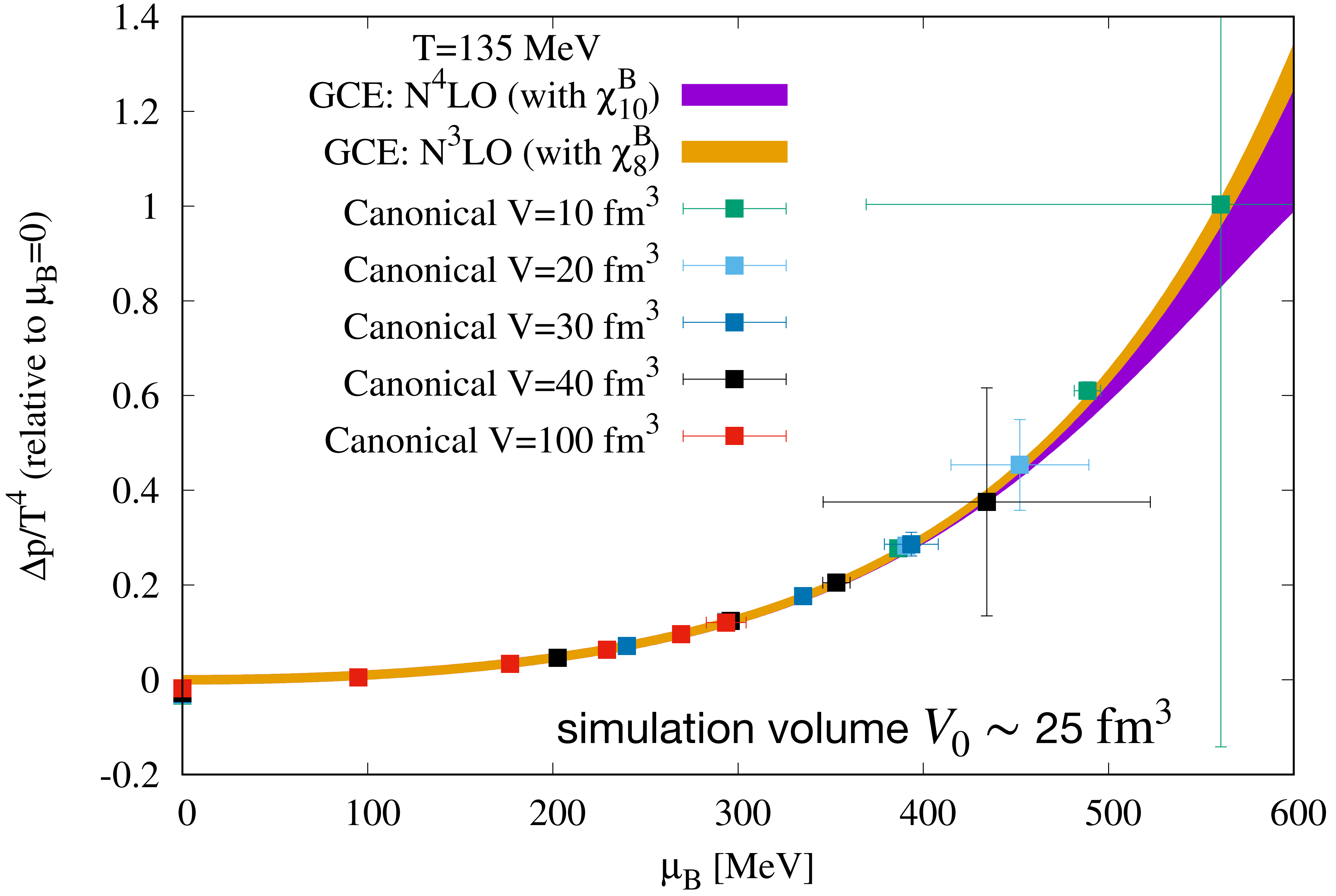
looking at same T, μ_B : it is a data point

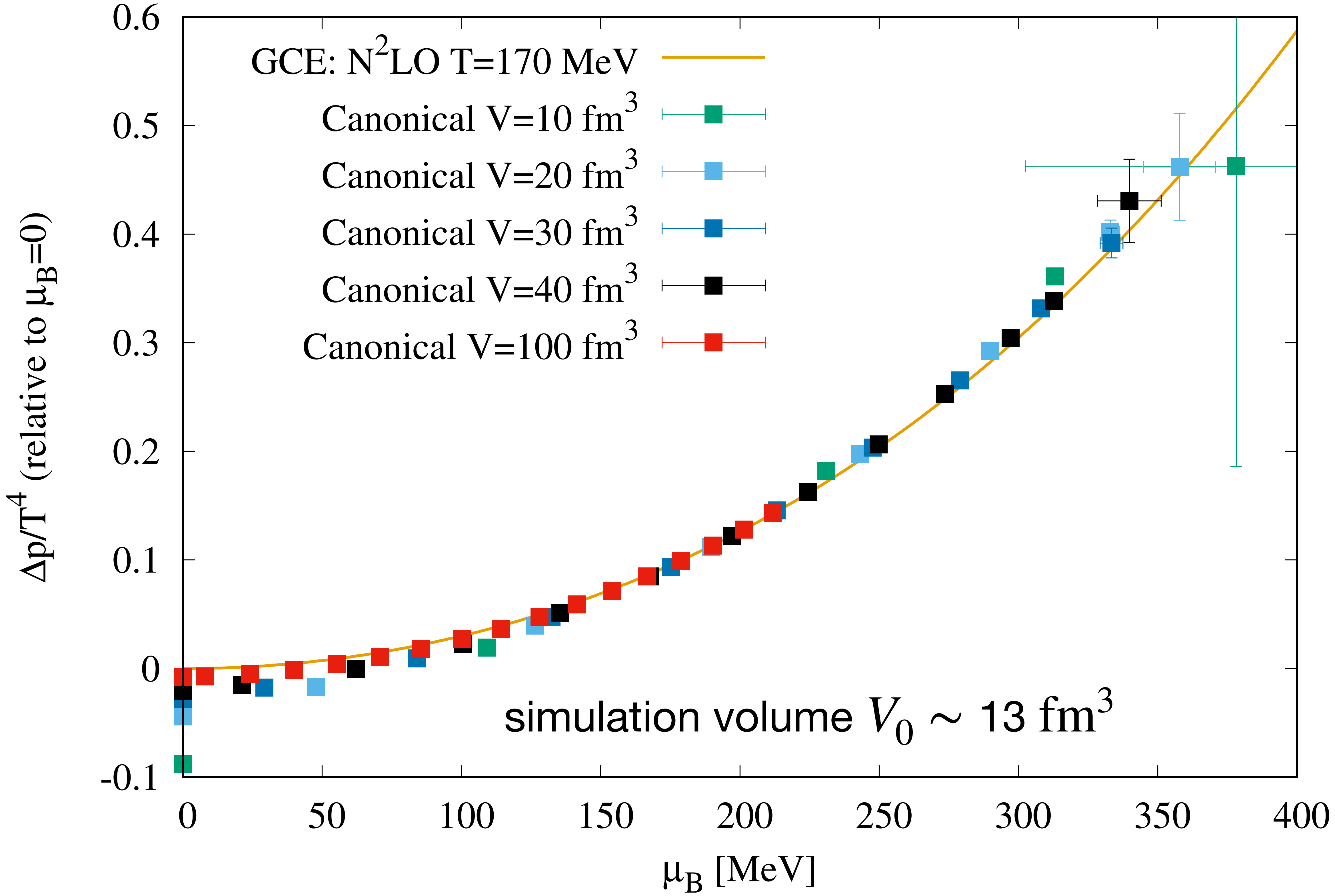
Different volume scaling in GCE and CE

$$P_C \underset{V\to\infty}{=} P_{GC}$$

$$Z_C(T,V,N) = \frac{1}{2\pi}\int_0^{2\pi} \exp\left[\frac{V}{V_0}\log Z_{GC}(T,V_0,\mu_B)\right]\cos(N\phi_B)\,d\phi_B$$

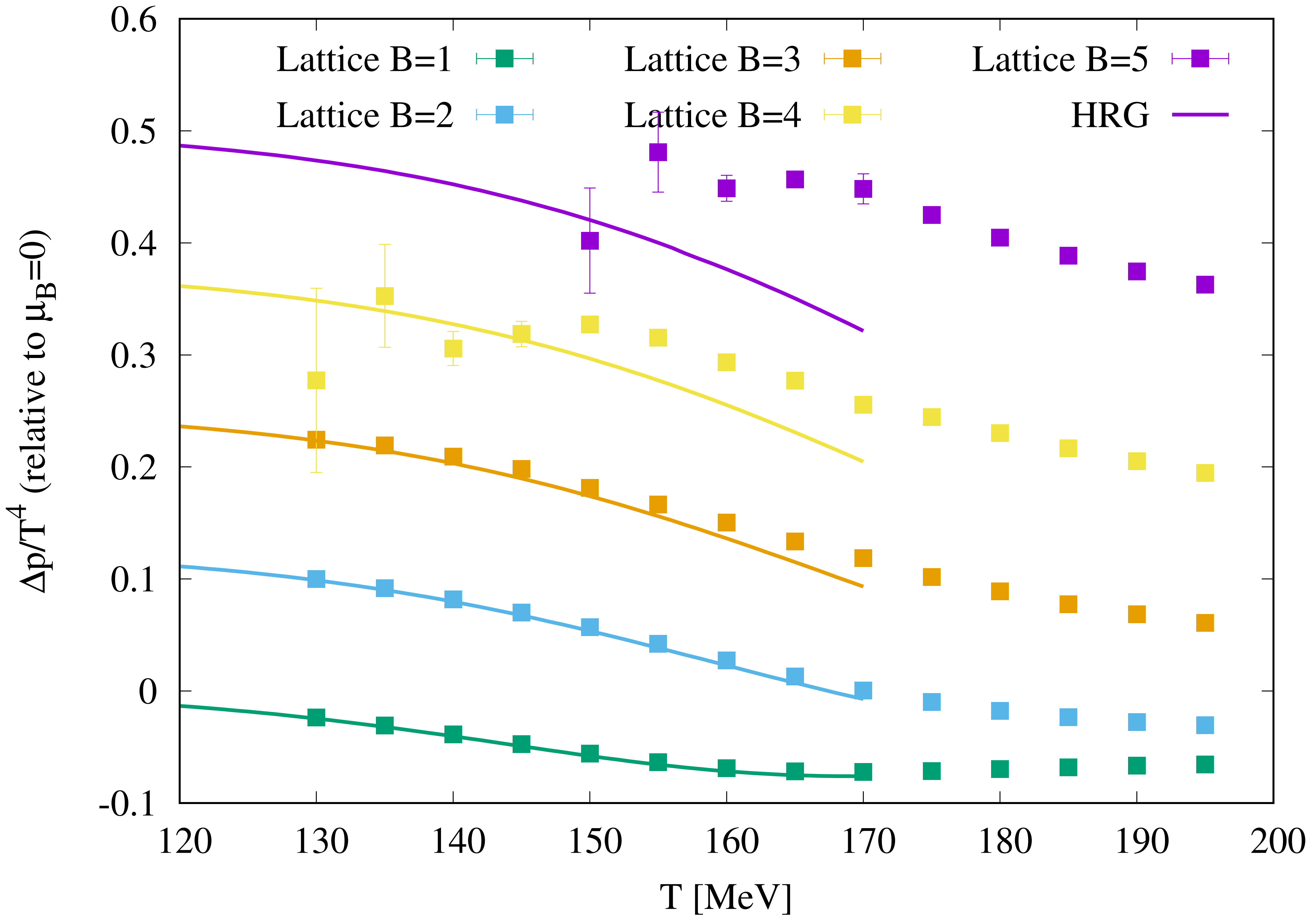
$$\frac{p_C(T,V,N)}{T^4} - \frac{p_{GC}(\mu=0)}{T^4} = \frac{1}{VT^3}\frac{\frac{1}{\pi}\int_0^\pi Z_{GC}(i\phi)^{V/V_0}\log\left(\frac{Z_{GC}(i\phi)}{Z_{GC}(0)}\right)\cos(N\phi)\,d\phi}{\frac{1}{\pi}\int_0^\pi Z_{GC}(i\phi)^{V/V_0}\cos(N\phi)\,d\phi}$$

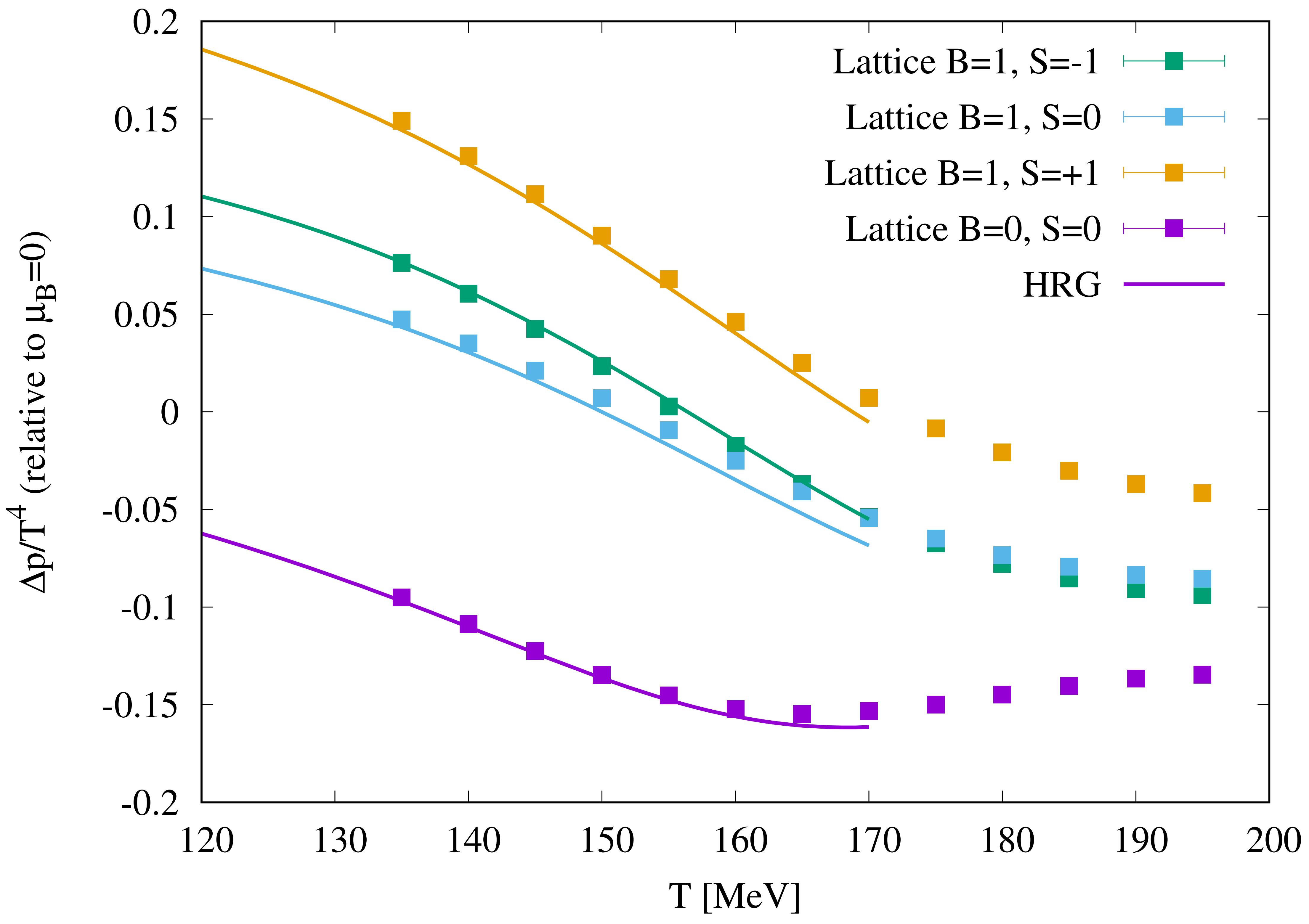




Some comparisons with HRG

- HRG: hadron resonance gas (non-interacting particles)





$$Z_{BS} = \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} Z_{GC}(T, V, \mu_B, \mu_S)\, e^{-iB\phi_B}\, e^{-iS\phi_S}\, d\phi_B\, d\phi_S$$

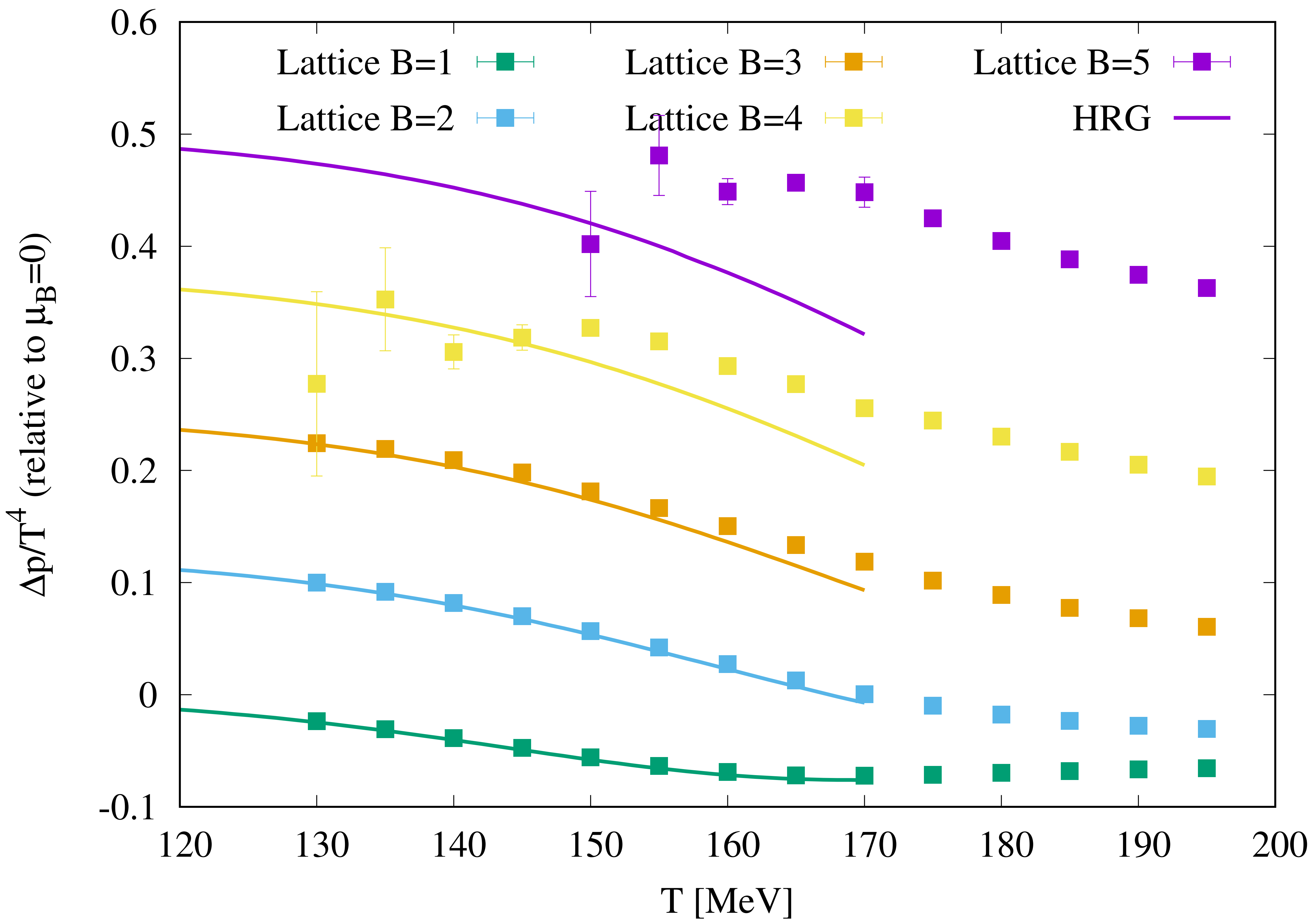
Conclusions

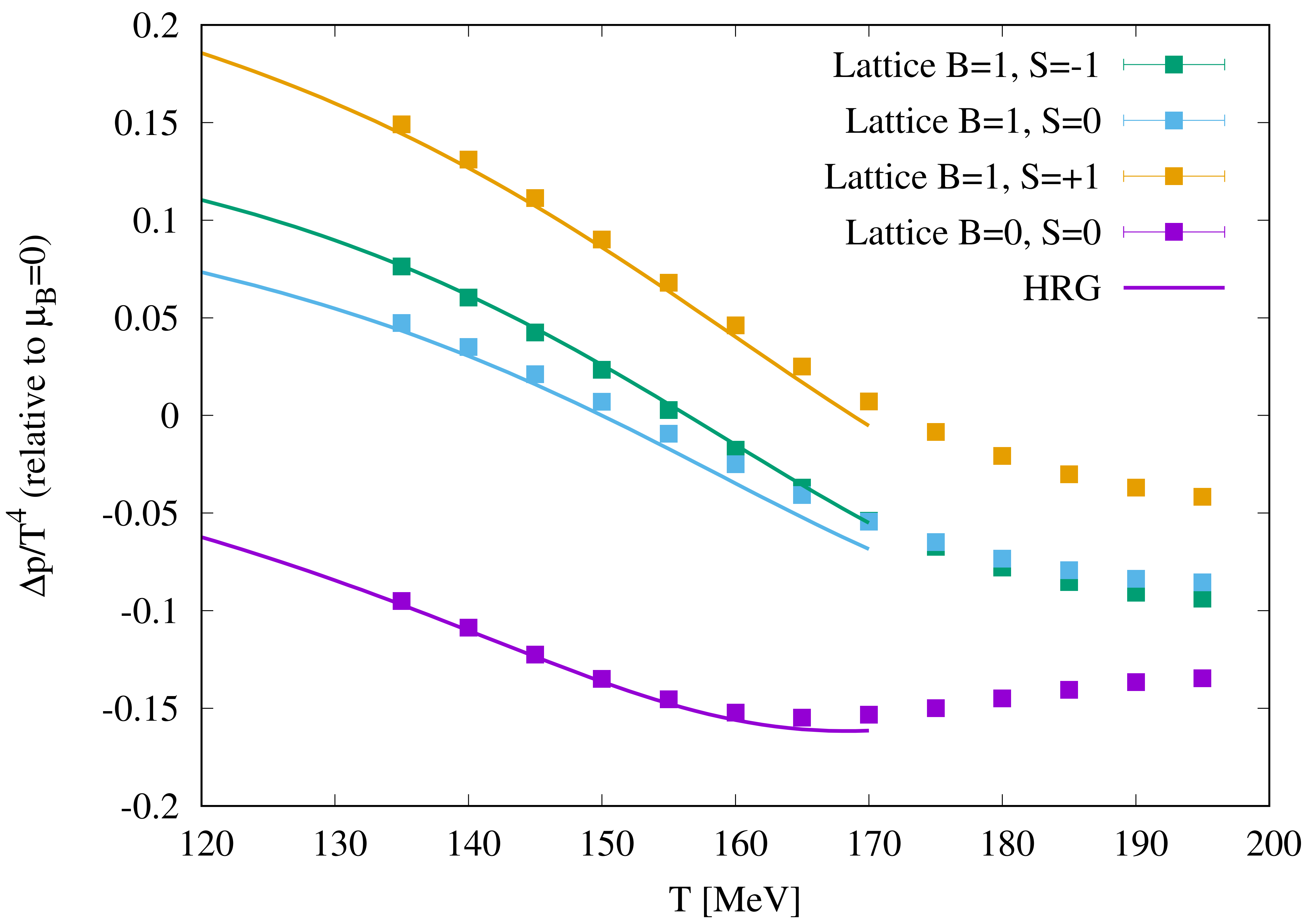
- We explore some techniques to overcome the sign problem in lattice QCD
- We focus mainly on Taylor expansions and a canonical approach
- Taylor methods
    - have an uncontrolled truncation in μ_B
    - need small lattice volumes to reach high μ_B
- In canonical lattice QCD
    - it is not numerically easy to compute high N coefficients
    - at large densities the error explodes (but they are already stat+syst!!)

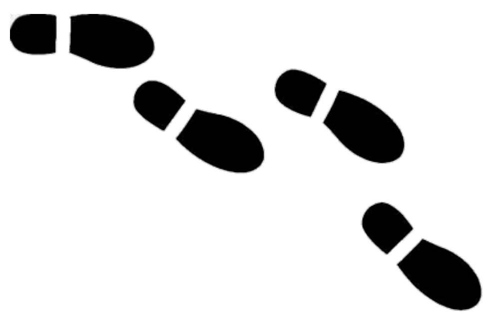
Backup slides

Some comparisons with HRG

- HRG: hadron resonance gas (non-interacting particles)





A small trip in 

Reweighting with staggered fermions

arXiv:2308.06105

- Staggered fermions: rooting

- We look at 2+1 flavours theory with $\mu_u = \mu_d = \mu_q, \mu_s = 0$

- $Z_{2+1}(T, \mu_q) = \int DU\, e^{-S_G[U]} \det M(U, m_q, \mu_q)^{\frac{1}{2}} \det M(U, m_s, 0)^{\frac{1}{4}}$

- $\dfrac{Z_{2+1}(\mu_q)}{Z_{2+1}(0)} = \left\langle \dfrac{\det M(U, m_q, \mu_q)^{\frac{1}{2}}}{\det M(U, m_q, 0)^{\frac{1}{2}}} \right\rangle_{\mu_B=0}$ can be computed with reduced matrix formalism

- the eigenvalues $\{\lambda_k\}$ of the reduced matrix do not depend on μ_q
- solve the rooting ambiguity: take the square root for each eigenvalue
- $$\frac{\det M(U, m_q, \mu_q)^{\frac{1}{2}}}{\det M(U, m_q, 0)^{\frac{1}{2}}} = e^{-3N_s^3\mu_q/T} \prod_{k=1}^{6N_s^3} \sqrt{\frac{\lambda_k[m, U] - e^{\mu_q/T}}{\lambda_k[m, U] - 1}}$$
- it could have an overlap problem (long tails in the weights) but we crosscheck with other 2 reweighting methods
  - phase reweighting $\frac{Z_{2+1}}{Z_{2+1}^{PQ}} = \left\langle \frac{\det M(U, m_q, \mu_q)^{\frac{1}{2}}}{|\det M(U, m_q, \mu_q)^{\frac{1}{2}}|} \right\rangle_{PQ}$
  - sign reweighting $\frac{Z_{2+1}}{Z_{2+1}^{SQ}} = \left\langle \frac{\mathrm{Re}\det \mathrm{M(U, m_q, \mu_q)}^{\frac{1}{2}}}{|\mathrm{Re}\det \mathrm{M(U, m_q, \mu_q)}^{\frac{1}{2}}|} \right\rangle_{SQ}$

- Now, let's look at the light quark density (e.g. for equation of state studies)

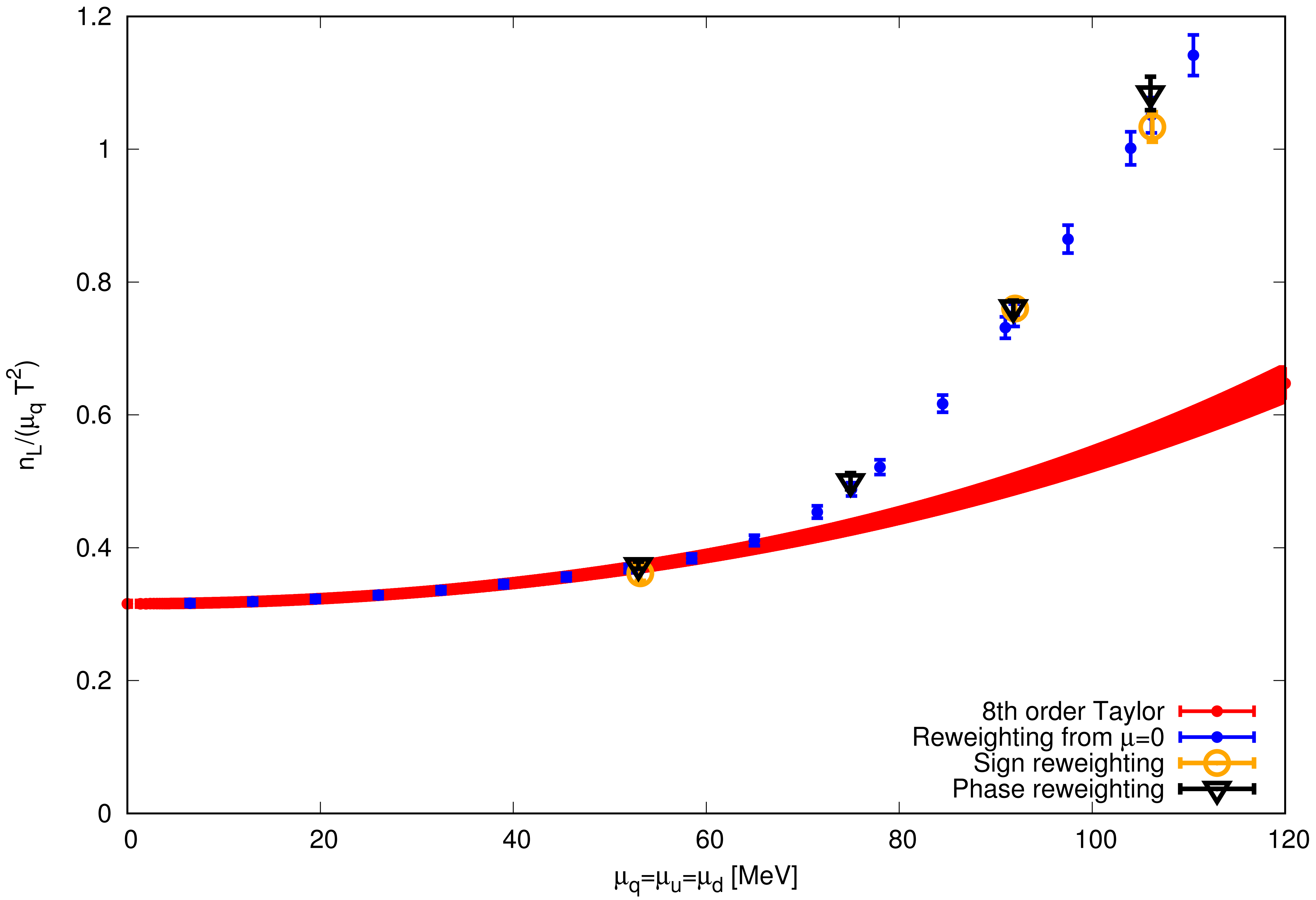
- Plot: $\hat{n}_L/\hat{\mu}_q$, $16^3 \times 8$ lattice, $m_\pi = 135$ MeV

A steep rise at $\mu_q \sim \dfrac{m_\pi}{2}$!! **Why?**

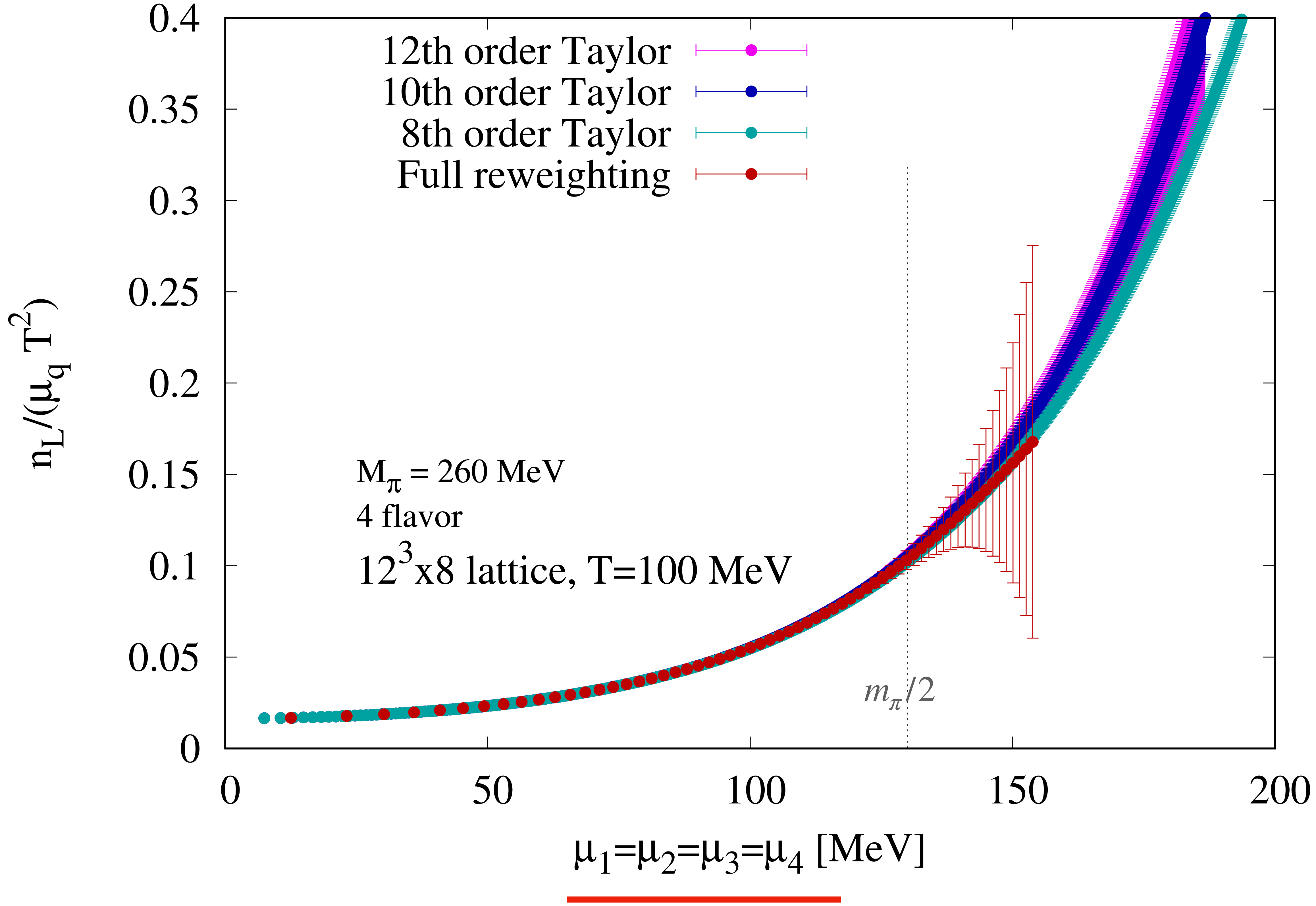
- Is it an overlap problem?

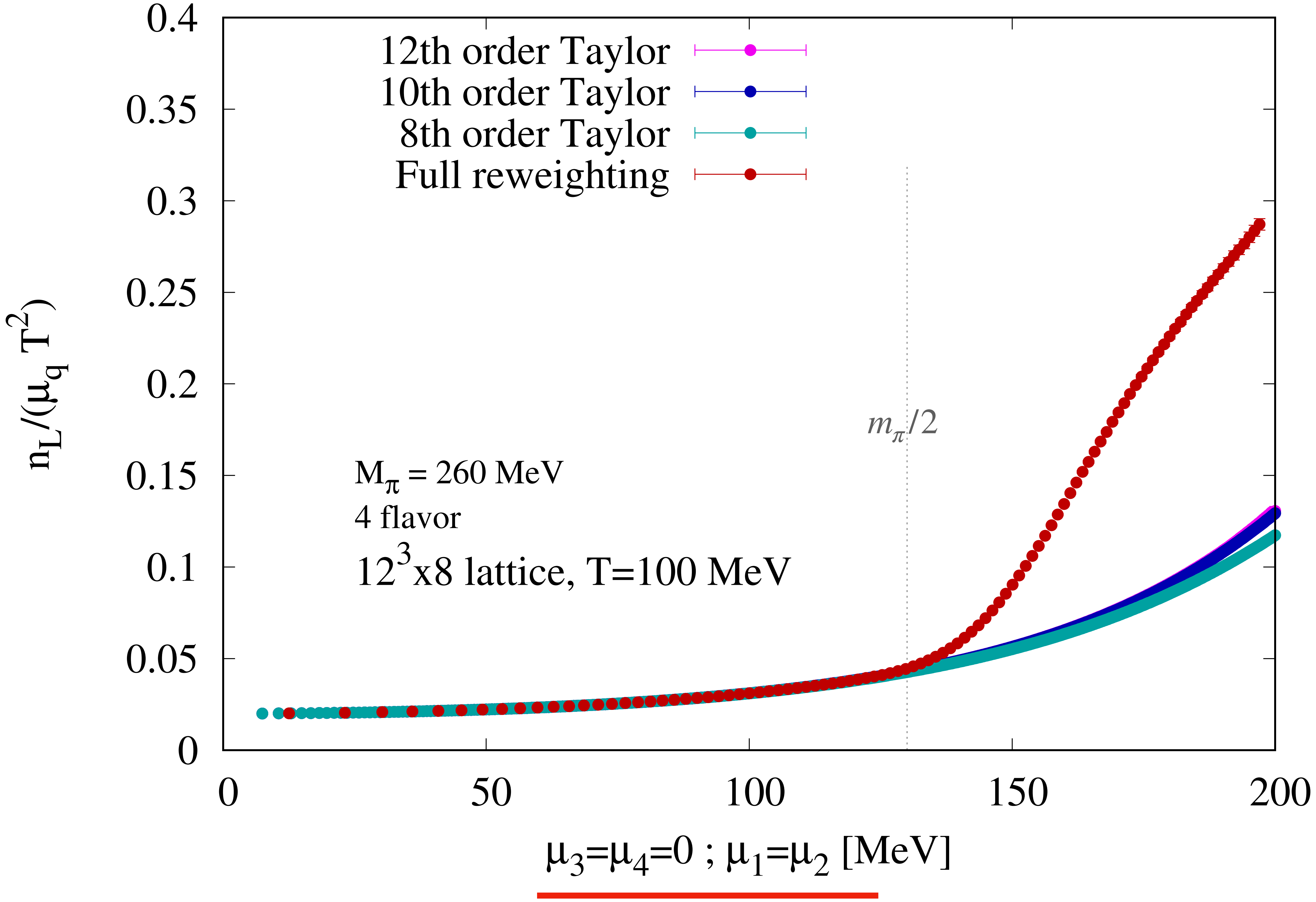
- No, the 3 reweighting techniques do the same

- It also a discretisation effect



T=130 MeV. 2 stout smearing,





- → no rooting
- reweighting and Taylor (up to 12th order) agree

- rise at $m_\pi/2$ for the reweighted case

- the culprit is actually the rooting!

- it seems that at the moment our favourite technique is Taylor method then
- But also there we need to be careful

Cancellations problem in Taylor method

- Goal: derivatives of an observable O w.r.t. μ_i (i: flavour) $\partial_i O$
- Given $A_i = \dfrac{\partial \log(\det M)^{\frac{1}{4}}}{\partial \mu_i} = \dfrac{1}{4}\mathrm{Tr}(\mathrm{M_i^{-1}M_i'}) \rightarrow \ <A_i> = \ \partial_i \log Z$
- for O we have the generic chain rule formula
- $\partial_i < O > = \ < O A_i > + < \partial_i O > - < O > < A_i >$

- the bigger is the order n of derivative, the more terms we have…
- and the bigger is the cancellation between them!

- Below: $\partial^n \log Z / \partial\mu^n$ (ignoring the flavour)

$n = 1$

$$< A >$$

$n = 2$

$$< A^2 > + < A' > - < A >^2$$

$n = 3$

$$< A^3 > +2 < A >^3 -3 < A > < A^2 >$$
$$+ < A'' > +3 < AA' > -3 < A > < A' >$$

$n = 4$

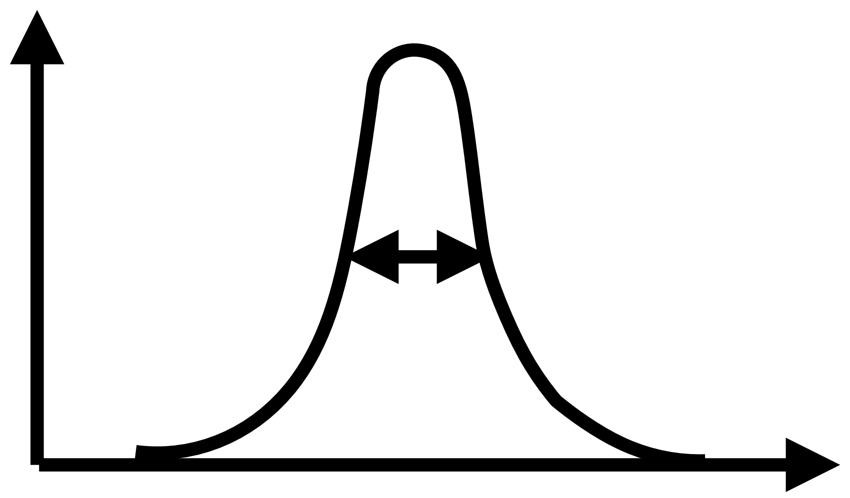
$$< A^4 > +4 < AA'' > + < A''' > -4 < A > < A^3 > -4 < A > < A'' >$$
$$+6 < A^2 A' > +3 < A'A' > -6 < A^2 > < A' > -3 < A' > < A' >$$
$$+12 < A > < A > < A' > -12 < A > < AA' >$$
$$+12 < A > < A > < A^2 > -3 < A^2 > < A^2 > -6 < A >^4$$

$$\cdots$$

- This cancellation actually scales with the volume → how?
- Derivatives of $\log Z$ are related to quark number susceptibilities

$$\chi_{ijk}^{uds}(T, \mu_u, \mu_d, \mu_s) = \frac{T}{V} \frac{\partial^{i+j+k} \log Z}{(\partial_u)^i (\partial_d)^j (\partial_s)^k}$$

- $\chi_1^u \sim < u > \sim n_u$
- $\chi_2^u \sim \frac{1}{V} < u^2 > - < u >^2$: a variance / V, we except $O(1)$

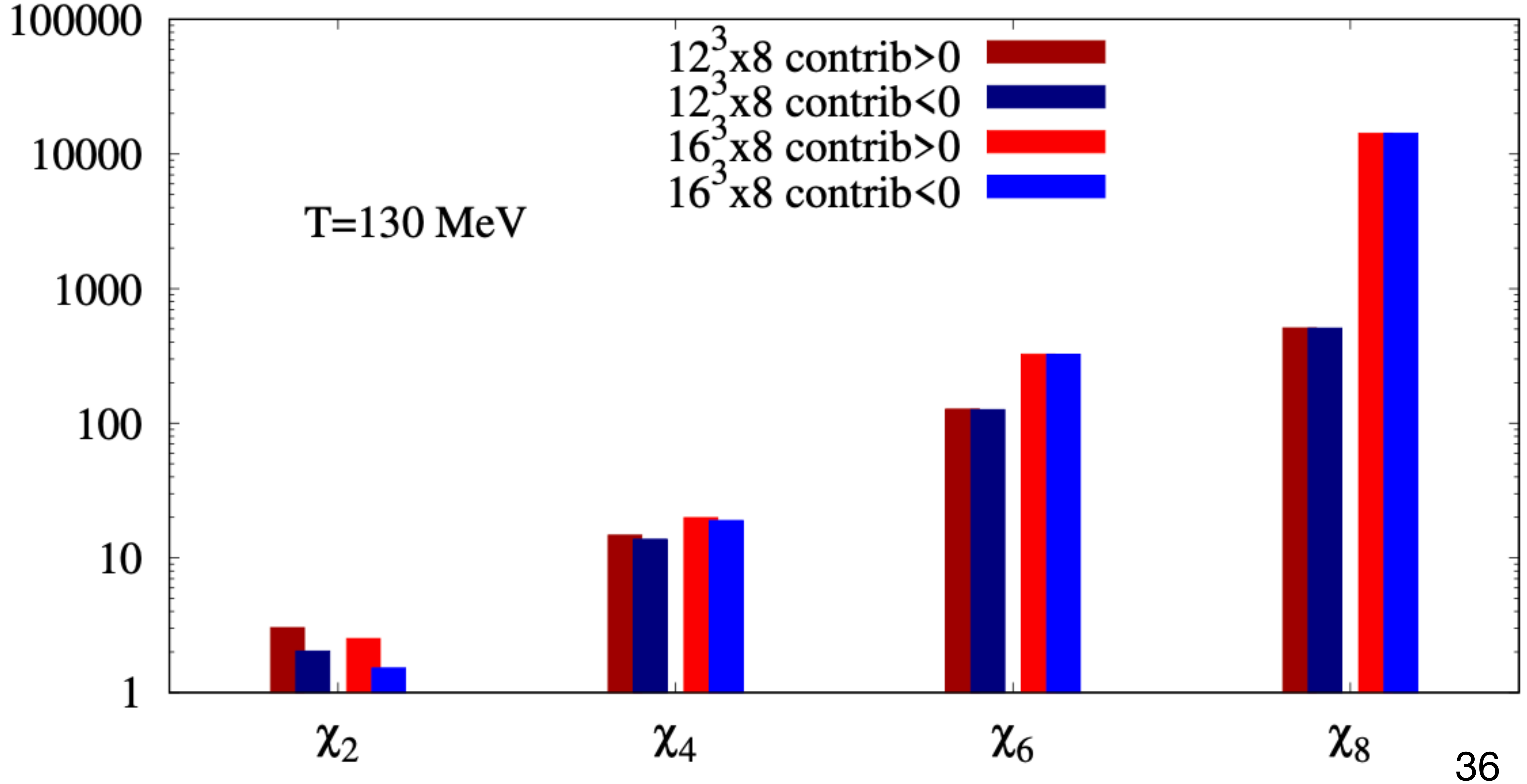


- χ_2^u contains terms like $\frac{1}{V}(< A^2 > - < A >^2) \to \; < A^2 > \sim V$

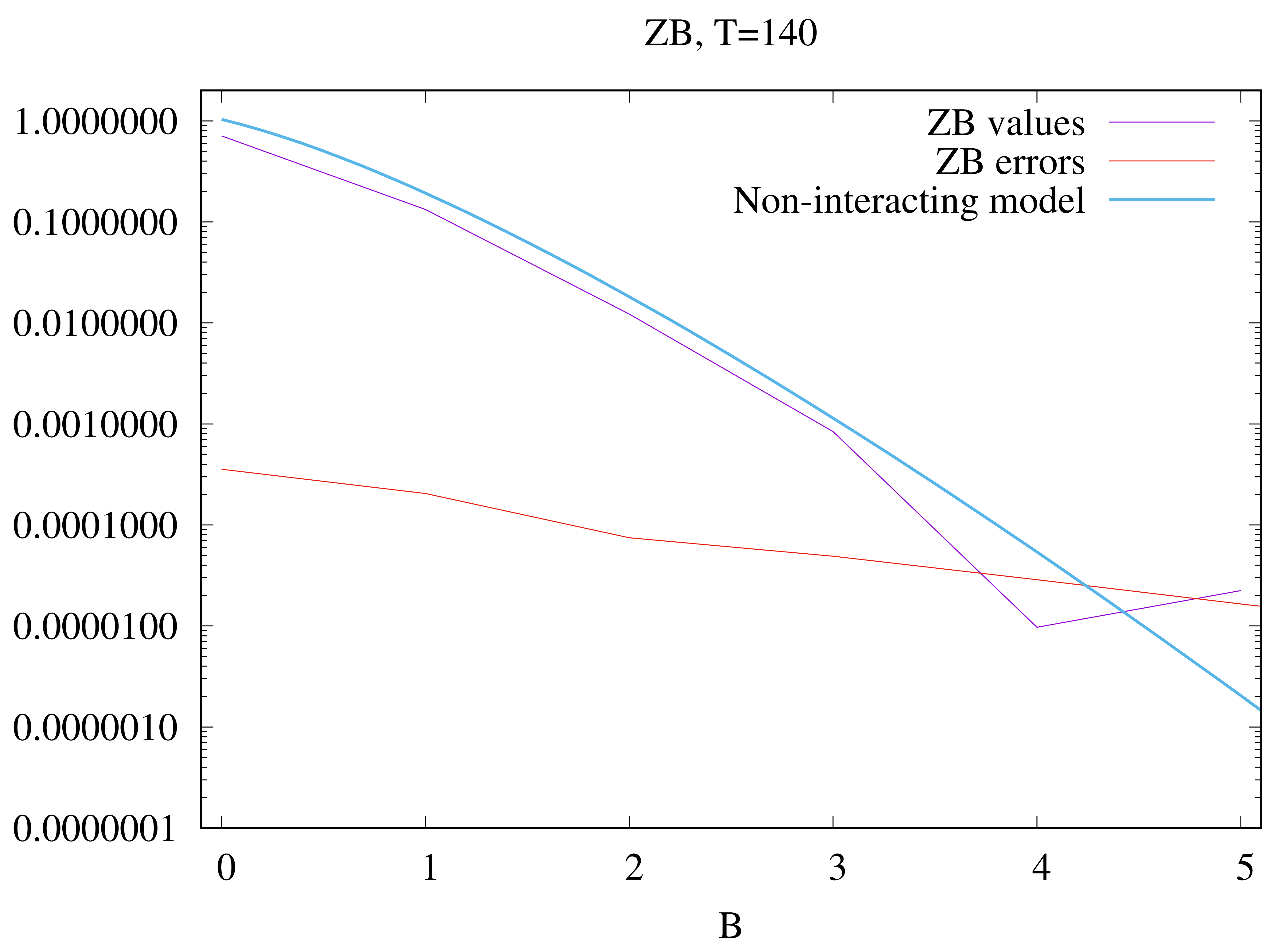
- Inside χ_4^u we have couples of terms like $\frac{1}{V}(\underbrace{<A^4>}_{O(V^2)} - 3\underbrace{<A^2>^2}_{O(V^2)}) \sim O(1)$ $\quad O(V^2) \leftarrow O(V^2)$
- the cancellation is $O(V)$
- Inside χ_6^u: $\frac{1}{V}(<A^6> - 15<A^2>^3) \sim O(1)$
- the cancellation is $O(V^2)$

- χ_{2n}: cancellation is $O(V^{n-1})$
- we need small volumes!!

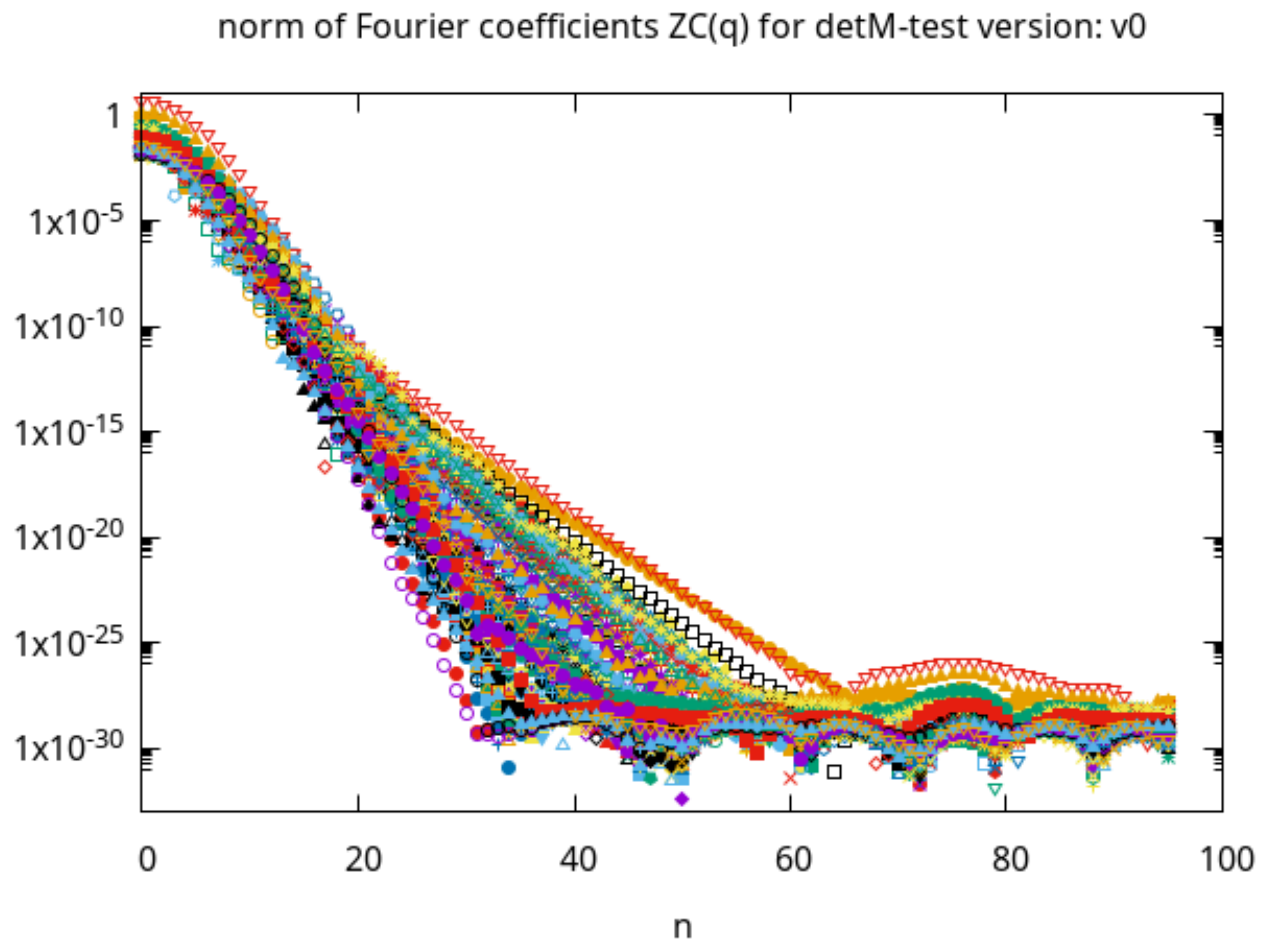
contributions normalised to sum

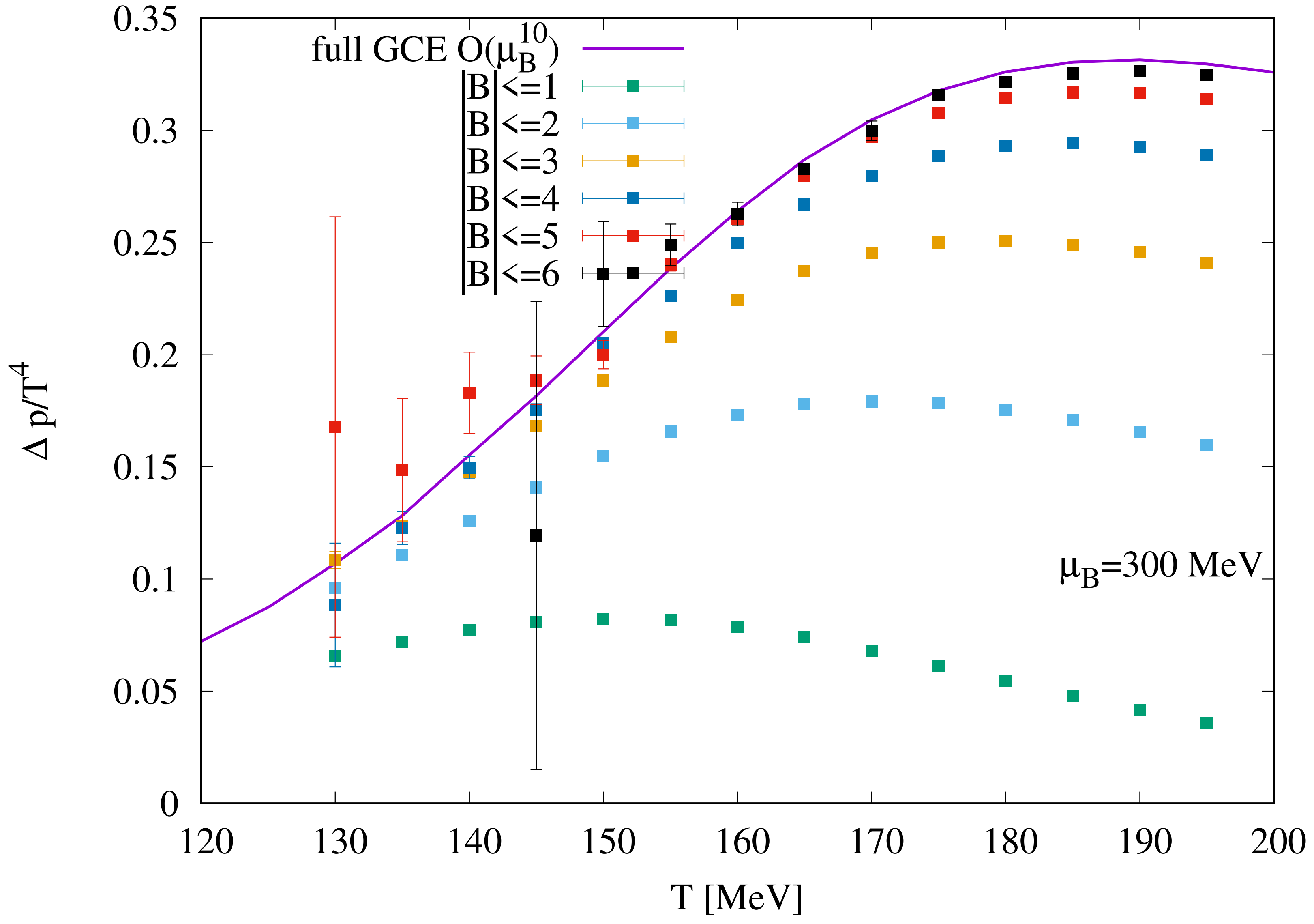


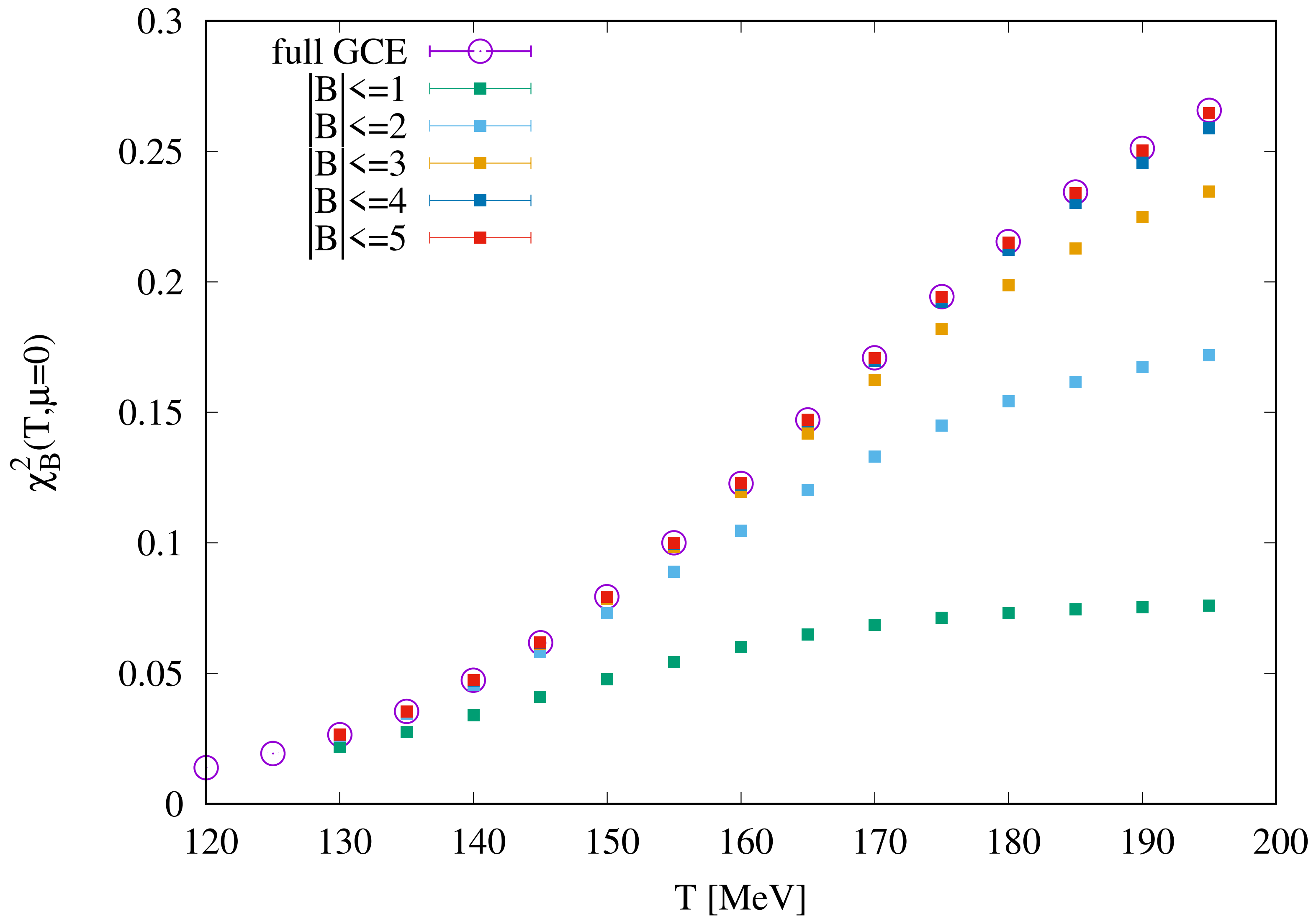
Technical difficulty of canonical approach

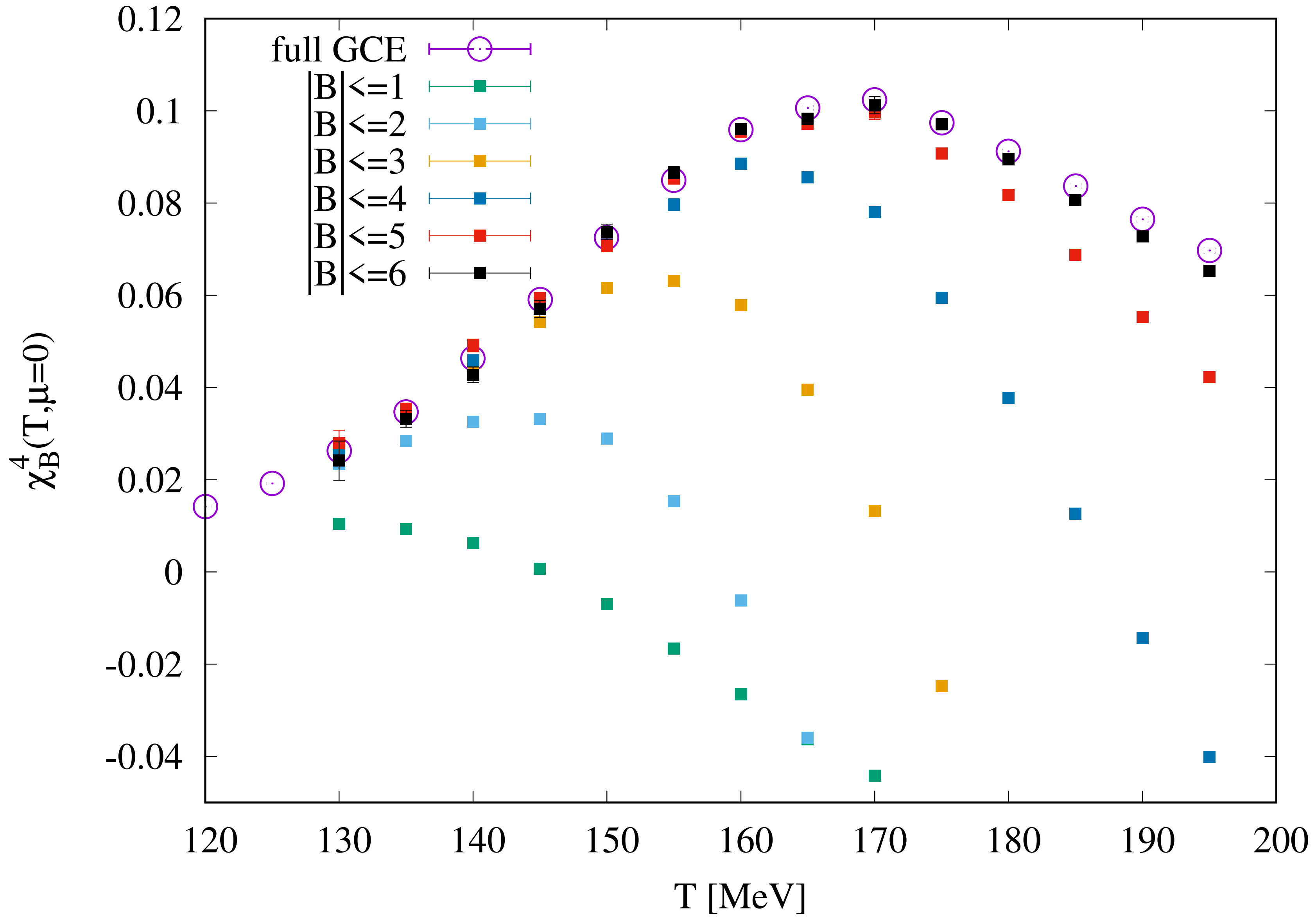


- We can compute only a few Fourier coefficients









- $$\chi_B^2 = \frac{\sum_{N_B} \left(N_B - \langle N_B \rangle\right)^2 Z_C(T,V,N_B) e^{N_B \mu_B / T}}{\sum_B Z_C(T,V,N_B) e^{N_B \mu_B / T}}$$