Conjecture about the QCD Phase Diagram

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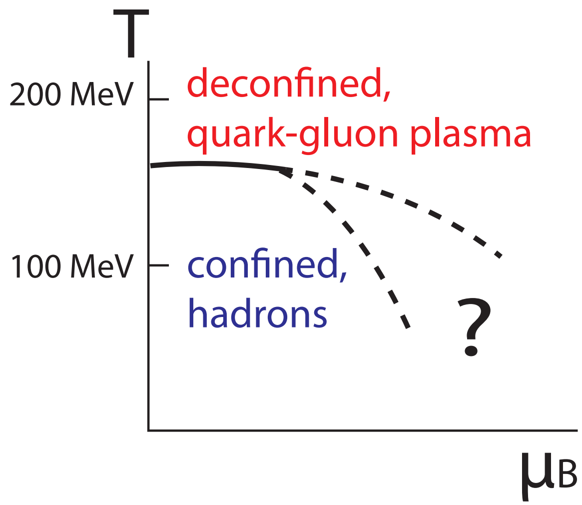
- **O(4) model as an effective theory for 2-flavor QCD: universality, dimensional reduction, topological charge $\sim$ baryon number**

- **Inclusion of chemical potential and quark mass in the Monte Carlo algorithm without any sign problem**

- **Phase diagram in the chiral limit, and with light quarks: where is the Critical Endpoint (CEP) ?**

Hypothetical QCD phase diagram:



$\mu_B = 0$:

- $N_f = 2$: $m_u = m_d = 0$: 2^{nd} order phase transition
  $N_f = 3$: $m_u = m_d = 0$, m_s physical: $T_{\mathrm{c}} \simeq 132$ MeV [Ding et al. '19]
  $2+1+1$ flavors: $T_{\mathrm{c}} \simeq 134$ MeV [Kotov et al. '21]

- $m_u = m_d > 0$ crossover
  m_s physical: pseudo-critical $T_{\mathrm{x}} \simeq 155$ MeV
  [Borsanyi et al. '10, Bhattacharya et al. '14 . . .]

Monte Carlo simulations on Euclidean space-time lattices

Sign problem at $\mu_B > 0$ still unsolved: $p[U] \propto \exp(-S[U]) \notin \mathbb{R}_+$
Conjectures on the phase diagram based on effective theories.

Here: **O(4) non-linear σ-model**

Assumed to be in universality class of $N_f = 2$ chiral QCD.

[Gasser/Leutwyler, Pisarski/Wilczek '83]

$$S[\vec{e}] = \int d^4x \left[\frac{F_\pi^2}{2} \partial_\mu \vec{e}(x) \cdot \partial_\mu \vec{e}(x) - \vec{h} \cdot \vec{e}(x) \right]$$

$$\vec{e}(x) \in \mathbb{R}^4 \, , \quad |\vec{e}(x)| \equiv 1$$

$\vec{h}$ external "magnetic field"
$\vec{h} = \vec{0}$: global O(4) symmetry, can break spontaneously to O(3)
$\vec{h} \neq \vec{0}$ adds explicit symmetry breaking, like quark masses $m_u = m_d > 0$

Local isomorphy to chiral flavor symmetry:

$$\{ \ \mathrm{SU}(2)_\mathrm{L} \otimes \mathrm{SU}(2)_\mathrm{R} = \mathrm{O}(4) \ \} \quad \longrightarrow \quad \{ \ \mathrm{SU}(2)_{\mathrm{L}=\mathrm{R}} = \mathrm{O}(3) \ \}$$

Same symmetry groups before and after symmetry breaking

Assume $T = 1/\beta$ high enough for **dimensional reduction:**

$$S[\vec{e}] = \int_0^\beta dt_\mathrm{E} \int_V d^3x \ \Big[\frac{F_\pi^2}{2} \partial_i \vec{e}(x) \cdot \partial_i \vec{e}(x) - \vec{h} \cdot \vec{e}(x) \Big] \simeq \beta H[\vec{e}]$$

3d O(4) model (with periodic b.c.) has topological sectors, $\pi_3(S^3) = \mathbb{Z}$.

- [Skyrme '61,'62, Witten '79, Adkins/Nappi/Witten '83, Zahed/Brown '86, . . .] :
  top. charge Q corresponds to baryon number B
  $\vec{e}(x)$ pion field, but in this way the model accounts for baryons.

$\Rightarrow$ Baryon chem. potential $\mu_B \stackrel{\wedge}{=}$ imaginary vacuum angle θ,

$$H[\vec{e}] = \cdots - \mu_B Q[\vec{e}] \in \mathbb{R} \ , \qquad Q[\vec{e}] \ \text{top. charge}$$

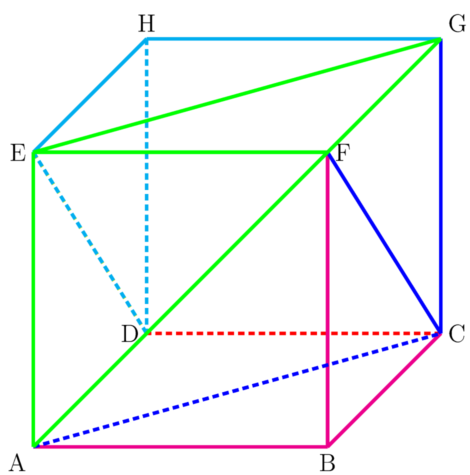
Standard lattice formulation,

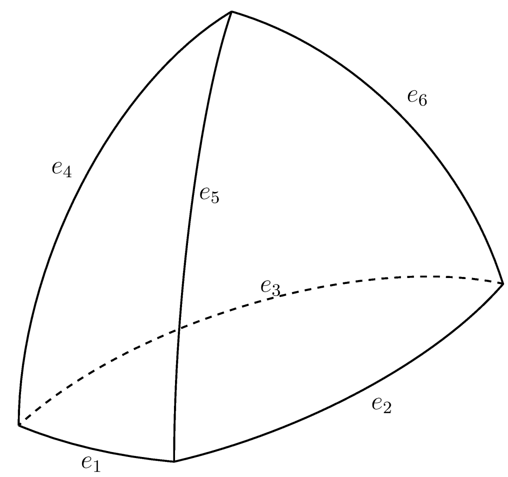
$$S_{\text{lat}}[\vec{e}] = -\beta_{\text{lat}} \Big(\sum_{\langle x,y \rangle} \vec{e}_x \cdot \vec{e}_y + \vec{h}_{\text{lat}} \cdot \sum_x \vec{e}_x + \mu_{B,\text{lat}} Q[\vec{e}] \Big)$$

x: lattice sites; $\langle x, y \rangle$: nearest neighbor sites

Topological charge on the lattice: geometric definition:

Split lattice unit cubes into 6 tetrahedra; the 4 spins at the vertices of one tetrahedron, $(\vec{e}_w, \vec{e}_x, \vec{e}_y, \vec{e}_z)$, span a **spherical tetrahedron** on S^3 (edges $e_1 \dots e_6$: geodesics in S^3).





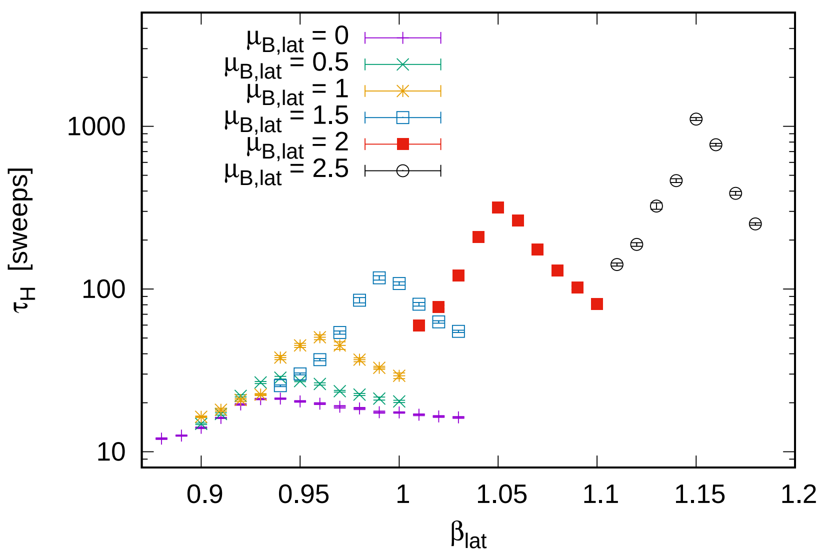
Topological density of a tetrahedron = volume of oriented spherical tetrahedron, $V_{w,x,y,z}[\vec{e}] \in (-\pi^2, \pi^2)$,

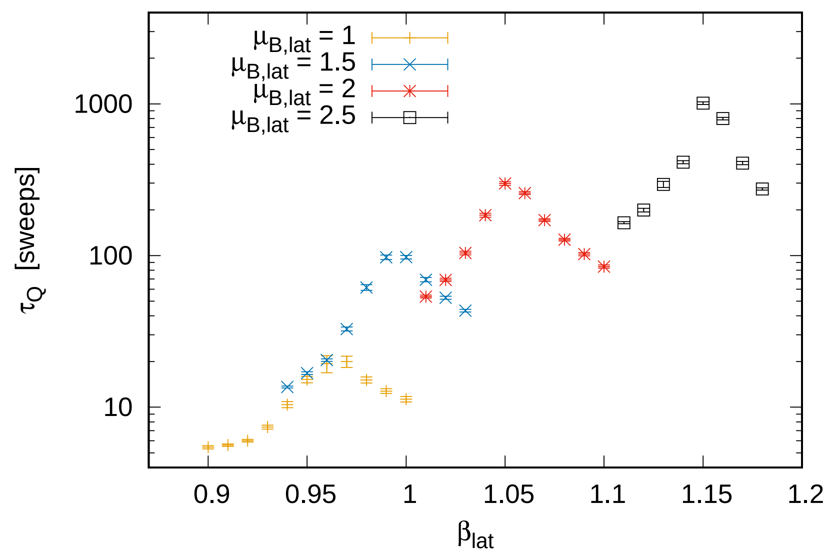
$$Q[\vec{e}] = \frac{1}{2\pi^2} \sum_{\langle w,x,y,z \rangle} V_{w,x,y,z}[\vec{e}] \in \mathbb{Z}$$

Prescription to compute $V_{w,x,y,z}[\vec{e}]$ by Murakami, '12.

Cluster algorithm: another benefit of the O(4) model as an effective theory.

Still, increasing μ_B causes a rapid increase in auto-correlation time τ: this limits the range of reliable simulations to $\mu_{B,\mathrm{lat}} \leq 2.5$.





τ in multi-cluster updates with respect to H and Q ($L = 20$, $h = 0$).

I. Results in the chiral limit, $h = 0$

Physical units by referring to $T_c = 1/\beta_c$ at $\mu_B = 0$:

$\beta_{c,\text{lat}} = 0.9359(1)$ [Oevers, '96] $\Leftrightarrow$ $T_c \approx 132$ MeV [Ding et al. '19]

$$\mu_B = \frac{\beta_{c,\text{lat}}}{\beta_c}\,\mu_{B,\text{lat}} \approx 124\ \text{MeV}\ \mu_{B,\text{lat}}$$

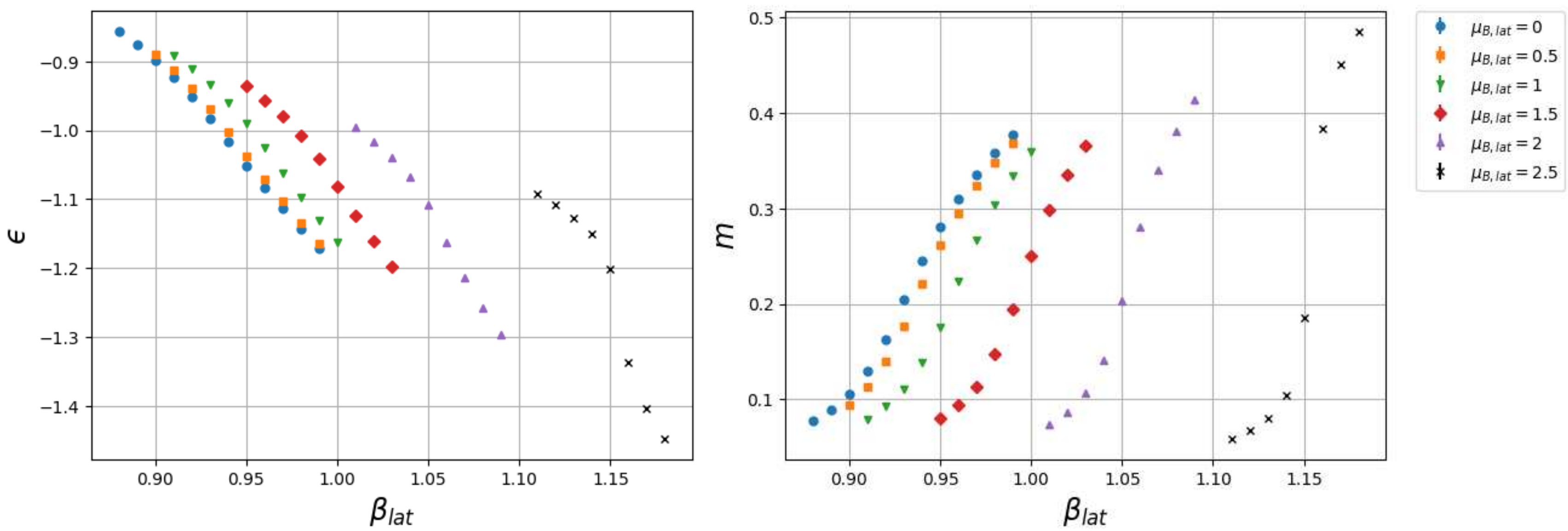
Simulation parameters:

$\mu_{B,\text{lat}} = 0,\ 0.1,\ 0.2,\ \ldots 1.5;\ 2, 2.5 \ \Leftrightarrow\ \mu_B = 0 \ldots 309$ MeV

Lattice volumes L^3, $L = 10,\ 12,\ 16,\ 20$ (problem: huge τ)

For each parameter set: 10^4 measurements, perfectly decorrelated

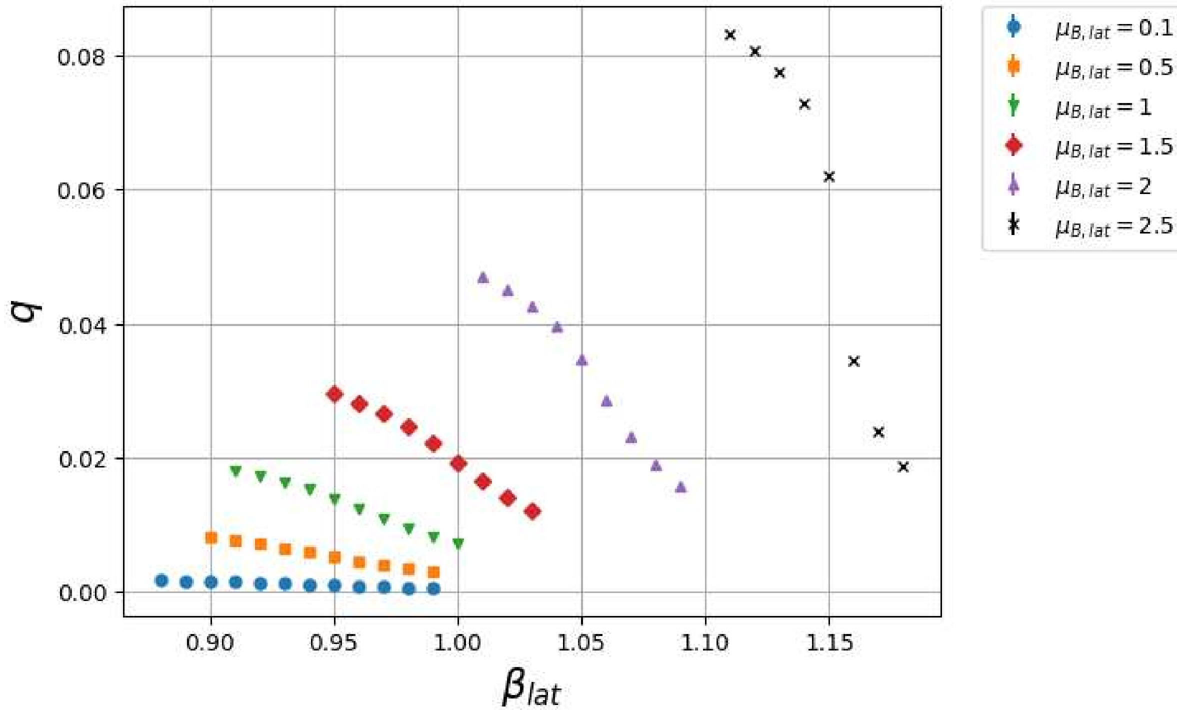
Observables: 1^{st} and 2^{nd} derivatives of $F = -T \ln Z$.



Energy density $\epsilon = \langle H \rangle / V$ (left) and magnetization density (order parameter) $m = \langle |\vec{M}| \rangle / V$, $\vec{M} = \sum_x \vec{e}_x$ (right), $L = 20$.

Increase $\mu_{B,\mathrm{lat}}$ at fixed β: larger ϵ, lower m,
interval of maximal slope moves to larger $\beta \approx \beta_{\mathrm{c}}$.

$\mu_{B,\mathrm{lat}} = 2.5$: quasi-jumps, 1$^{\mathrm{st}}$ order phase transition near-by ?

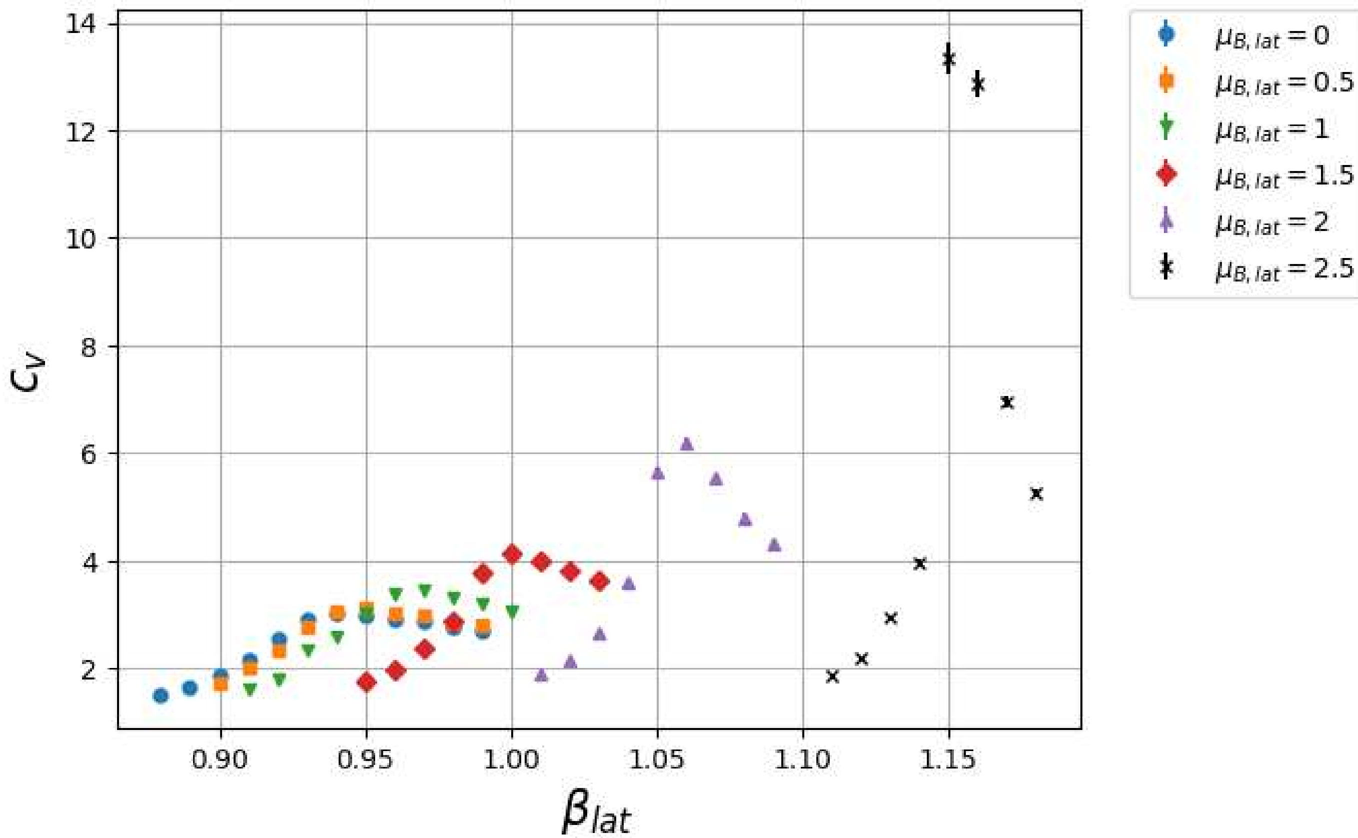


Top. charge density $q = \langle Q \rangle / V$

At $\mu_B = 0$: $q = 0$ due to parity symmetry.

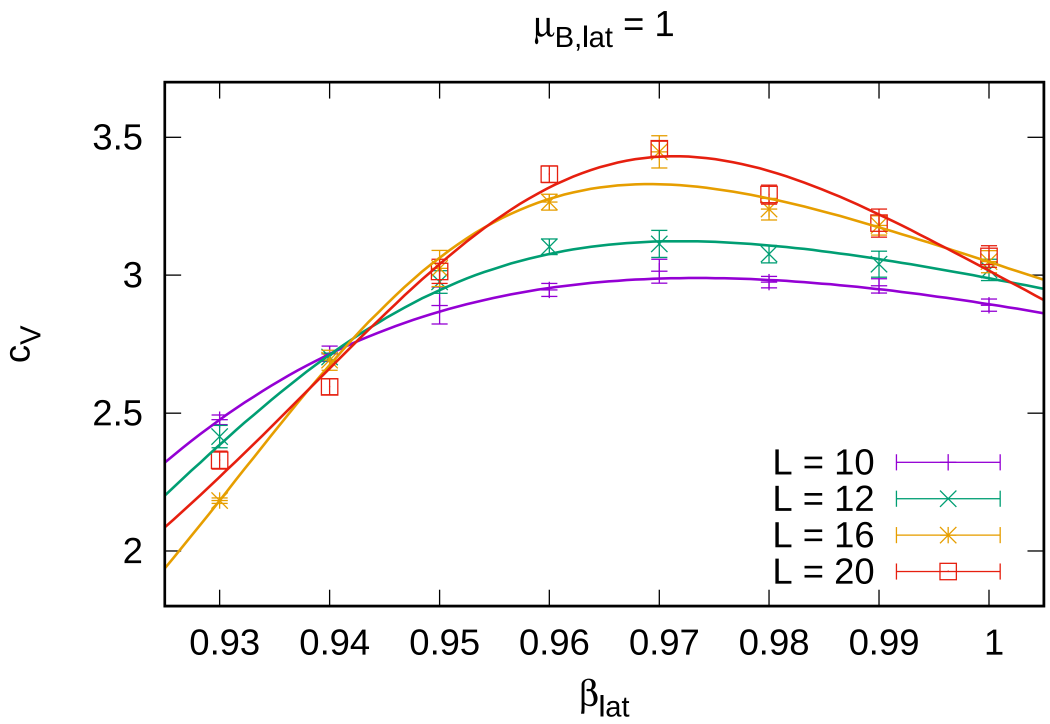
$\mu_B > 0$ enhances $Q > 0$, up to $\langle Q \rangle > 600$.

Again: quasi-jump for $\mu_{B,\mathrm{lat}} = 2.5$, to be clarified by 2^{nd} derivatives of F.



Specific heat $c_V = \frac{\beta^2}{V}\left(\langle H^2\rangle - \langle H\rangle^2\right)\ , \quad L = 20$

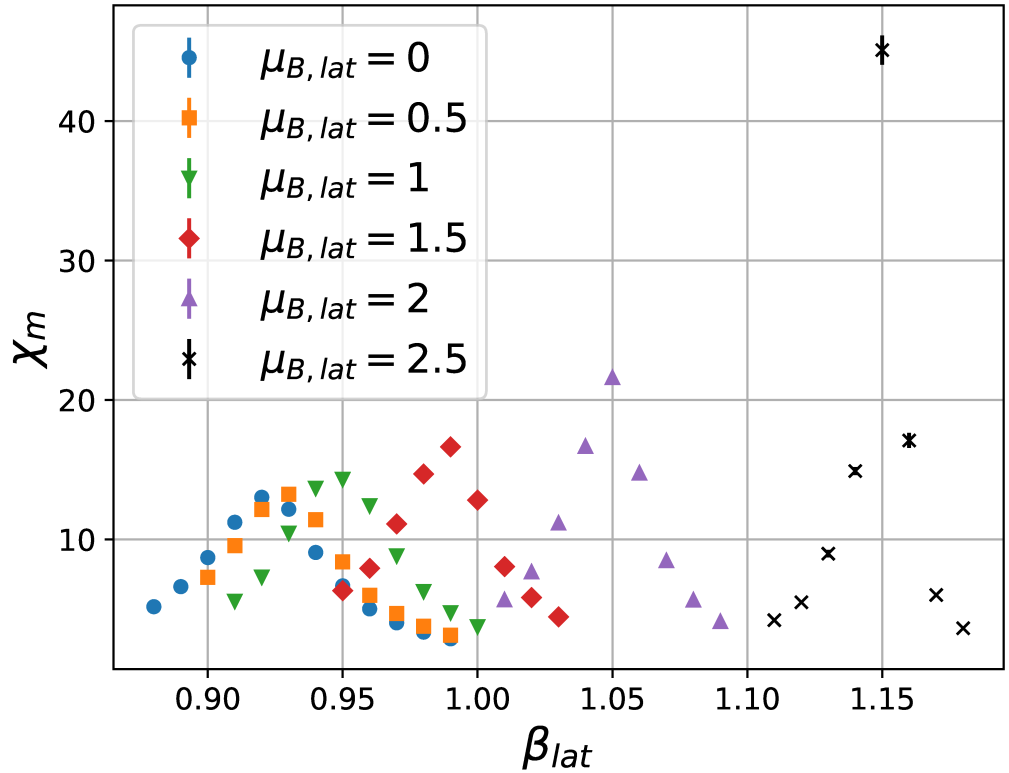
Peak most pronounced at $\mu_{B,\mathrm{lat}} = 2$ and 2.5, likely still 2nd order.



Peak of c_V identified with fits to Johnson's S_U-function for each $\mu_{B,\mathrm{lat}}$.

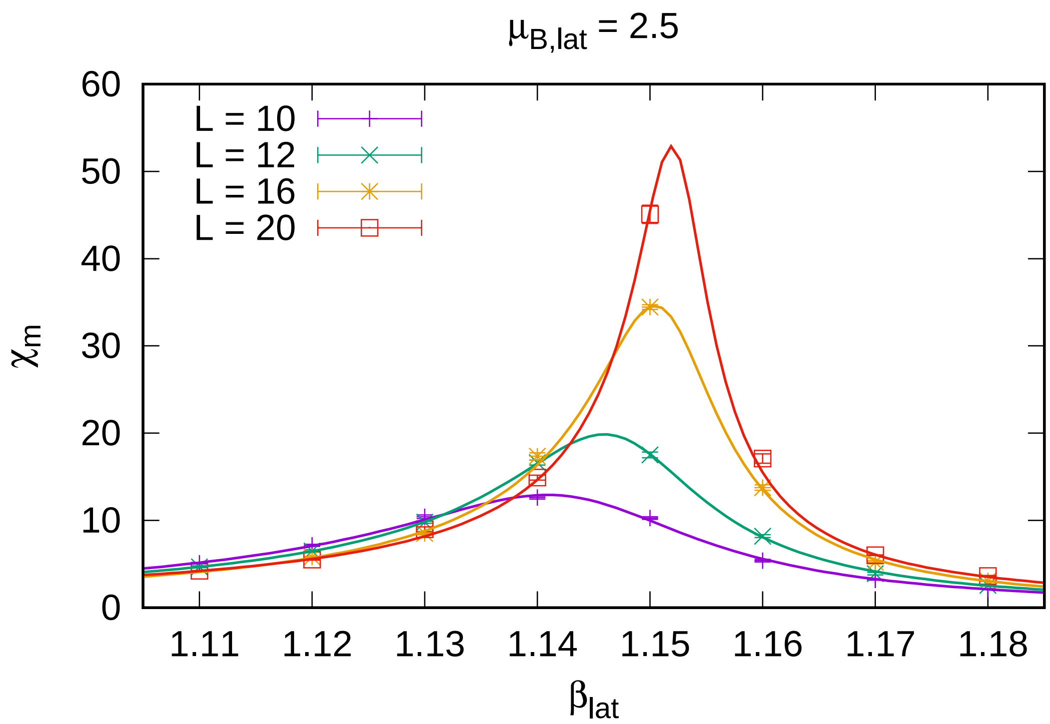
Peak location hardly moves with V, extrapolation to β_c simple.

For 2$^{\mathrm{nd}}$ order we expect (peak height) $\propto L^{\alpha/\nu}$; at $\mu_{B,\mathrm{lat}} = 2$: $\alpha/\nu \approx 0.2$.



Magnetic susceptibility $\chi_{\mathrm{m}} = \frac{\beta}{V}\left(\langle \vec{M}^2 \rangle - \langle |\vec{M}| \rangle^2\right)$, $\quad L = 20$

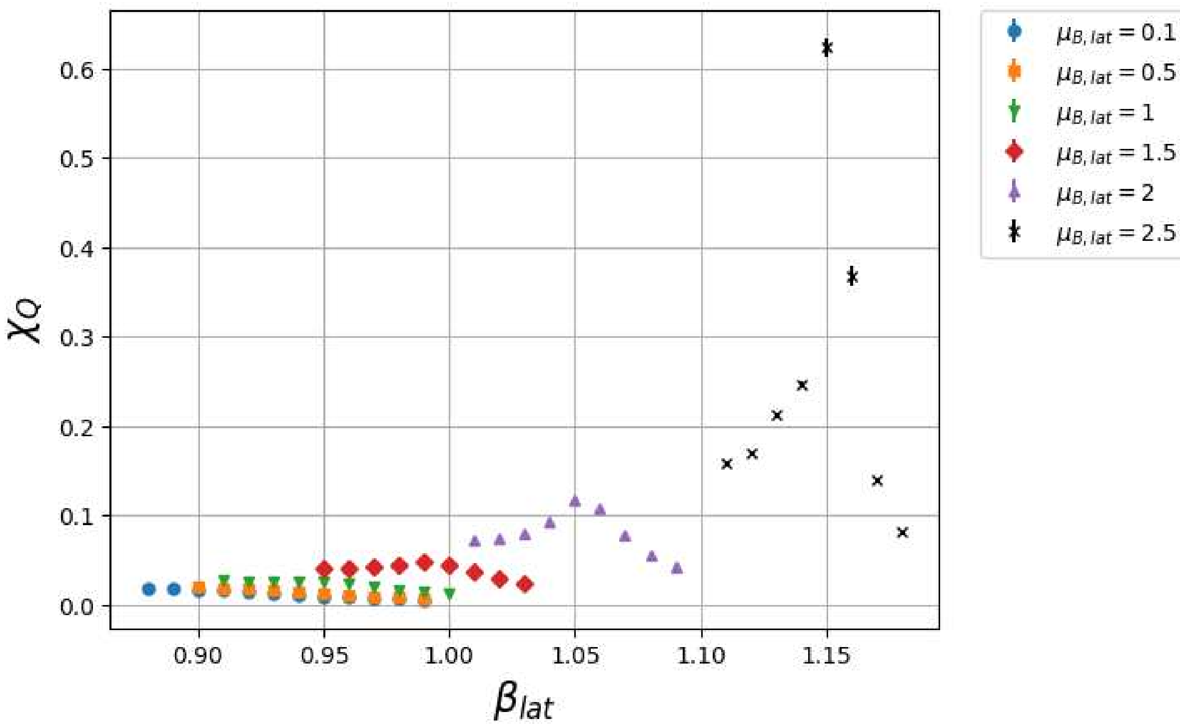
Peak most pronounced at $\mu_{B,\mathrm{lat}} \geq 1$, supports 2^{nd} order.



Peak of χ_m moves with V, extrapolation to β_c consistent with other criteria.

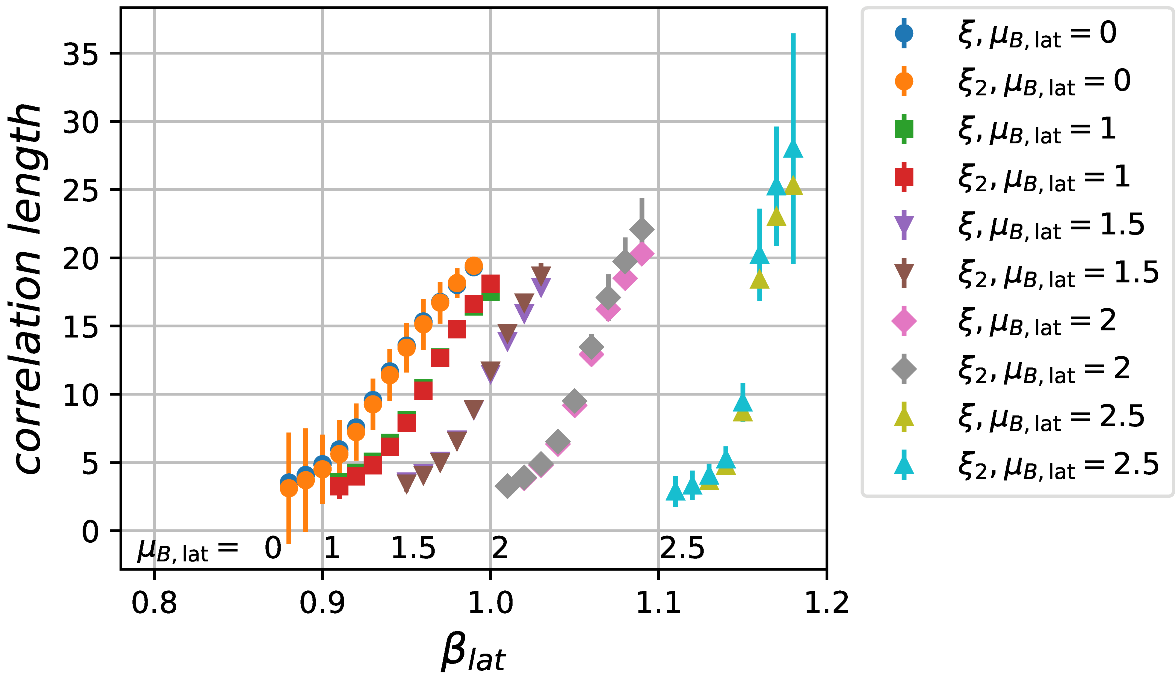
2^nd order: (peak height) $\propto L^{\gamma/\nu}$, $\frac{\gamma}{\nu}(\mu_{B,\mathrm{lat}}) \in [1.7 \ldots 2.1]$
at $\mu_B = 0$ compatible with 1.970 [Engels/Fromme/Seniuch, '03]

Strongly supports 2^nd order, along with auto-correlation time τ.

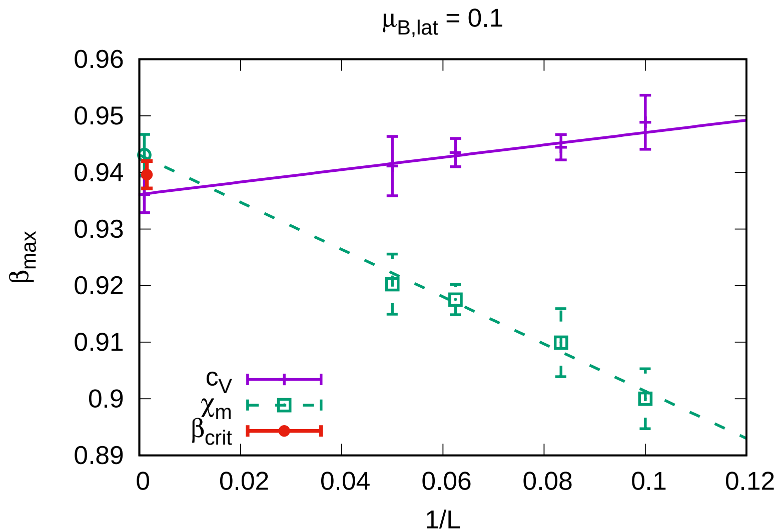


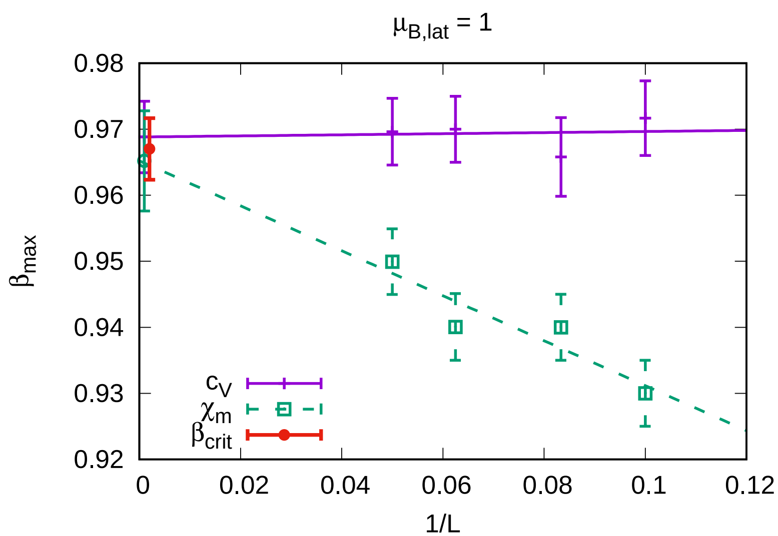
Topological susceptibility $\chi_Q = \frac{1}{V}\Big(\langle Q^2\rangle - \langle Q\rangle^2\Big)$

Peak most pronounced at $\mu_{B,\text{lat}} \geq 1.5$, supports 2$^{\text{nd}}$ order, consistent with previous determinations of β_c. One might try to introduce a new critical exponent θ: $\chi_Q(T_c) \propto L^{\theta/\nu}$, *e.g.* $\frac{\theta}{\nu}|_{\mu_{B,\text{lat}}=0} \simeq 0.2$, $\frac{\theta}{\nu}|_{\mu_{B,\text{lat}}=1} \simeq 0.3$

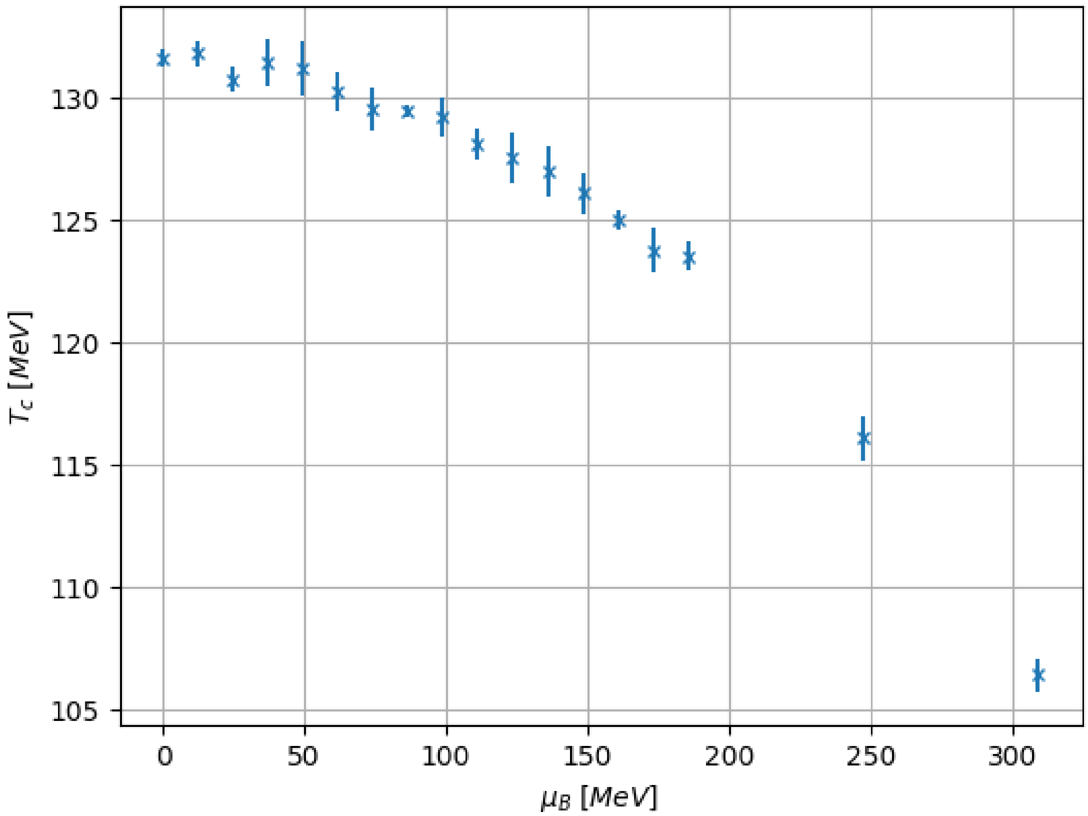


Correlation length ξ
(or "2$^{\mathrm{nd}}$ moment correlation length" $\xi_2 \simeq \xi$, easier to measure):
peaks at $L = 20$ are again consistent
most compelling evidence for 2$^{\mathrm{nd}}$ order phase transition





Large-volume extrapolations of β_{max} to β_{c}
Consistent for each value of $\mu_{B,\mathrm{lat}}$



Combine all determinations of $\beta_{\mathrm{c,lat}}(\mu_{B,\mathrm{lat}})$ (steepest slopes and peaks, extrapolated $V \to \infty$), convert to physical units: final phase diagram in the chiral limit. Shape as expected, but no Critical Endpoint — *i.e.* no change to 1$^{\mathrm{st}}$ order — in the regime $\mu_B \lesssim 309$ MeV and $T \gtrsim 106$ MeV.

II. Preliminary results at physical pion mass, $h = |\vec{h}| > 0$

Estimate of physical units

$$\beta_{\rm c,lat} \simeq 0.936 \,, \quad T_{\rm x} \simeq 155 \text{ MeV}$$
$$h = h_{\rm lat} \frac{\beta_{\rm c,lat}^4}{\beta_{\rm x}^4} = h_{\rm lat} \, (145 \text{ MeV})^4$$

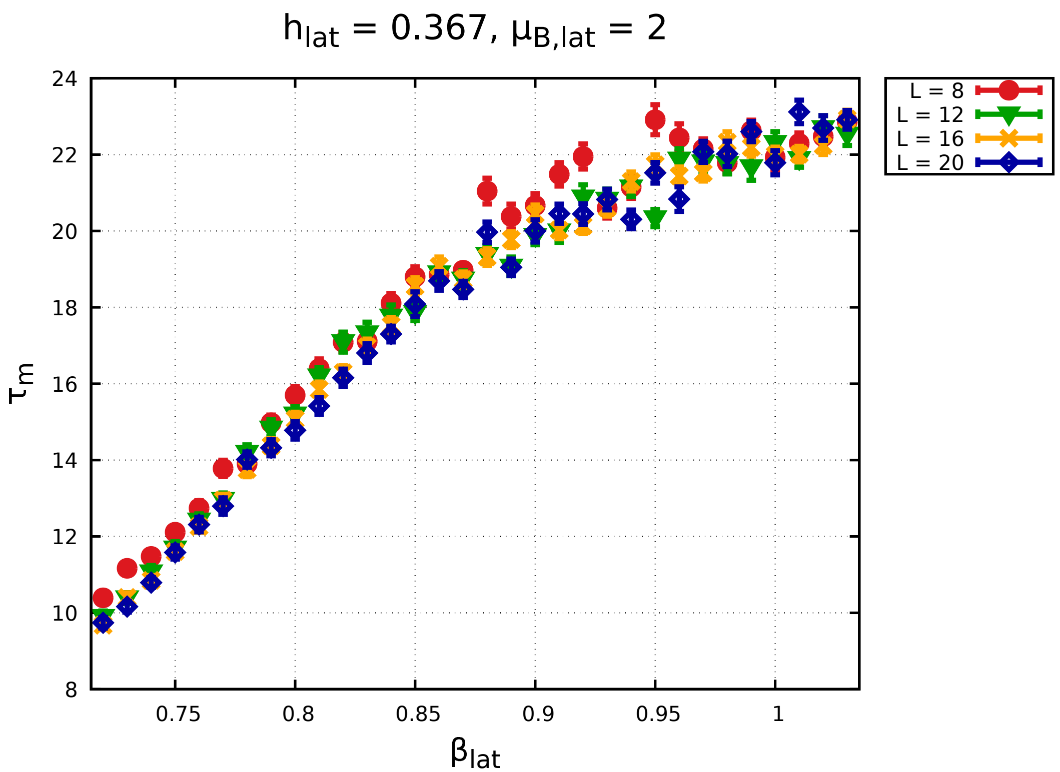
$\beta_{\rm x,lat} \approx 0.87$ ambiguous, see below.

We fix h by the Gell-Mann–Oakes–Renner relation:

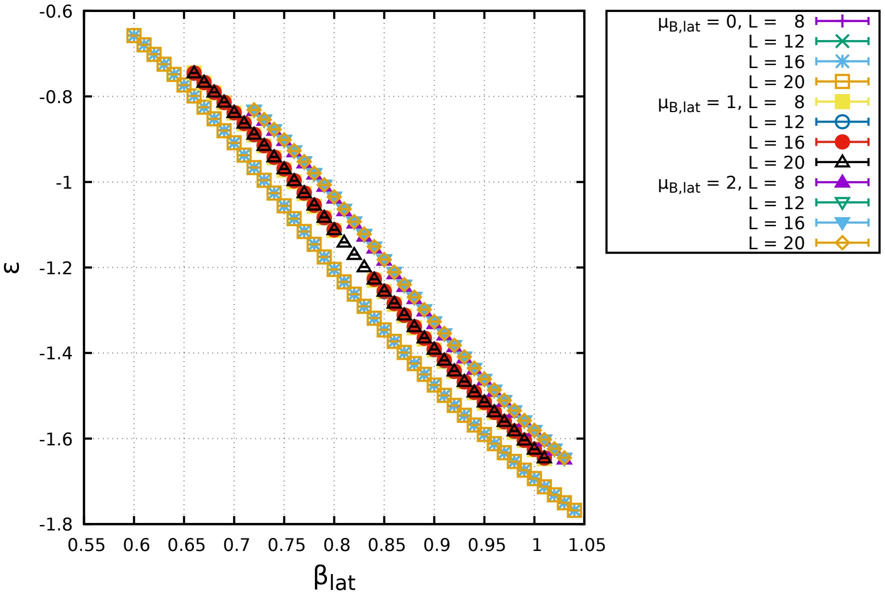
$$h = m_q \Sigma \stackrel{!}{=} F_\pi^2 \, M_\pi^2 \simeq (92.4 \text{ MeV})^2 \, (138 \text{ MeV})^2 \;\Rightarrow\; h_{\rm lat} = 0.367$$

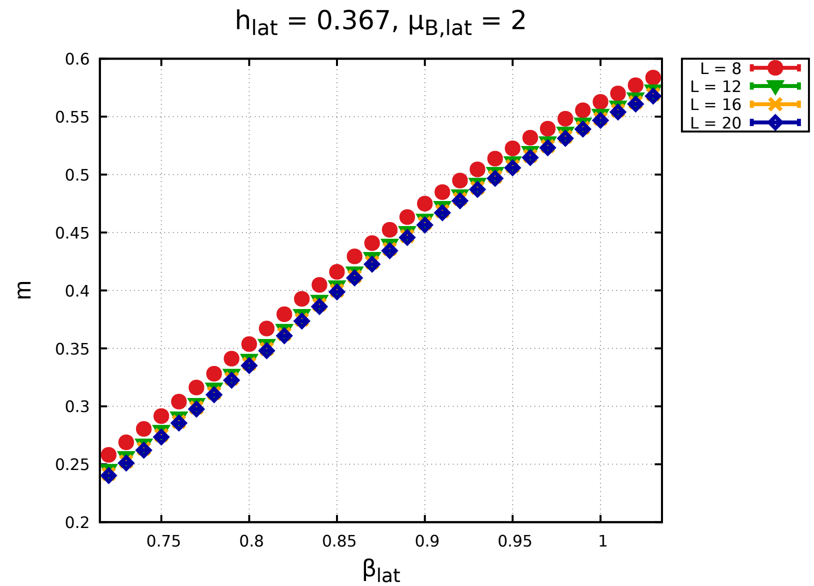
with $\Sigma = -\langle \bar{\psi} \psi \rangle \simeq (250 \, \text{MeV})^3$, this corresponds to $m_q \simeq 5 \, \text{MeV}$

Growth of auto-correlation times τ is strongly alleviated by crossover: τ does not diverge at β_x, **no critical slowing down**.



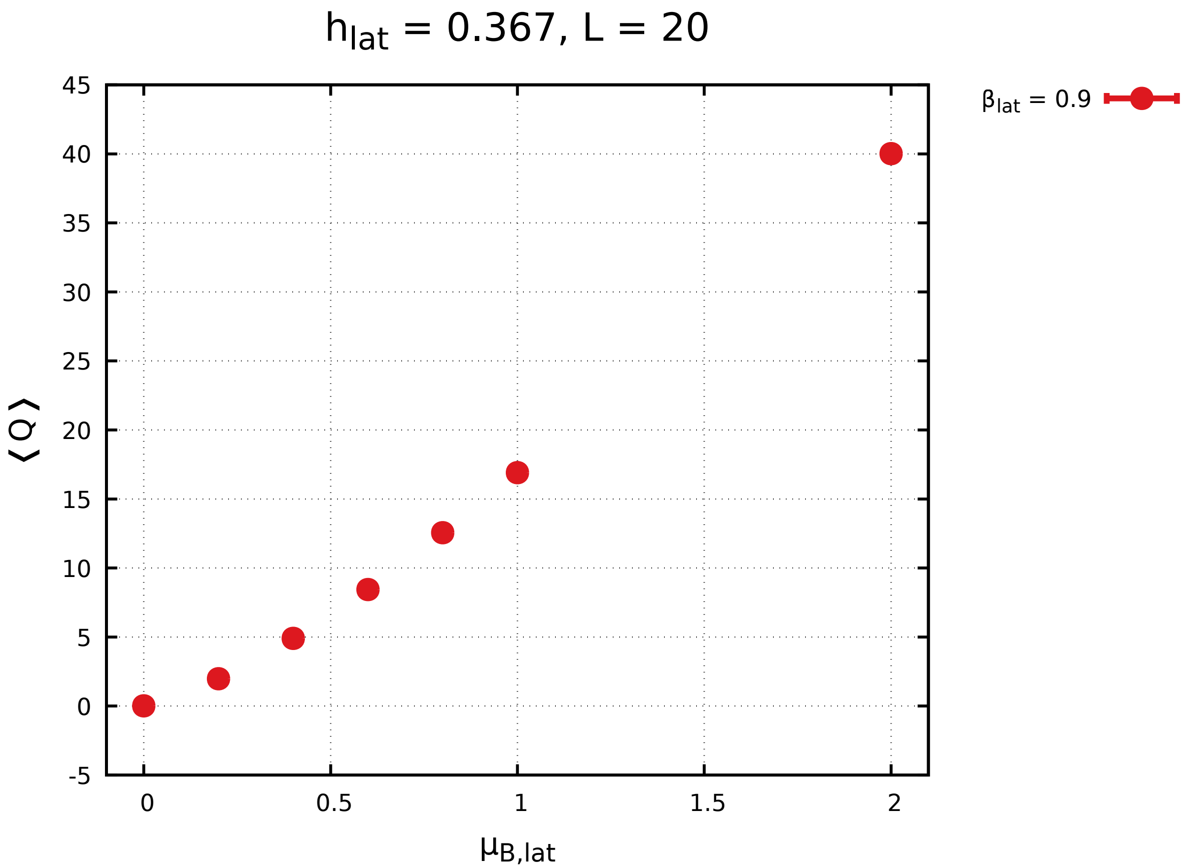
Magnetic auto-correlation time $\tau_{\rm m}$





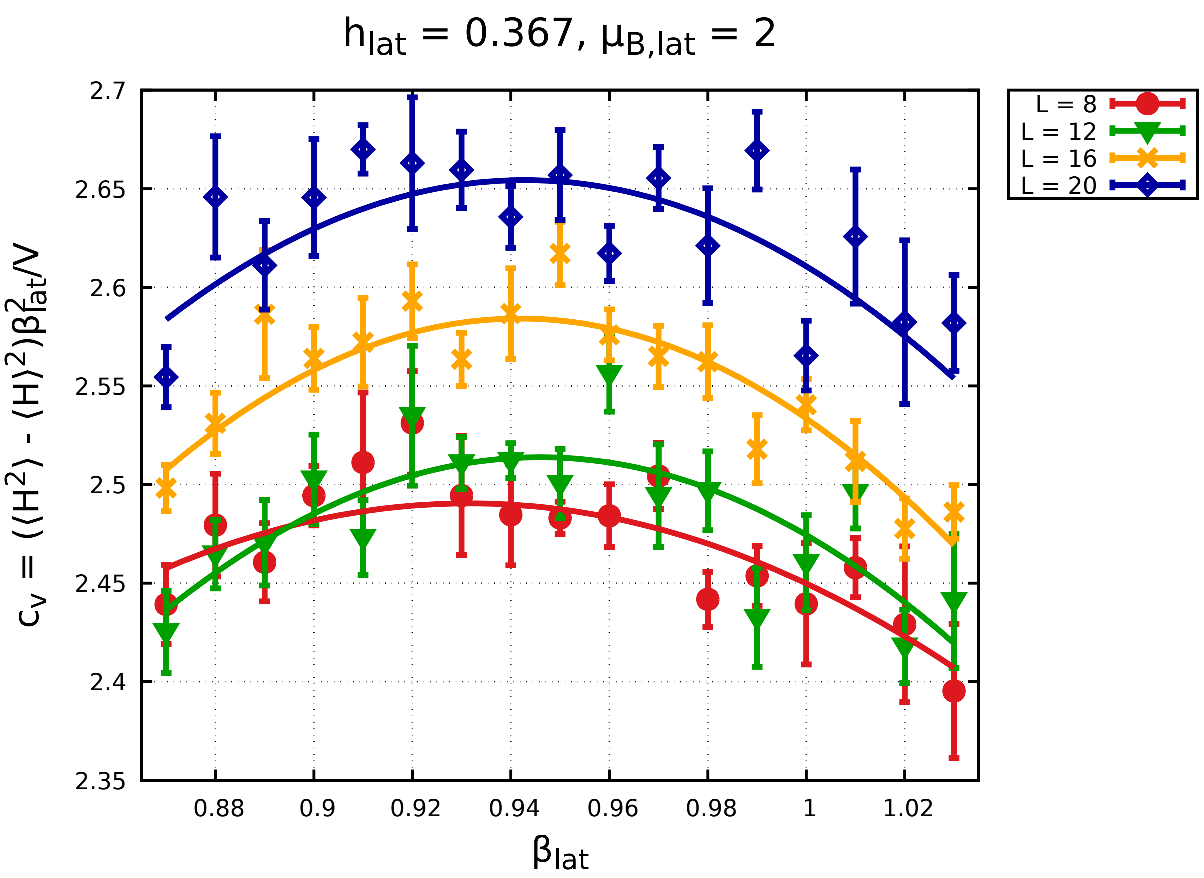
Left: Energy density $\epsilon = \langle H \rangle / V$ hardly depends on L. Shift for $\mu_{B,\text{lat}} = 0,\ 1,\ 2$.
Right: Magnetization density $m = \langle |\vec{M}| \rangle / V$ at $\mu_{B,\text{lat}} = 2$. Modest finite-size effects.

No interval of extraordinary slope (as L grows):
2^{nd} order phase transition smeared out to a crossover.



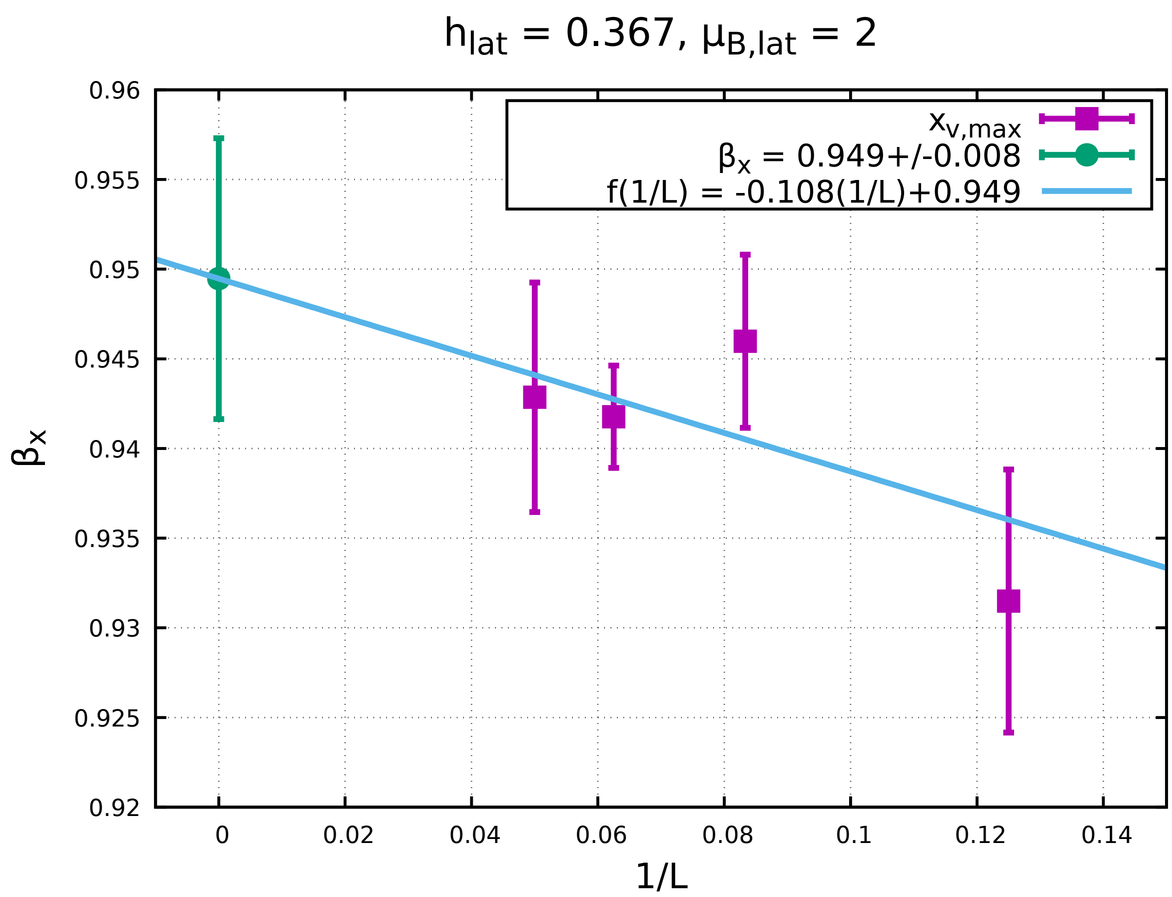
$\langle Q \rangle$ at $\beta_{\text{lat}} = 0.9,\ L = 20.$

$\langle Q \rangle \triangleq \langle$ baryon number $\rangle$, enhanced by $\mu_{B,\text{lat}}$



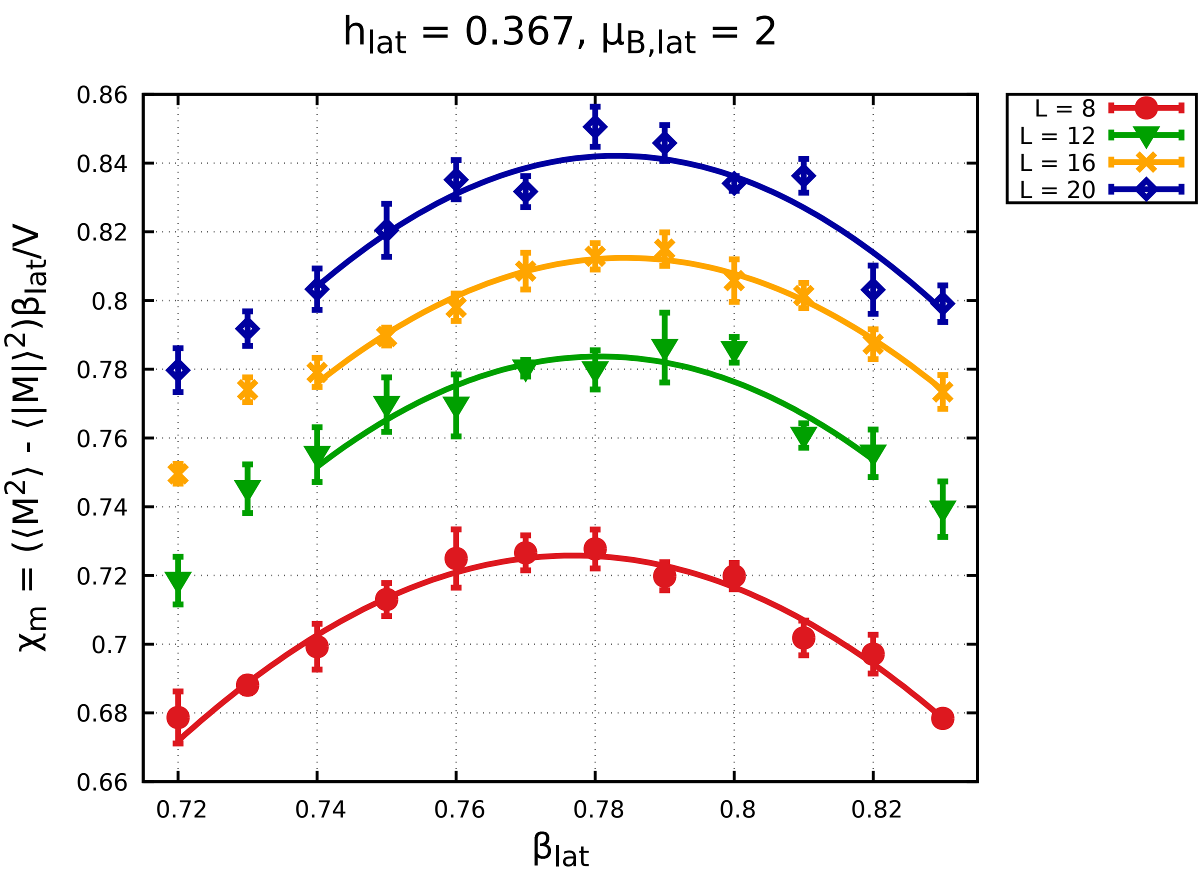
Specific heat c_V

Peak washed out by mass term; located by Gaussian fits

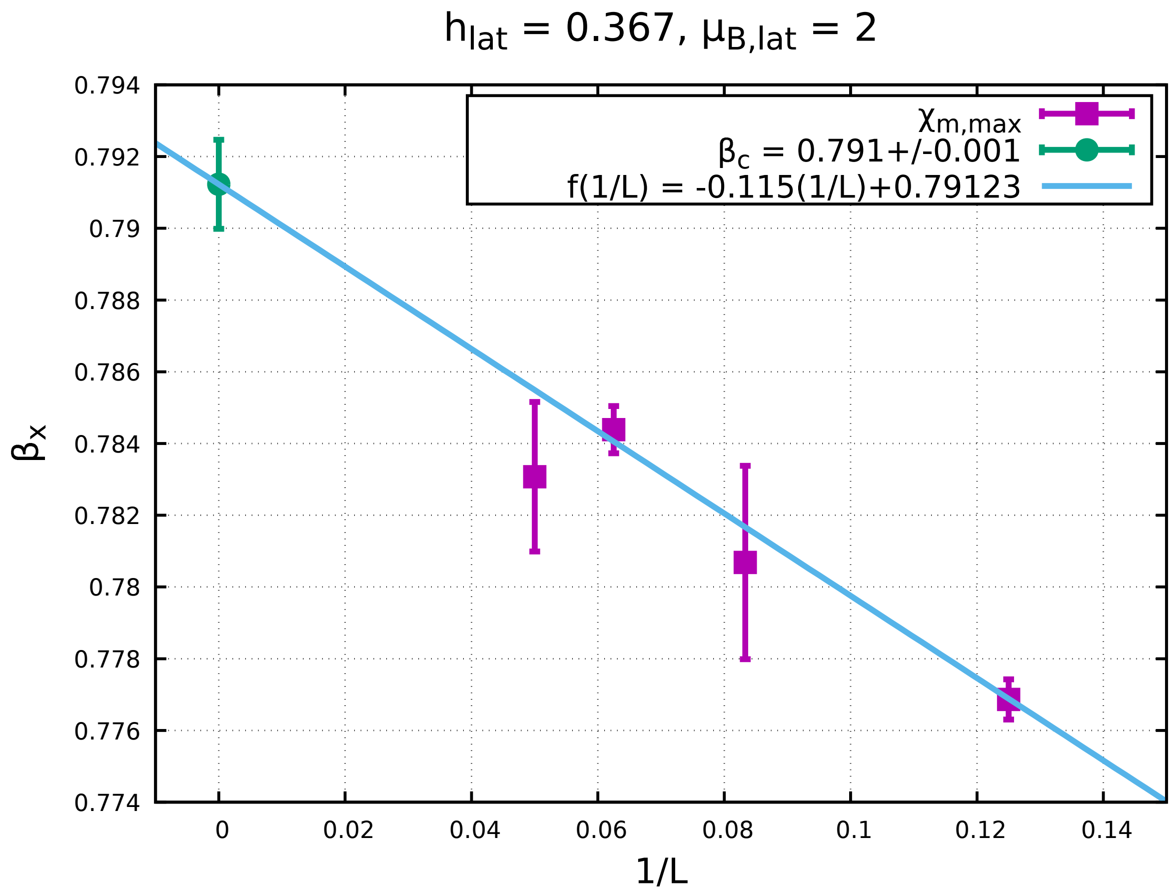


Large-L extrapolation of c_V peak locations $\rightarrow \beta_{\mathrm{x,lat}}$

Performed at each $\mu_{B,\mathrm{lat}}$ to monitor the crossover.

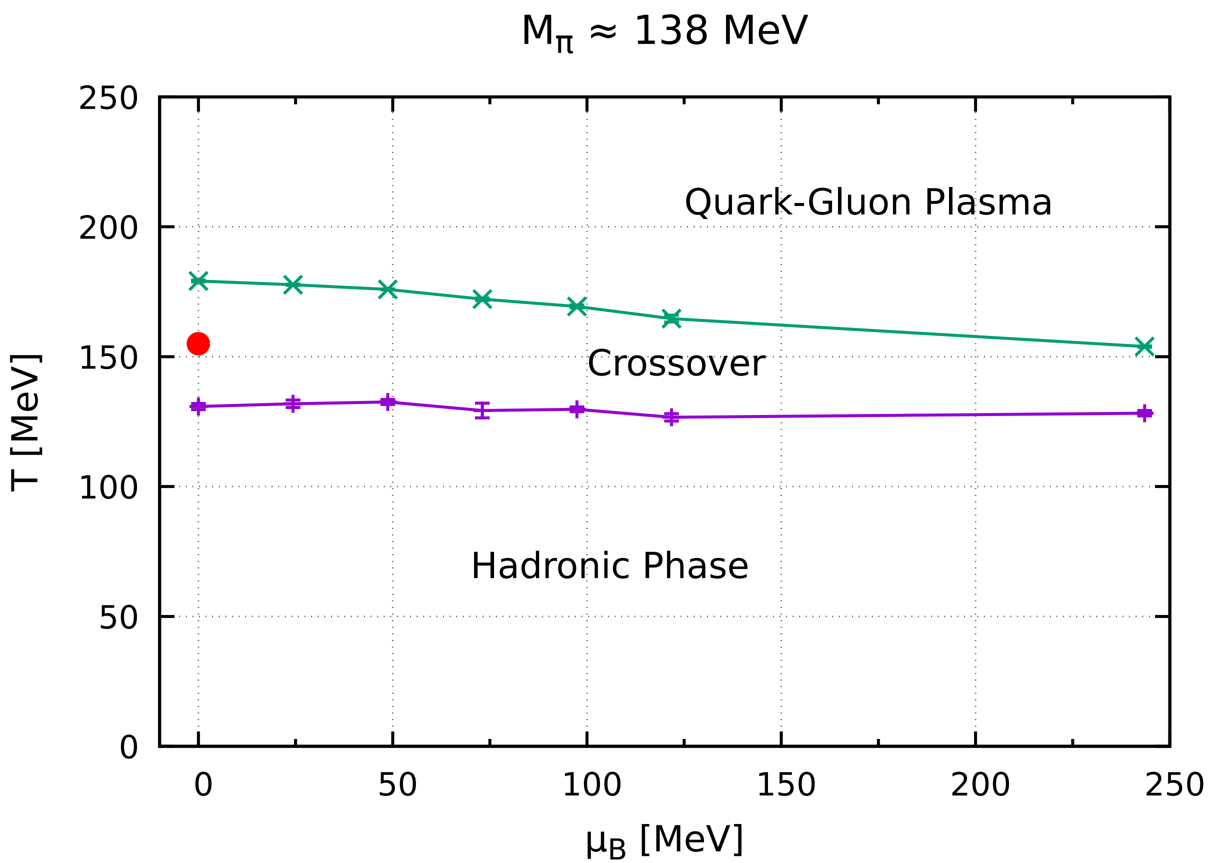


Magnetic susceptibility $\chi_{\rm m}$ at $\mu_{B,\rm lat} = 2$. Again: peak washed out, localized by Gaussian fits. Another criterion to search $\beta_{\rm x}$.



Large-L extrapolation of $\chi_{\rm m}$ peak locations $\rightarrow \beta_{\rm x,lat}$

Below values obtained from c_V; typical for a crossover.



Phase diagram at finite quark mass: broad crossover region; T_x hardly decreases up to $\mu_B = 244\ \mathrm{MeV}$. No indication of a Critical Endpoint.

Conclusions

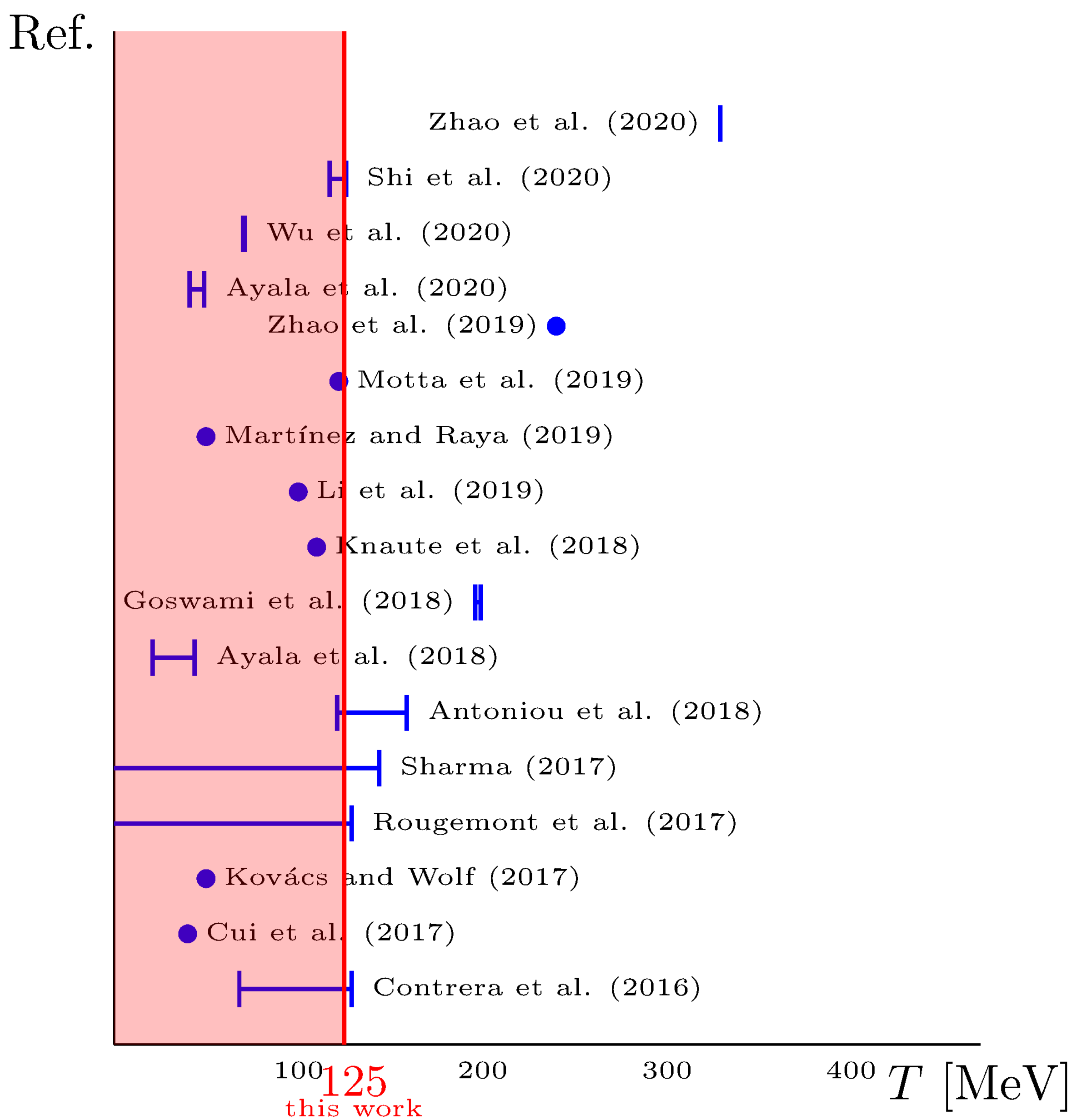
We assume the O(4) model to be in the universality class of 2-flavor QCD in the chiral limit.

High-T dimensional reduction to 3d O(4) leads to topological charge, identified with the baryon number.

Model can be simulated with baryon chemical potential, without sign problem, and with a powerful cluster algorithm.

We monitor the critical line up to $\mu_B \simeq 309$ MeV, $T_c \simeq 106$ MeV. $T_c(\mu_B)$ decreases monotonically; no Critical Endpoint found, but hints for it to be near-by.

At physical pion mass: T_x varies little with μ_B, crossover in some T-interval; up to $\mu_B \simeq 244$ MeV again no CEP.


Ref.
Zhao et al. (2020)
Shi et al. (2020)
Wu et al. (2020)
Ayala et al. (2020)
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Martínez and Raya (2019)
Li et al. (2019)
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Antoniou et al. (2018)
Sharma (2017)
Rougemont et al. (2017)
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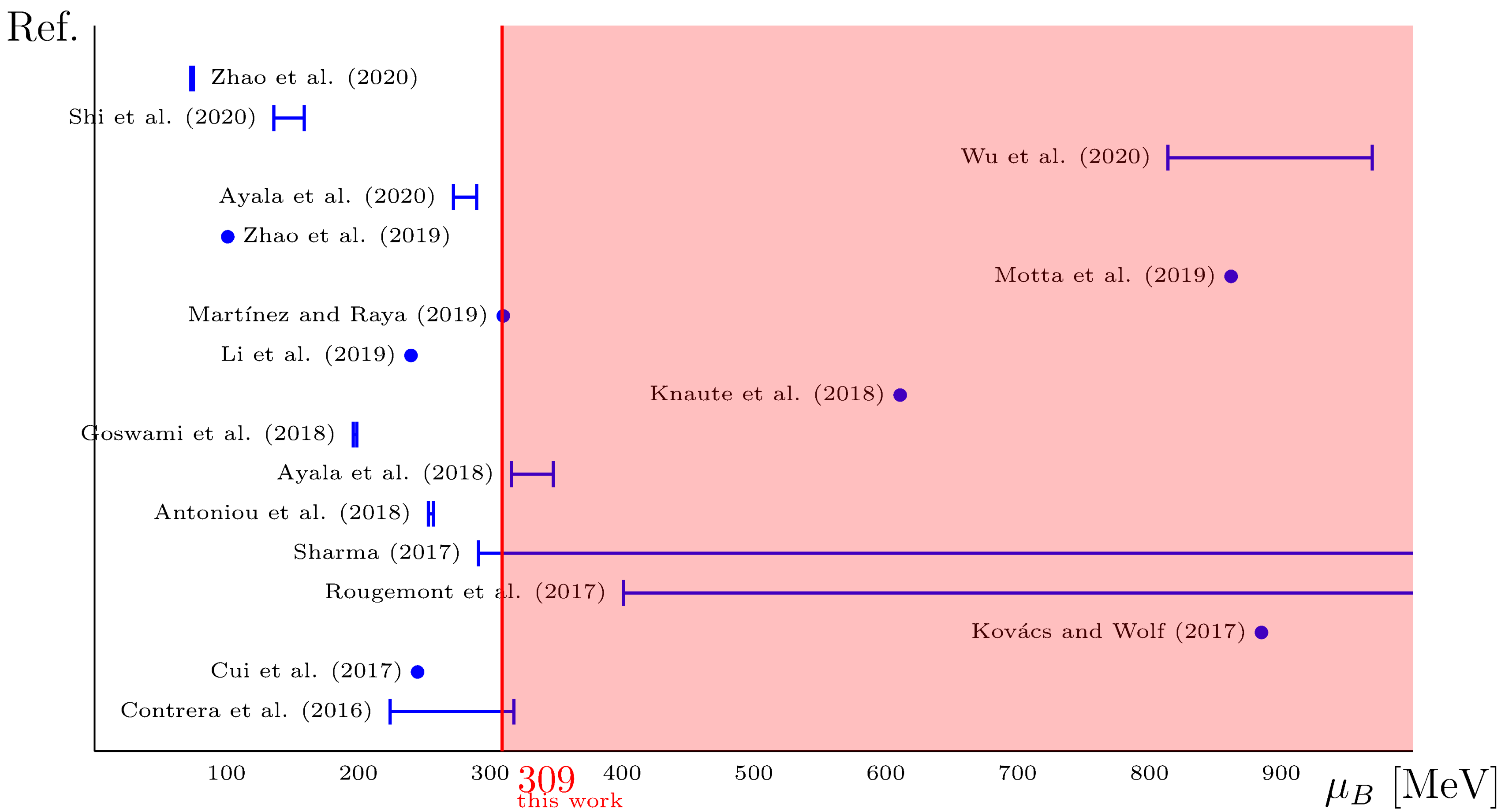
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