Conjecture about the QCD Phase Diagram

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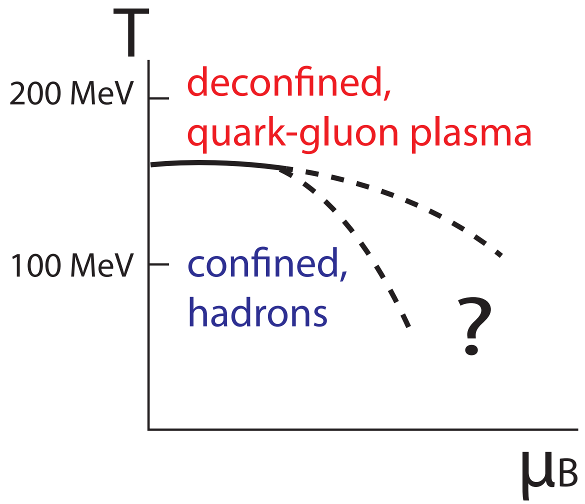
- **O(4) model as an effective theory for 2-flavor QCD: universality, dimensional reduction, topological charge $\sim$ baryon number**

- **Cluster algorithm, inclusion of quark mass and baryon chemical potential without sign problem**

- **Phase diagram in the chiral limit, and with light quarks** (preliminary)

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: $T_c \simeq 132$ MeV [Ding et al. '19]
  $2+1+1$ flavors: $T_{\mathrm{pc}} \simeq 134$ 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 . . .], agrees with $T_{\text{freeze-out}}$

Sign problem at $\mu_B > 0$ still unsolved.
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.

[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:

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

Same symmetry groups before and after symmetry breaking

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

$$S[\vec{e}] = \beta \int_V d^3x \left[\frac{F_\pi^2}{2}\,\partial_i \vec{e}(x)\cdot\partial_i \vec{e}(x) - \vec{h}\cdot\vec{e}(x)\right] = \beta H[\vec{e}]$$

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 $\mu_B \;\hat{=}\;$ imaginary vacuum angle θ,

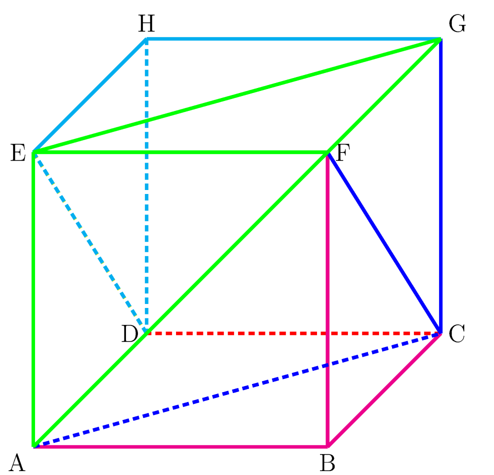
$$H[\vec{e}] = \cdots - \mu_B Q[\vec{e}] \in \mathbb{R}$$

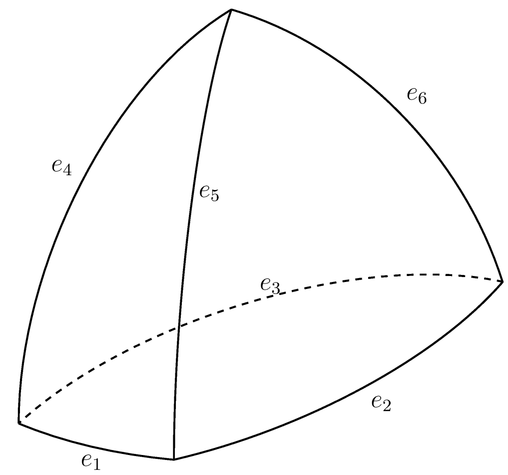
Standard lattice formulation,

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

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).





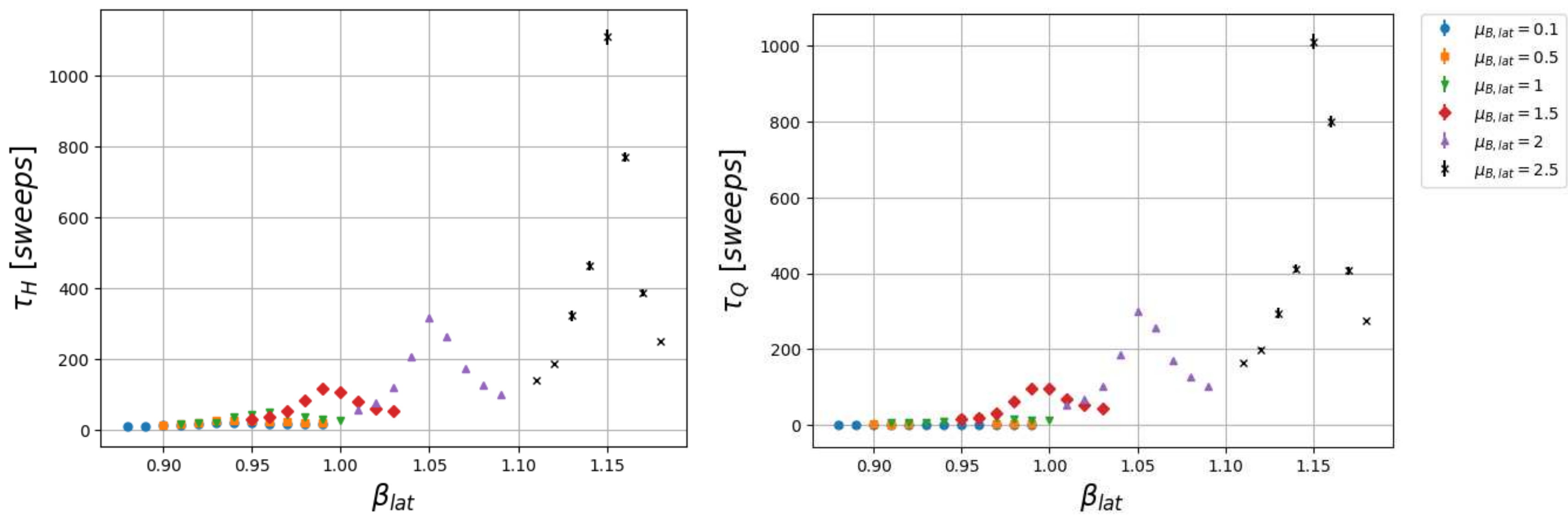
Topological density of a tetrahedron = (normalized) volume of oriented spherical tetrahedron, $V_{w,x,y,z}[\vec{e}] \in (-1/2,\, 1/2)$,

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

Implicit formulae for $V_{w,x,y,z}[\vec{e}]$ 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 (so far) 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 $T_{\rm c} = 1/\beta_{\rm c}$ at $\mu_B = 0$:

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

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

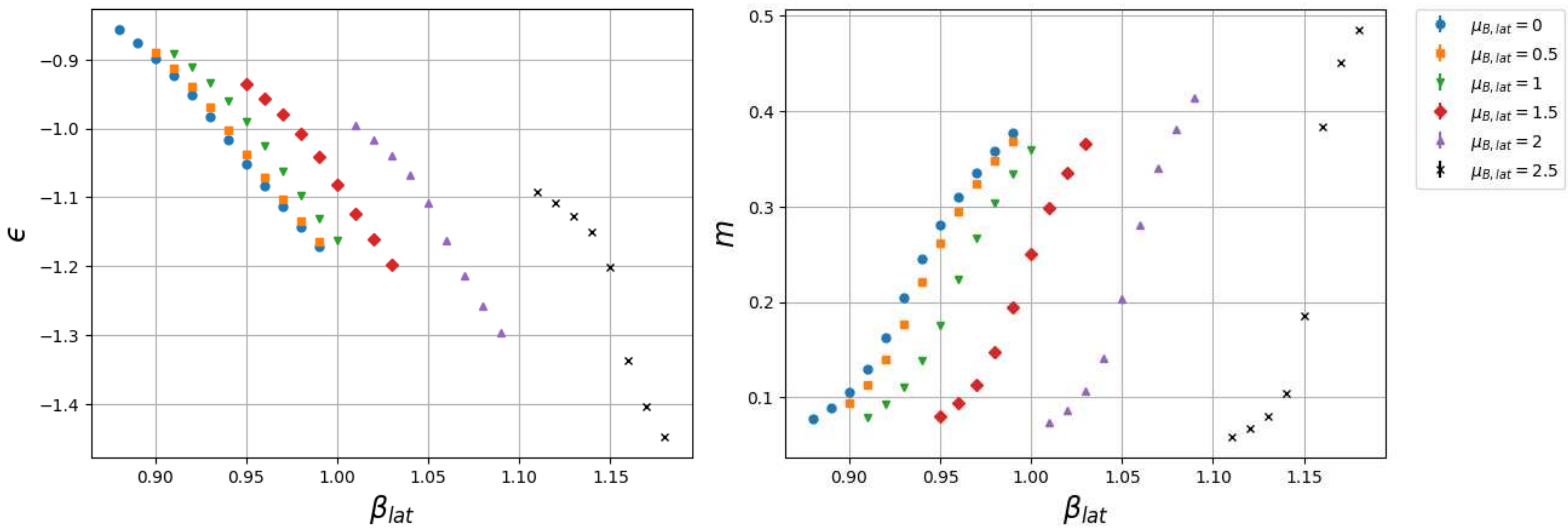
Simulation parameters:

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

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

For each parameter set: 10^4 confs., perfectly de-correlated

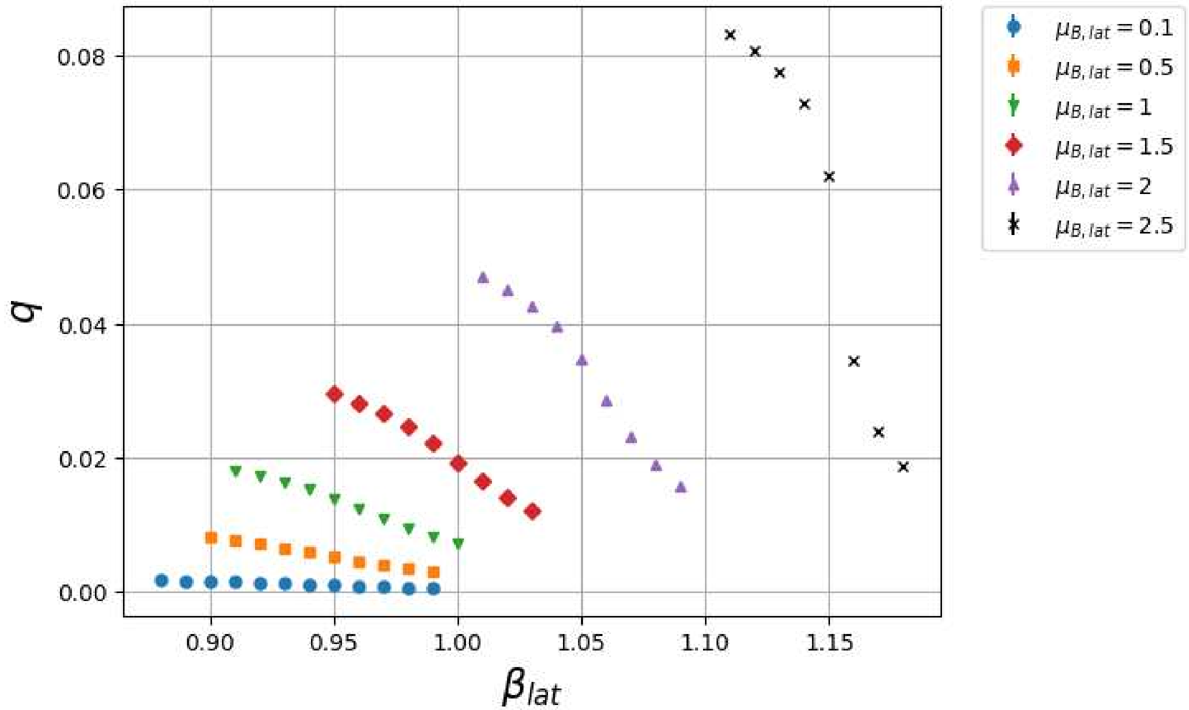
Observables: $1^{\rm st}$ and $2^{\rm nd}$ derivatives of $F = -T \ln Z$.



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 $\beta \approx \beta_{\mathrm{c}}$.

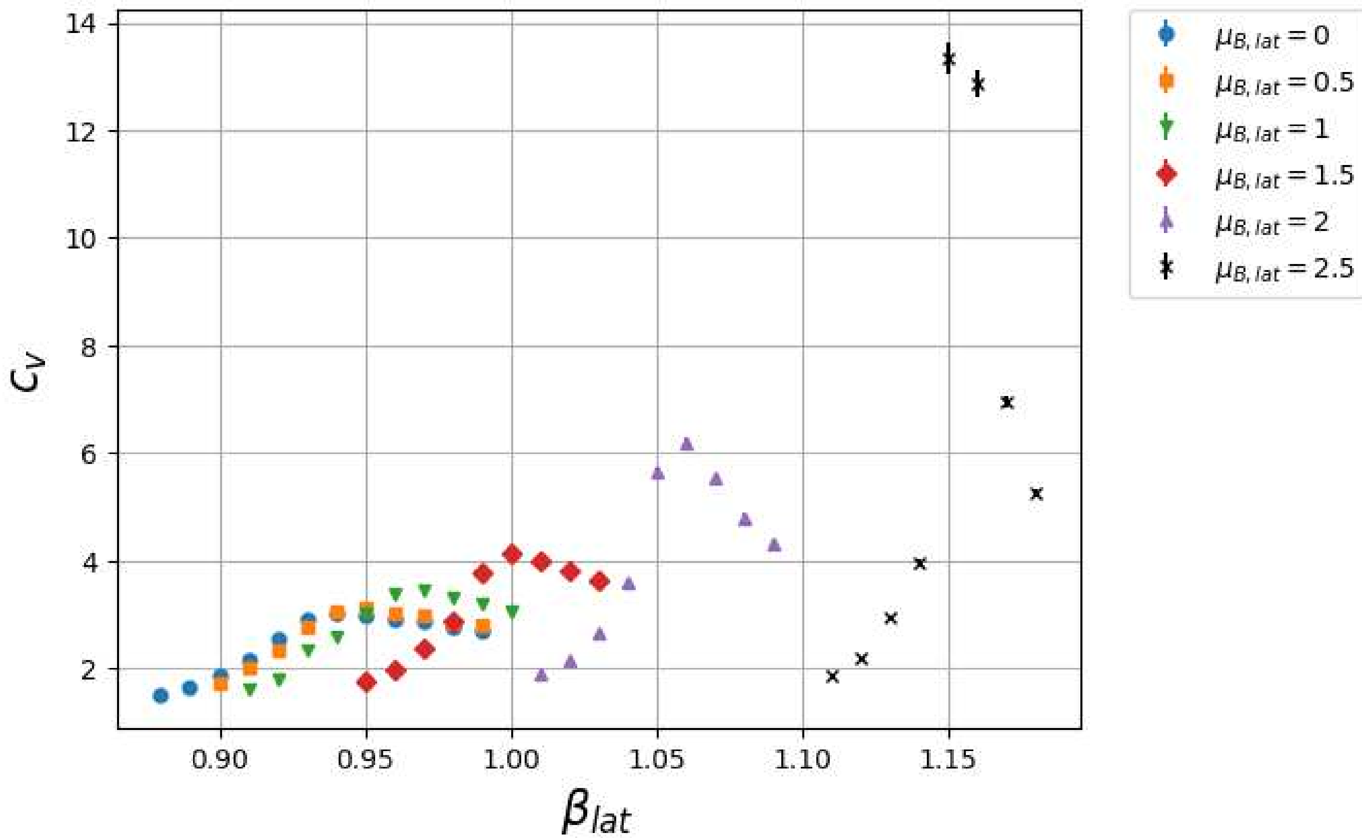
$\mu_{B,\mathrm{lat}} = 2.5$: quasi-jumps, 1^{st} order phase transition near-by ?



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

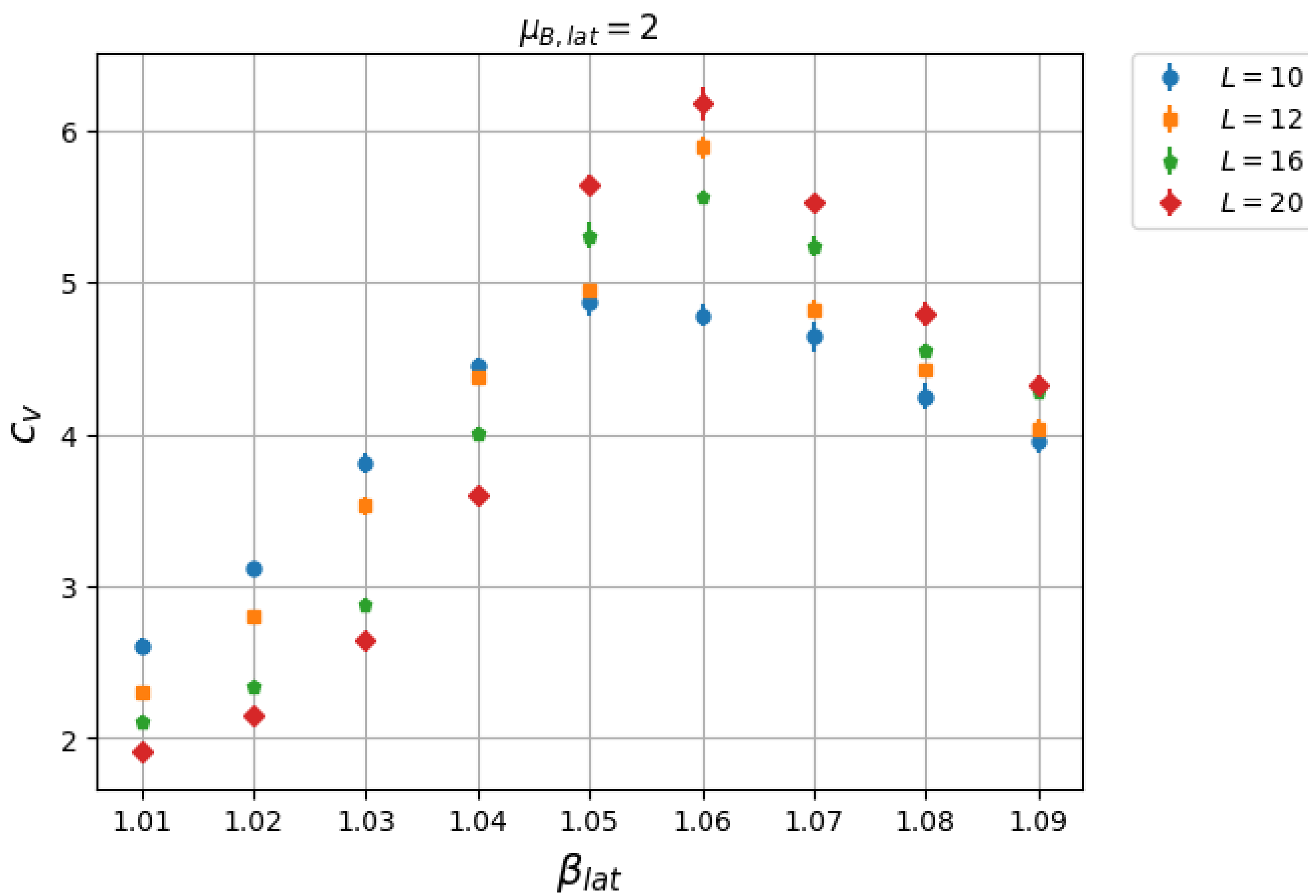
At $\mu_B = 0$: $q = 0$ due to parity symmetry. $\mu_B > 0$ enhances $Q > 0$.

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



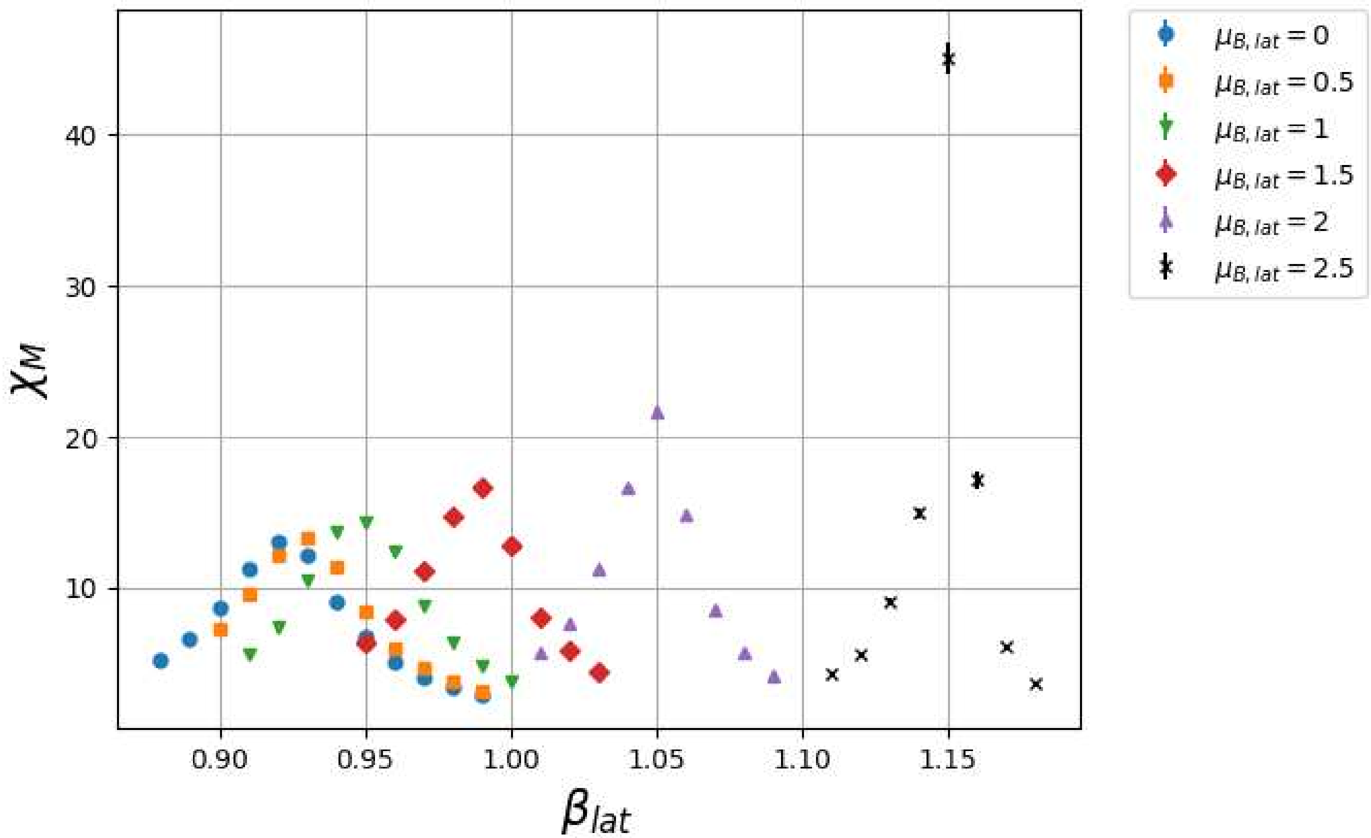
Specific heat $c_V = \frac{\beta^2}{V}\Big(\langle H^2\rangle - \langle H\rangle^2\Big)$

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



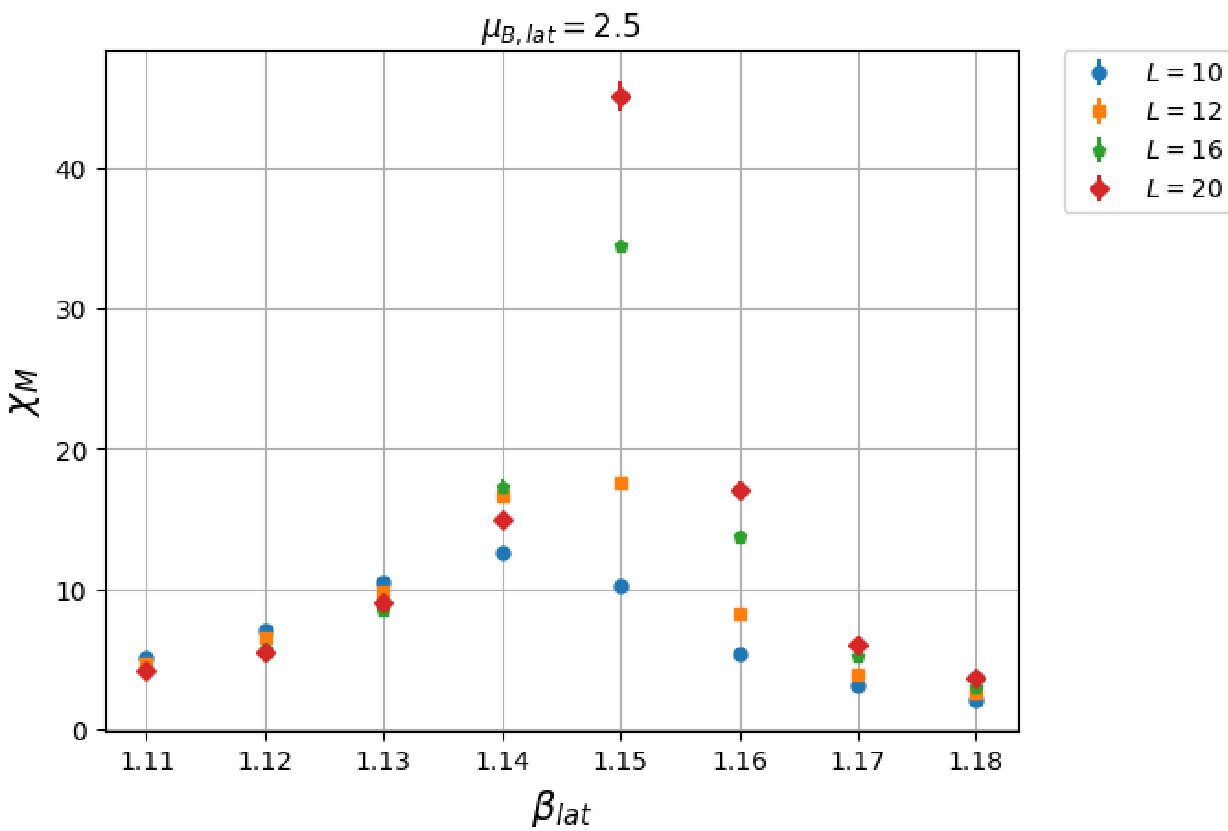
Peak of c_V hardly moves with V, extrapolation to β_c simple.

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



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

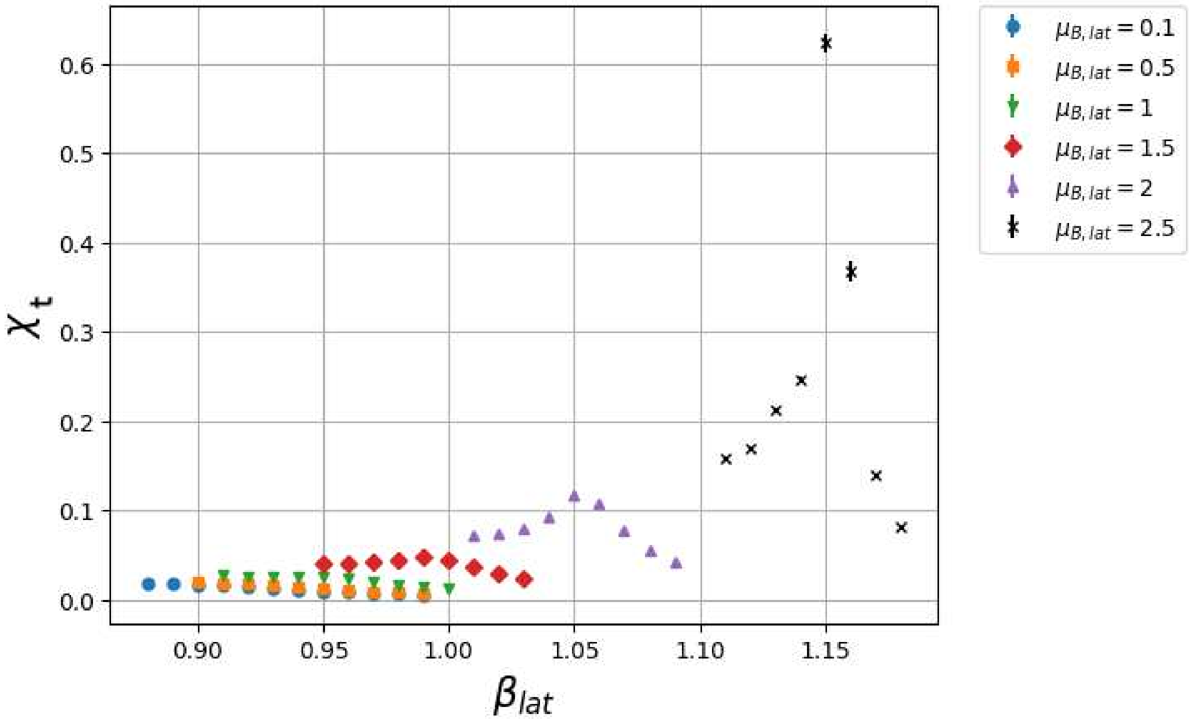
Peak most pronounced at $\mu_{B,\rm lat} \geq 1$, supports $2^{\rm nd}$ order.



Peak of $\chi_{\rm m}$ moves with V, extrapolation to $\beta_{\rm c}$ consistent with other criteria.

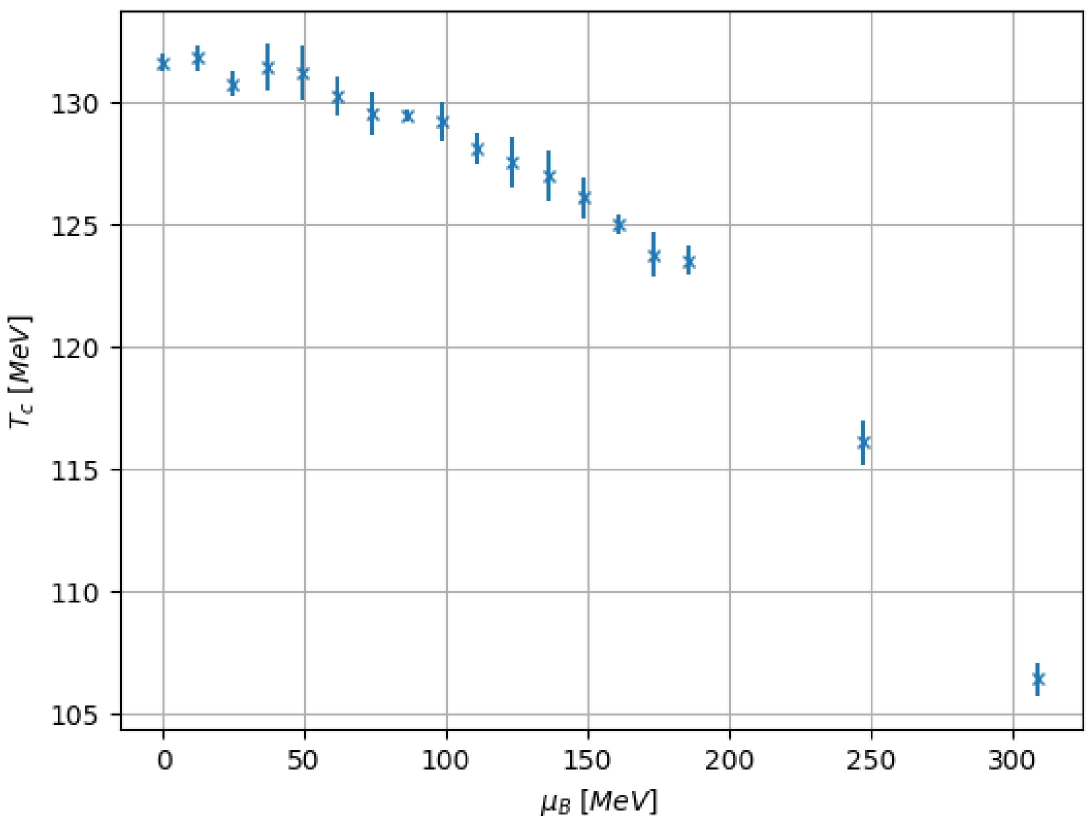
$2^{\rm nd}$ order: (peak height) $\propto L^{\gamma/\nu}$, $\frac{\gamma}{\nu}(\mu_{B,\rm lat}) \in [1.7 \dots 2.1]$
at $\mu_B = 0$ compatible with 1.970 [Engels/Fromme/Seniuch, '03]

Strongly supports $2^{\rm nd}$ order.



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

Peak most pronounced at $\mu_{B,\mathrm{lat}} \geq 1.5$, supports 2$^{\mathrm{nd}}$ order, consistent with previous determinations of β_c. Defines critical exponent x, $\chi_t(T_c) \propto L^{x/\nu}$, $e.g.$ $\frac{x}{\nu}|_{\mu_{B,\mathrm{lat}}=0} \simeq 0.2$, $\frac{x}{\nu}|_{\mu_{B,\mathrm{lat}}=1} \simeq 0.3$



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

Estimate of physical units

$$\begin{aligned} \beta_{\mathrm{c,lat}} &\simeq 0.9359 \;, \quad T_{\mathrm{x}} \simeq 155 \text{ MeV} \\ h &= h_{\mathrm{lat}} \frac{\beta_{\mathrm{c,lat}}^4}{\beta_{\mathrm{x}}^4} = h_{\mathrm{lat}} \, (145 \text{ MeV})^4 \end{aligned}$$

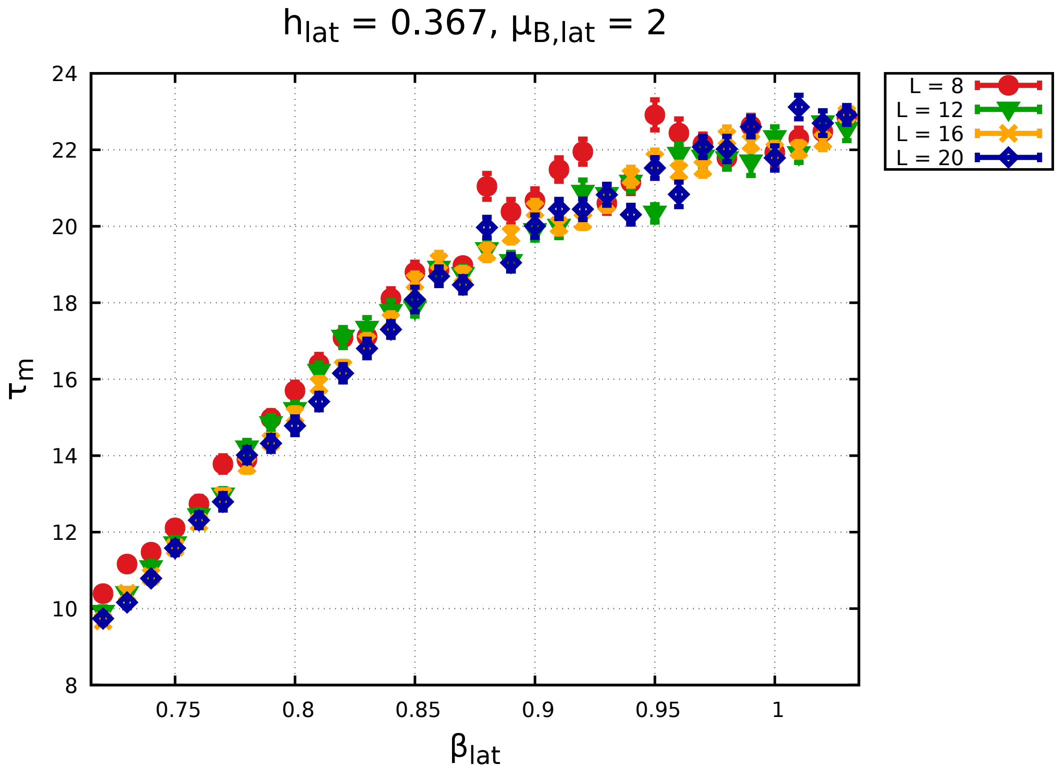
$\beta_{\mathrm{x,lat}} \approx 0.87$ ambiguous, see below.

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

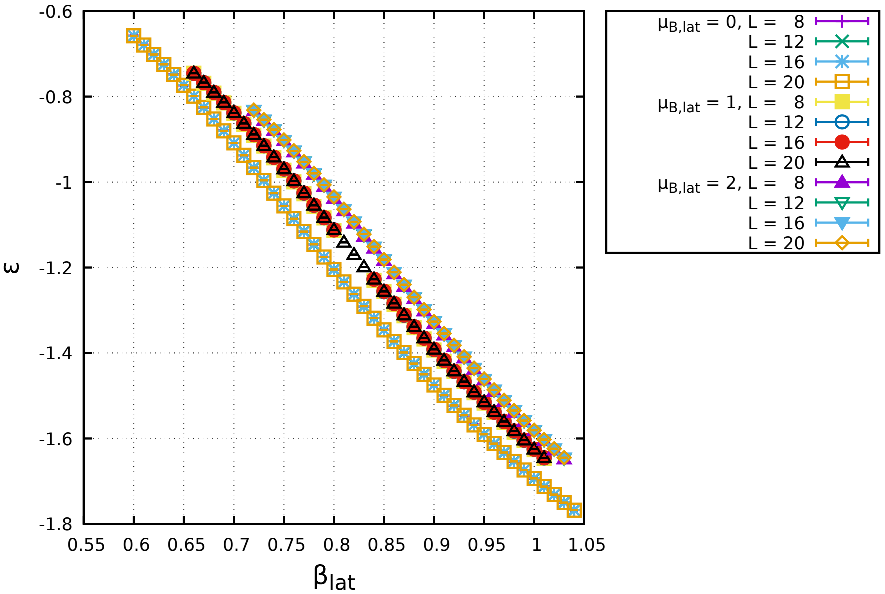
$$h = m_q \Sigma \stackrel{!}{=} F_\pi^2 \, M_\pi^2 \simeq (92.4 \text{ MeV})^2 \; (138 \text{ MeV})^2 \;\Rightarrow\; h_{\mathrm{lat}} = 0.367$$

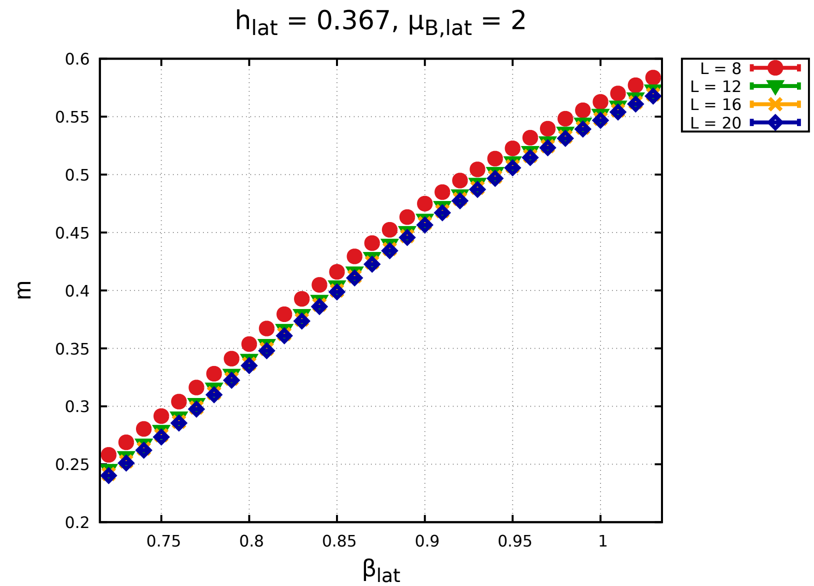
Inclusion by *modifying the cluster flip probability, directly or via global "ghost field".*

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 $\tau_{\rm m}$



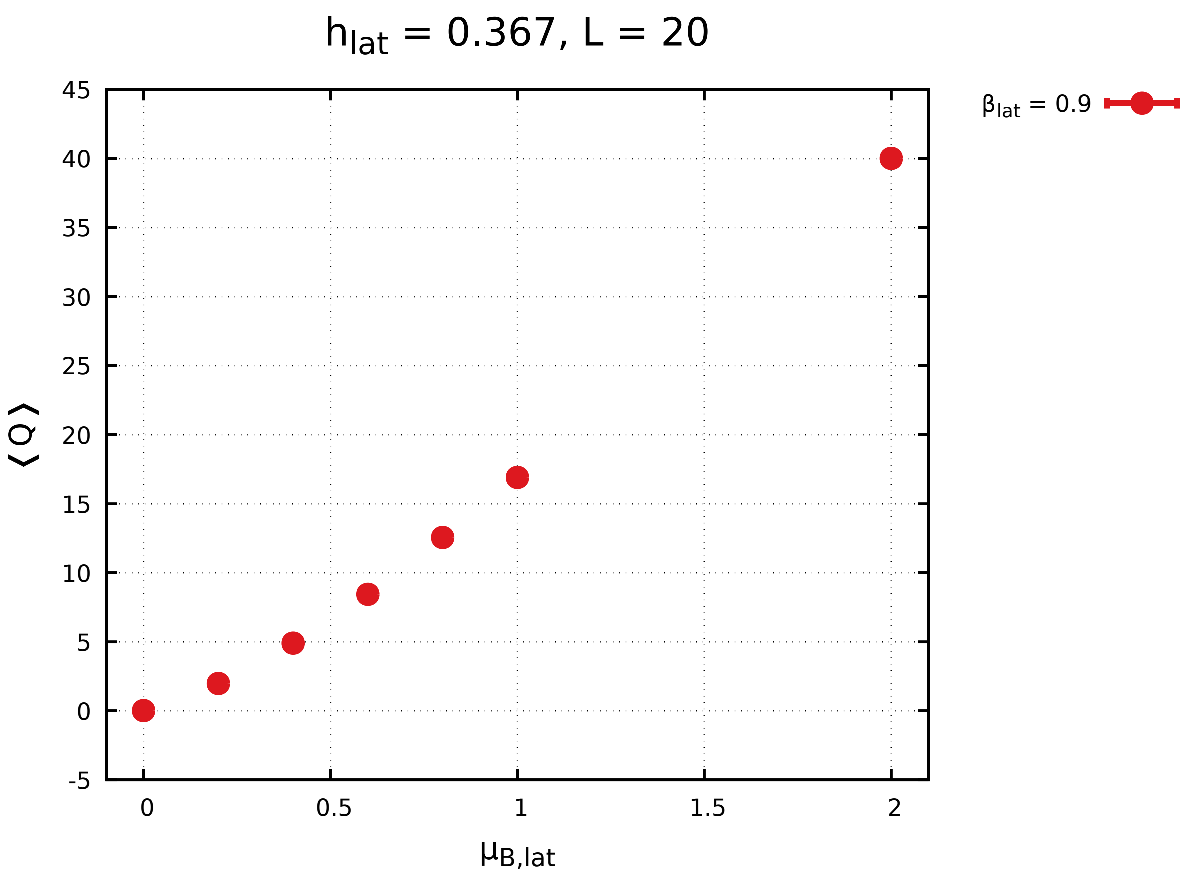


Left: Energy density $\epsilon = \langle H \rangle / V$ hardly depends on L. Shift for $\mu_{B,\mathrm{lat}} = 0,\ 1,\ 2.$

Right: Magnetization density $m = \langle |\vec{M}| \rangle / V$ at $\mu_{B,\mathrm{lat}} = 2.$ Modest finite-size effects.

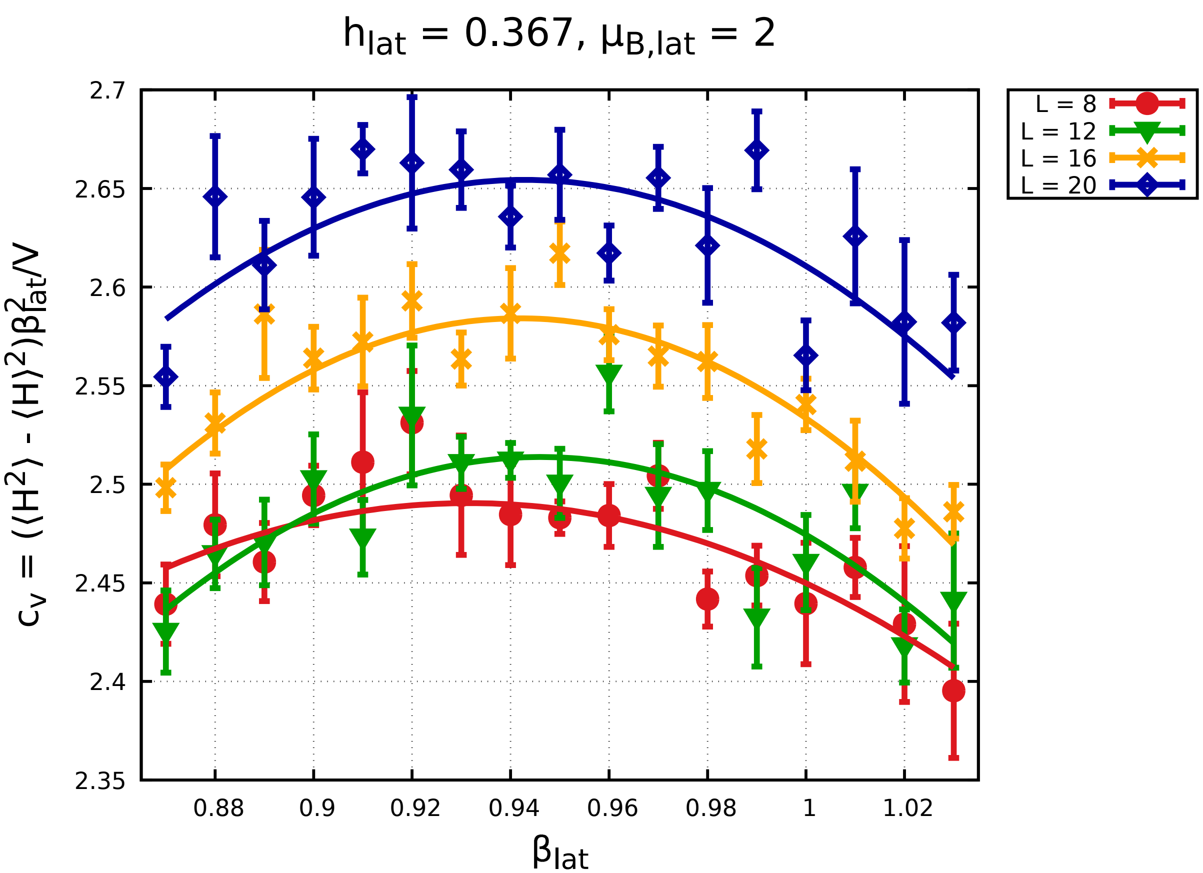
No interval of extraordinary slope (as L grows):

2^{nd} order phase transition smeared out to a crossover.



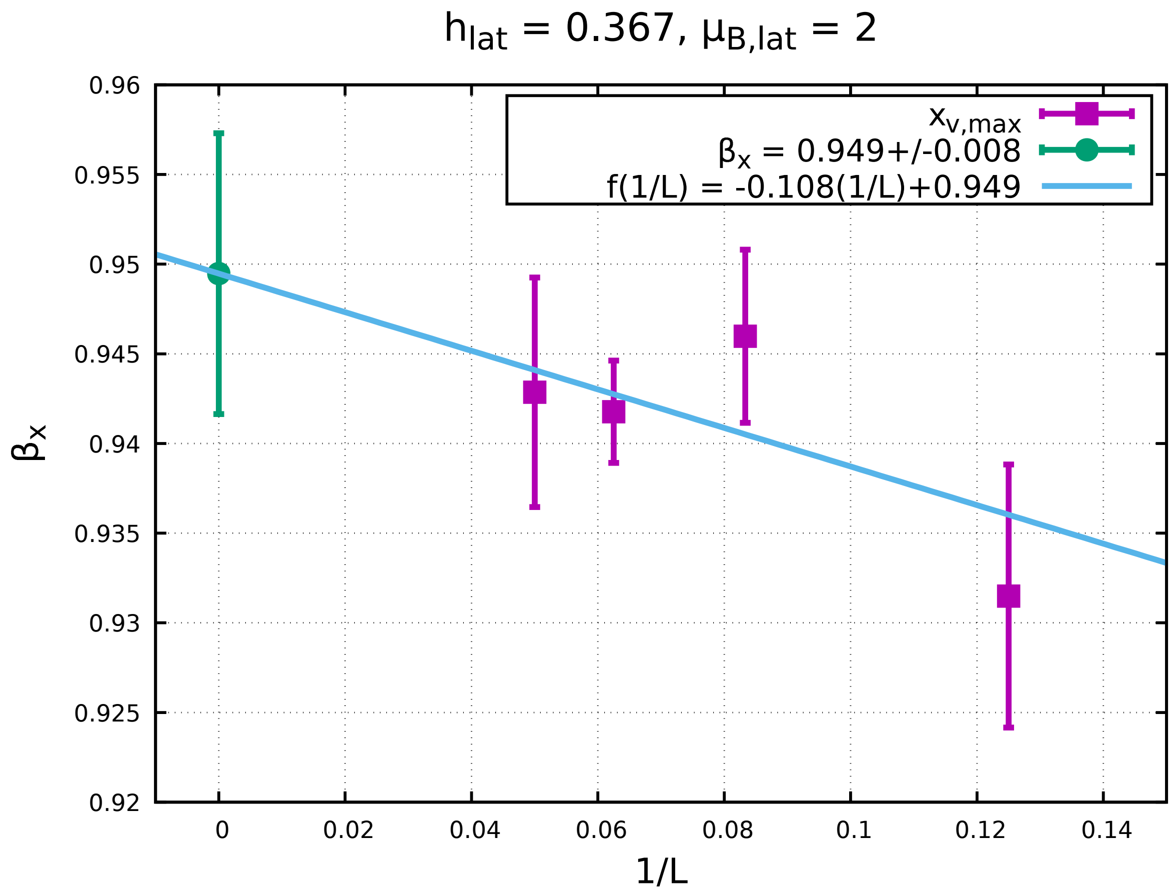
$\langle Q \rangle$ at $\beta_{\rm lat} = 0.9,\ L = 20.$

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



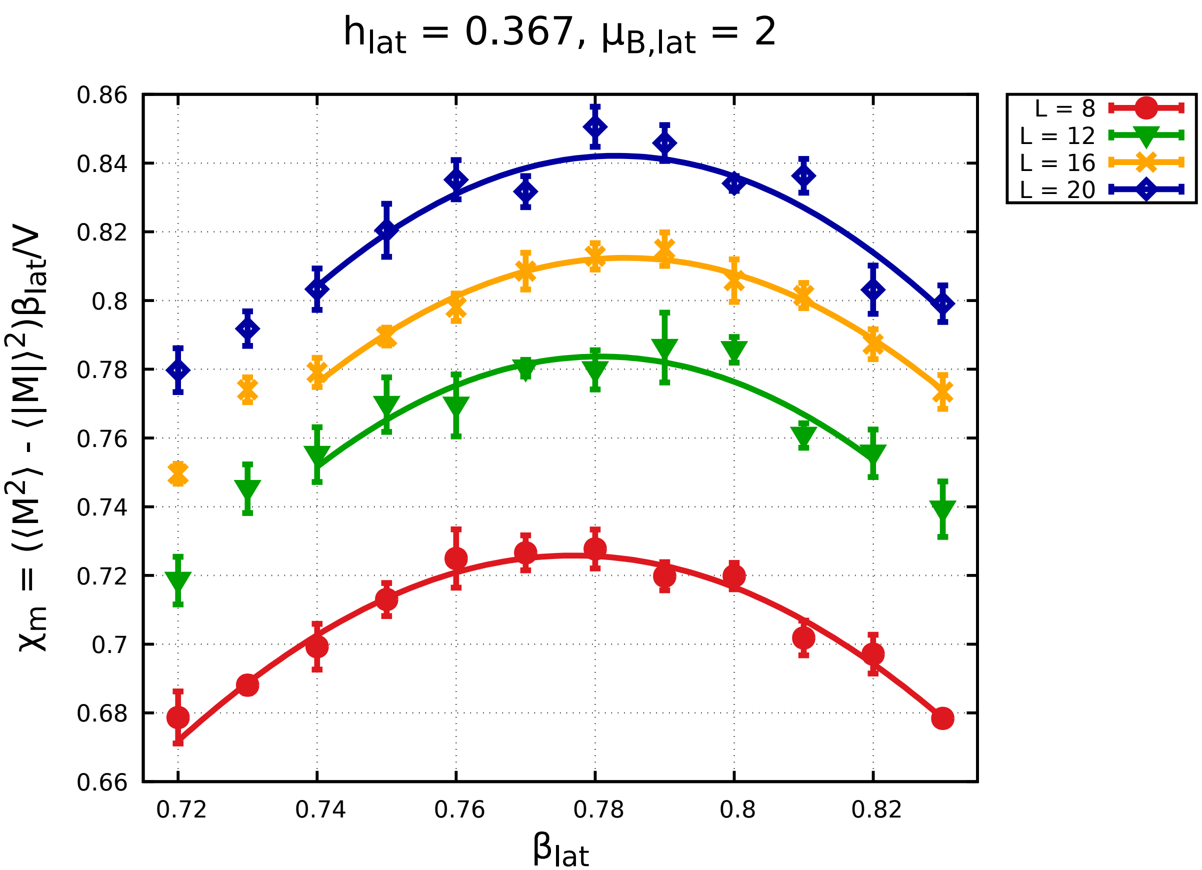
Specific heat c_V

Peak washed out by mass term; located by Gaussian fits

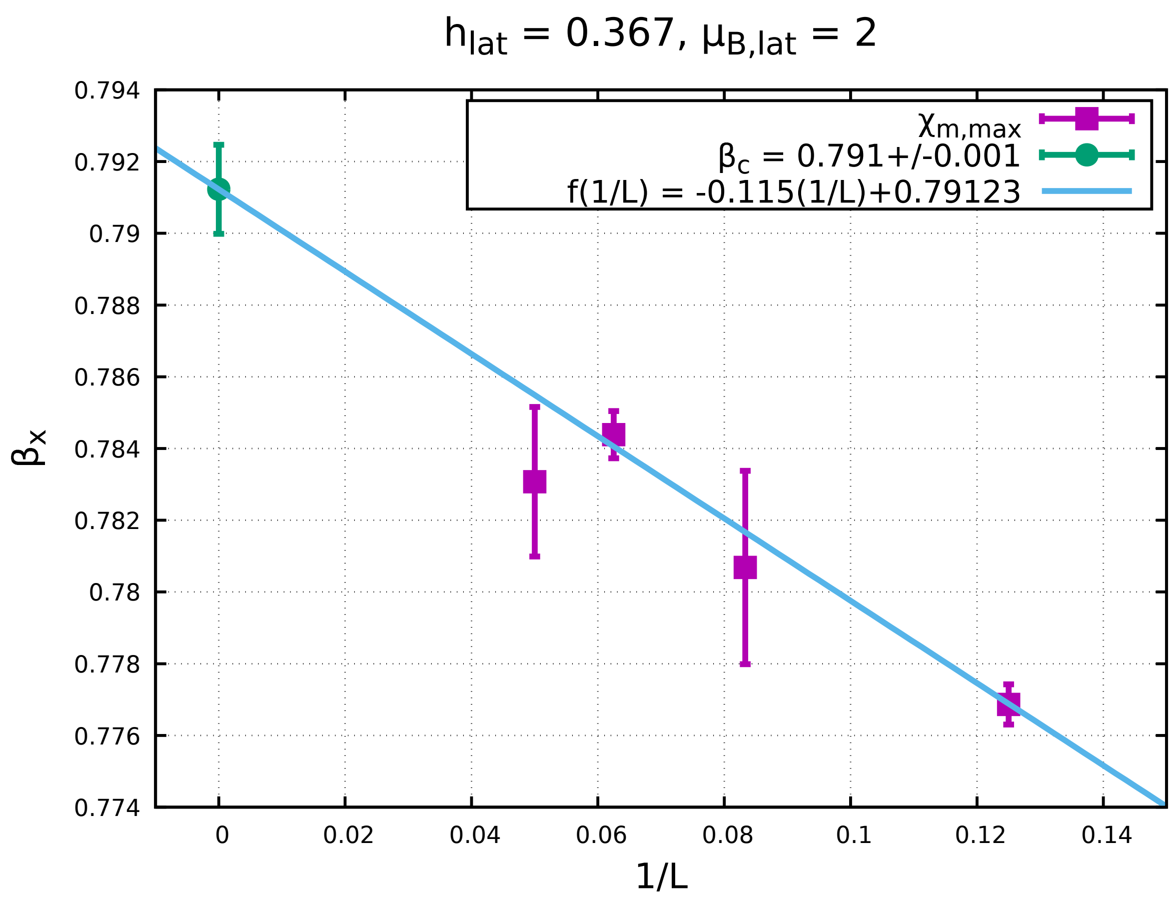


Large-L extrapolation of c_V peak locations $\rightarrow \beta_{\mathrm{x,lat}}$

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

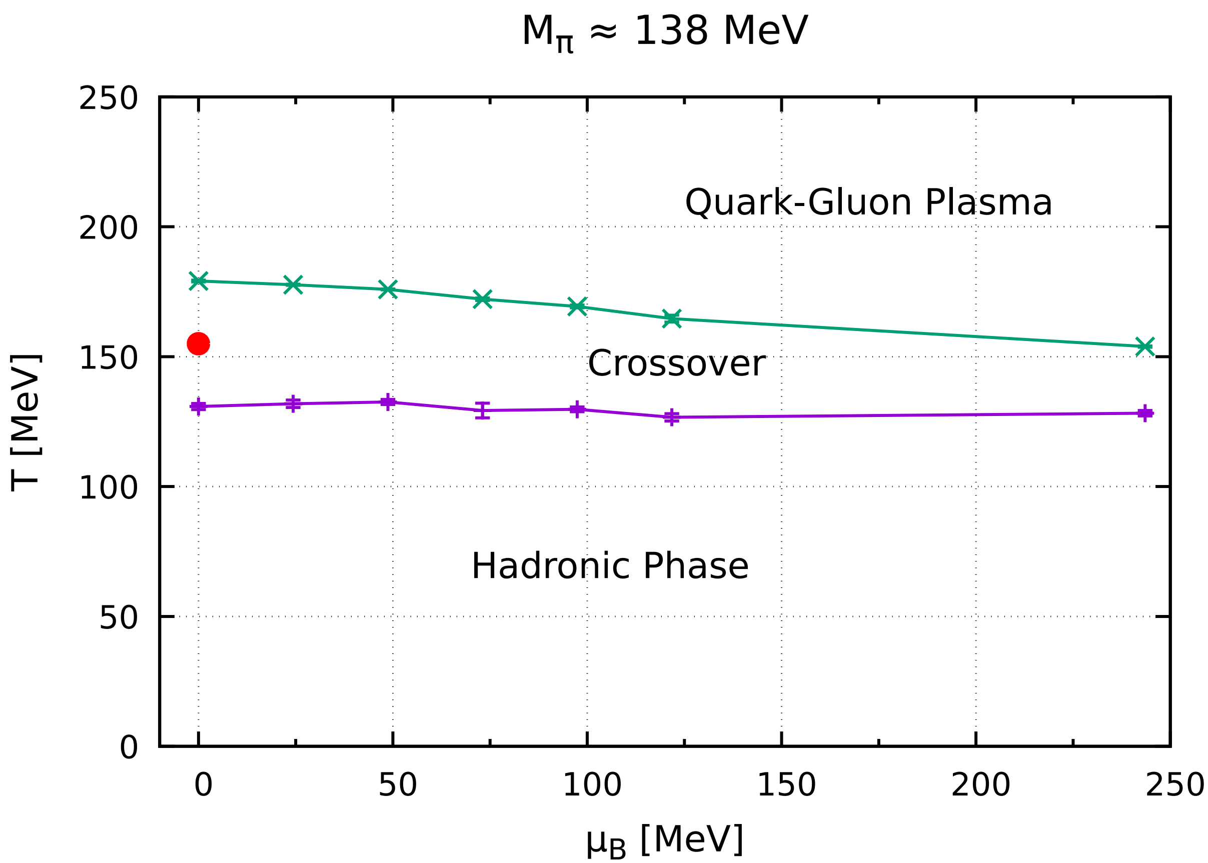


Magnetic susceptibility $\chi_{\rm m}$ at $\mu_{B,\rm lat} = 2$. Again: peak washed out, localized by Gaussian fits. Another criterion to search $\beta_{\rm x}$.



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

Below values obtained from c_V; typical for a crossover.



Phase diagram at finite quark mass: broad crossover region; $T_{\rm x}$ hardly decreases up to $\mu_B = 244$ 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.

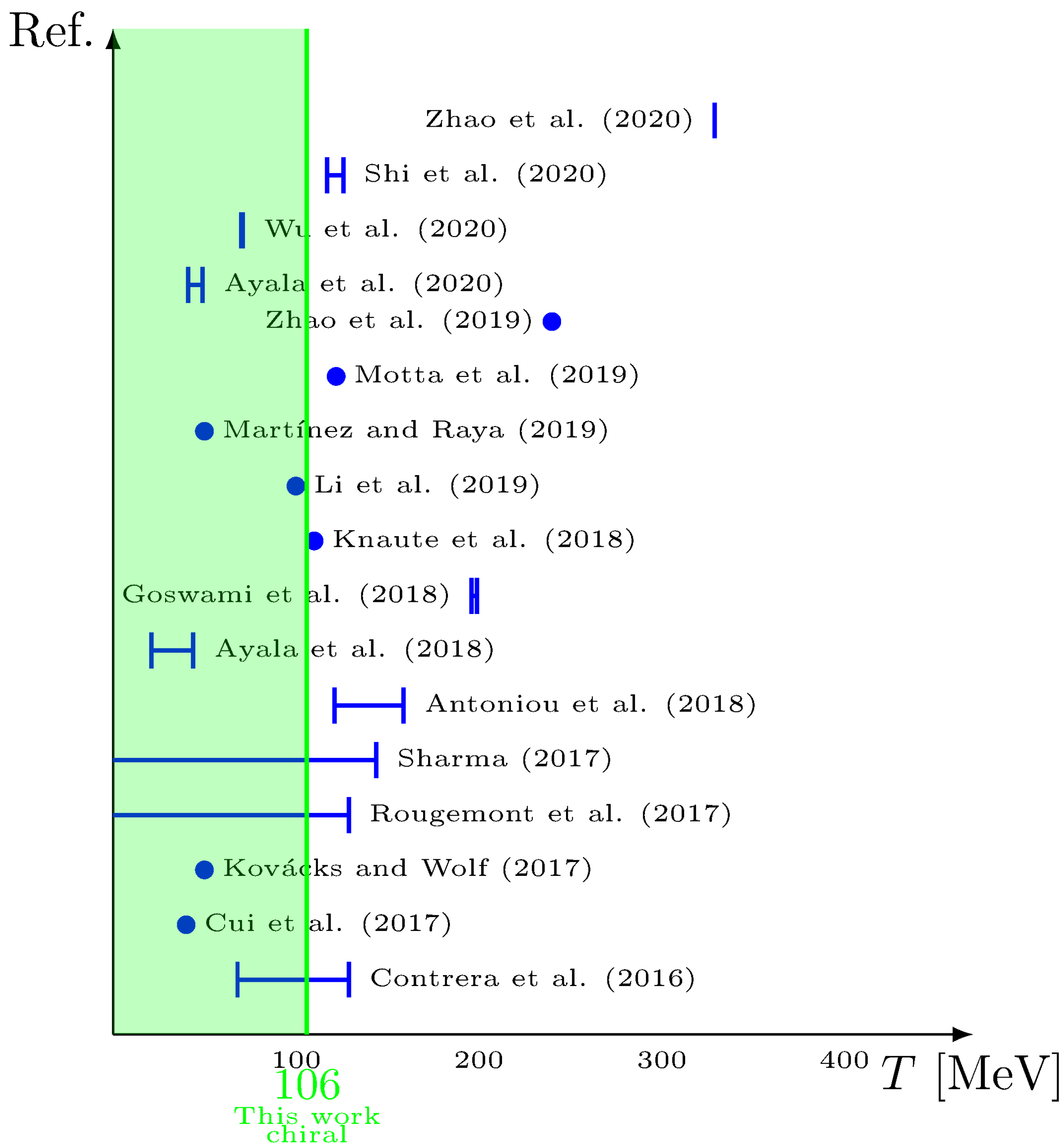
High-T dimensional reduction to 3d O(4) leads to topological charge, identified with the baryon number.

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 244 MeV again no CEP.

[Thanks to Tamer Boz, Arturo Fernández, Miguel Nava, Uwe-Jens Wiese]


Ref.
Zhao et al. (2020)
Shi et al. (2020)
Wu et al. (2020)
Ayala et al. (2020)
Zhao et al. (2019)
Motta et al. (2019)
Martínez and Raya (2019)
Li et al. (2019)
Knaute et al. (2018)
Goswami et al. (2018)
Ayala et al. (2018)
Antoniou et al. (2018)
Sharma (2017)
Rougemont et al. (2017)
Kovács and Wolf (2017)
Cui et al. (2017)
Contrera et al. (2016)
100
200
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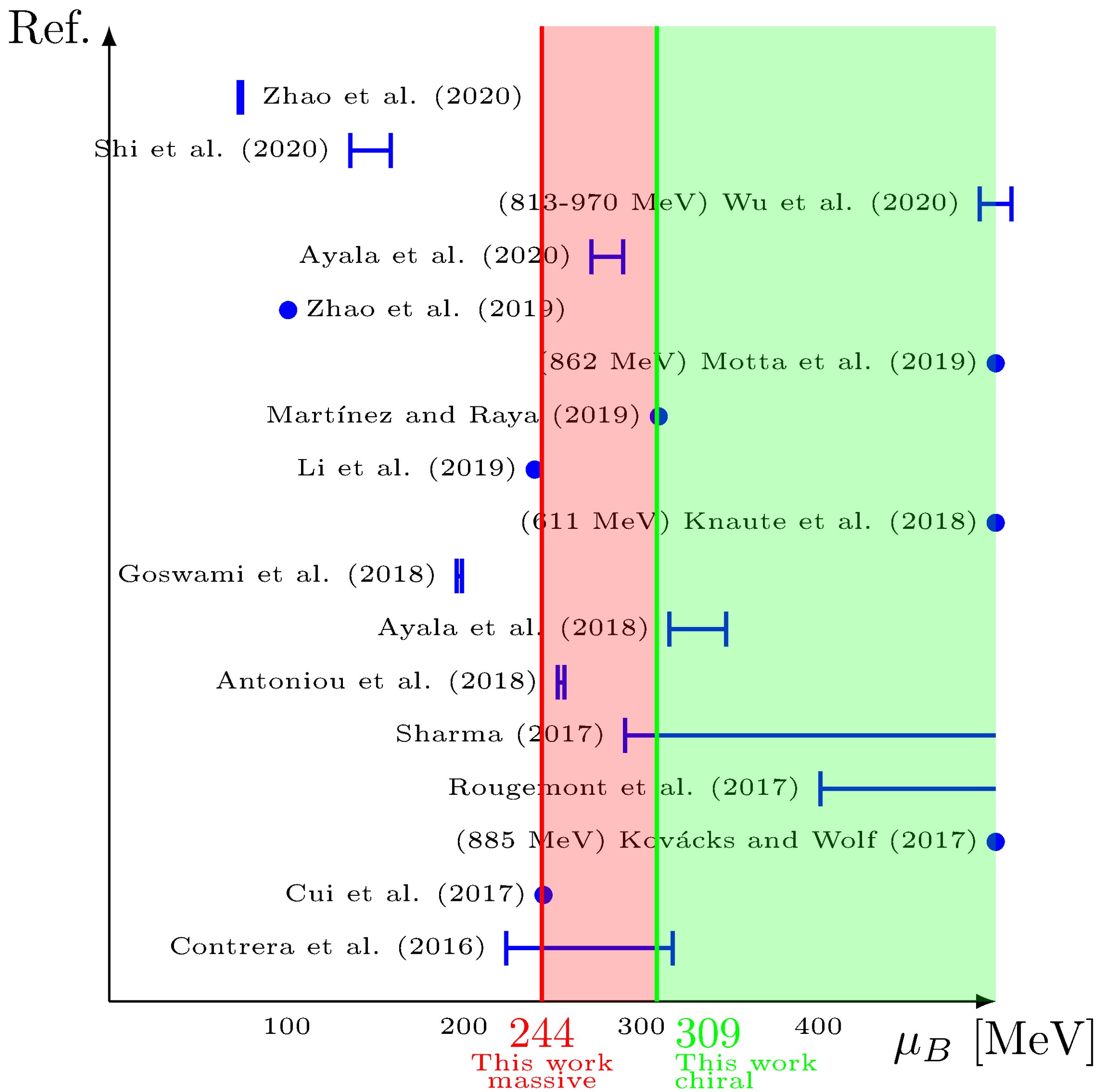
T [MeV]
106
This work
chiral



Ref.
Zhao et al. (2020)
Shi et al. (2020)
(813-970 MeV) Wu et al. (2020)
Ayala et al. (2020)
Zhao et al. (2019)
(862 MeV) Motta et al. (2019)
Martínez and Raya (2019)
Li et al. (2019)
(611 MeV) Knaute et al. (2018)
Goswami et al. (2018)
Ayala et al. (2018)
Antoniou et al. (2018)
Sharma (2017)
Rougemont et al. (2017)
(885 MeV) Kovácks and Wolf (2017)
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