Continuum limit of generalized charm susceptibilities at finite temperature

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Scale setting: Precision lattice QCD for particle and nuclear physics at ECT*, Trento, Italy

(Work done as part of the HotQCD Collaboration)

Motivation

- Generalized charm susceptibilities are useful to understand the charm thermodynamics.

$$\chi_{\mathrm{klmn}}^{\mathrm{BQSC}} = \frac{\partial^{(\mathrm{k+l+m+n})} \left[\mathrm{P}\left(\hat{\mu}_{\mathrm{B}}, \hat{\mu}_{\mathrm{Q}}, \hat{\mu}_{\mathrm{S}}, \hat{\mu}_{\mathrm{C}}\right)/\mathrm{T}^4\right]}{\partial\hat{\mu}_{\mathrm{B}}^{\mathrm{k}}\ \partial\hat{\mu}_{\mathrm{Q}}^{\mathrm{l}}\ \partial\hat{\mu}_{\mathrm{S}}^{\mathrm{m}}\ \partial\hat{\mu}_{\mathrm{C}}^{\mathrm{n}}}\Bigg|_{\vec{\mu}=0}$$

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PLB 850 (2024) 138520, arxiv:2312.12857

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- Have been used to establish chiral crossover as the onset of charmed hadron melting and appearance of charm quarks as new degrees of freedom, persistence of charmed hadrons in QGP.
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- Can be used to quantify the contribution of experimentally unobserved charmed hadrons to the partial charm pressure. arxiv:2501.01300

What do we calculate on lattice?

- Partition function of QCD with 2 light, 1 strange and 1 charm quark flavors is :

$$\mathcal{Z} = \int \mathcal{D}[\mathrm{U}]\{\det\ \mathrm{D}(\mathrm{m_l})\}^{2/4}\{\det\ \mathrm{D}(\mathrm{m_s})\}^{1/4}\{\det\ \mathrm{D}(\mathrm{m_c})\}^{1/4}\mathrm{e}^{-\mathrm{S_g}}.$$

  This can be used to calculate susceptibilities in the BQSC basis.
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- First derivative w.r.t μ_i will be $\left\langle \text{ Tr } \left(\mathrm{D}(\mathrm{m_i})^{-1}\frac{\partial \mathrm{D}(\mathrm{m_i})}{\partial \mu_\mathrm{i}}\right)\right\rangle$.

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- We used 500 random vectors to do unbiased stochastic estimation:

$$\langle \eta_\mathrm{i} \rangle = \lim_{\mathrm{N_s} \to \infty} \frac{1}{\mathrm{N_S}} \sum_{\mathrm{k=1}}^{\mathrm{N_S}} \eta_\mathrm{ki} = 0 \ , \quad (1)$$

$$\langle \eta_\mathrm{i} \eta_\mathrm{j} \rangle = \lim_{\mathrm{N_s} \to \infty} \frac{1}{\mathrm{N_S}} \sum_{\mathrm{k=1}}^{\mathrm{N_S}} \eta^*_\mathrm{ki} \eta_\mathrm{kj} = \delta_\mathrm{ij} \quad (2)$$

$$\text{Tr} \ (\mathrm{D(m_i)^{-1}}) = \frac{1}{\mathrm{N}} \sum_{\mathrm{k=1}}^{\mathrm{N}} \eta^\dagger_\mathrm{k} \underbrace{\mathrm{D(m_i)^{-1}} \eta_\mathrm{k}}_{\mathrm{x}} \ . \quad (3)$$

History of the lattice setup

- We used (2+1)-flavor HotQCD configurations generated using HISQ action and a Symanzik-improved gauge action for $\mathrm{m_s/m_l} = 27$ and $\mathrm{N}_\tau = 8, 12$ and 16. We treated charm sector in the quenched approximation.

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- The temperature is set using f_K.

$$af_K(\beta) = \left[\frac{c_0^K f(\beta) + \frac{10}{\beta} c_2^K f^3(\beta)}{1 + \frac{10}{\beta} d_2^K f^2(\beta)} \right], \quad (4)$$

with $c_0^K = 7486(25)$, $c_2^K = 41935(2247)$, $d_2^K = 3273(224)$.
Here, $f(\beta)$ is the 2-loop QCD beta function,
$f(\beta) = \left(\frac{10b_0}{\beta} \right)^{-b_1/2b_0^2} \exp\left(-\beta/(20b_0)\right)$, with b_0 and b_1 being its 1-loop perturbative expansion coefficients in 3-flavor QCD.

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- $T = (a N_\tau)^{-1} \implies$ three lattice spacings at a fixed temperature.

History of the lattice setup

- Strange quark mass was (mis)tuned by keeping the mass of fictitious pseudoscalar meson, $\eta_{s\bar{s}}$, fixed to 695 MeV (not 686 MeV). Conversion to MeV was done $r_1 \implies$ strange quark mass is 2.6% larger than its physical value. A. Bazavov et al, arXiv:1111.1710

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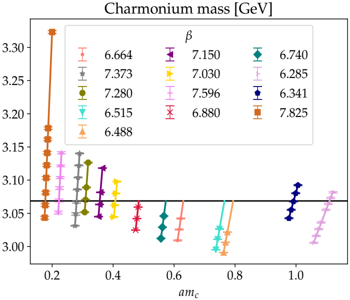
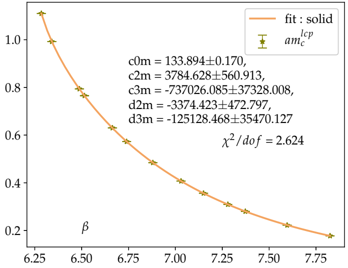
- However for finer lattices corresponding to $\beta > 7.03$, the resulting lattice mass of $\eta_{s\bar{s}}$ is larger than 695 MeV by about 3.5%. This drift from 695 MeV was further corrected by using lowest order χPT such that $M^2_{\eta_{s\bar{s}}} \propto m_s$ but the configuration generation did not take into account this corrected version of LCP. A. Bazavov et al, arXiv:1407.6387

Also discussed by Johannes H. Weber on Monday

Tuning charm quark mass on LCP[a]

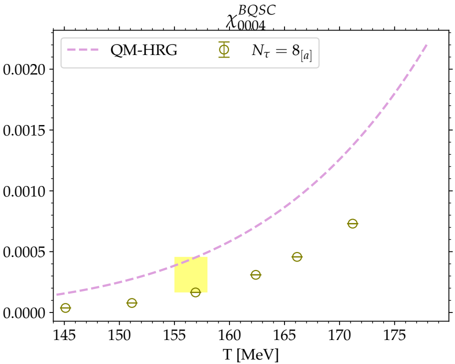




- We used spin-averaged charmonium to tune the bare charm quark at zero temperature.
- We used f_K to convert charmonium mass to physical units.
- The figure on the right fits an RG-inspired ansatz to the intersections of the colored lines and the black line (PDG value) in the left figure.

S.Sharma, arxiv:2212.11148

Quartic charm susceptibility



At T_{pc}, the physical expectation for χ_4^C, based on HRG, is roughly 2.7 times the result obtained for $N_\tau = 8$ ($\mathrm{a} \approx 0.16$ fm) on LCP$_{[a]}$ at the chiral crossover.

Different LCP prescriptions

- In the HRG phase, each charmed hadron contributes as $\left(\frac{m_i}{T}\right)^2 e^{-m_i/T}\ [1+\mathbb{O}((m_i/T)^{-1})]\mathsf{cosh}(B_i\hat{\mu}_B+Q_i\hat{\mu}_Q+S_i\hat{\mu}_S+C_i\hat{\mu}_C)$.

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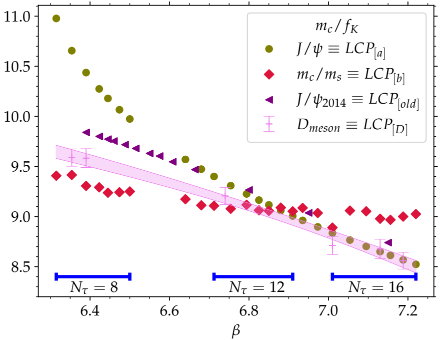
- This also holds true in the QGP phase where charm quarks and charmed hadrons coexist. arxiv:2312.12857
- We removed order $(am_c)^4$ tree level lattice artifacts by adding the so-called epsilon-term, which leads to sub-percent errors in observables linked to charm at $am_c \approx 0.5$ or $a \approx 0.08$ fm. [[HPQCD, UKQCD],2006]

Major source of cutoff effects



- In order to understand the cutoff effects, we investigated the sensitivity of χ_4^C to four different LCP prescriptions used to tune am_c values: LCP$_{[b]}$ fixes $m_c/m_s = 11.76$, LCP$_{[D]}$ is defined by the physical D-meson mass, LCP$_{[old]}$ is also defined by the charmonium mass A. Bazavov et al, arXiv:1404.4043

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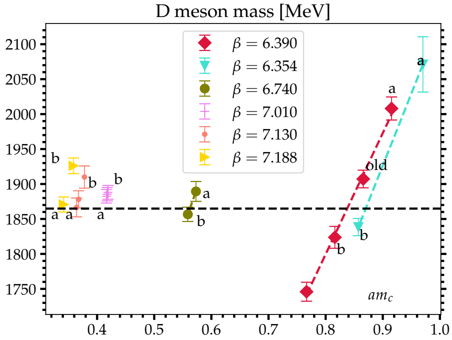
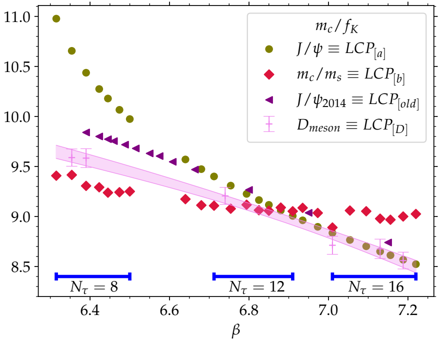


- The difference between mass of the most thermodynamicaly dominant hadron, i.e., D-meson, calculated on $\mathrm{LCP}_{[a]}$ and its physical value is less than 2% only for $\beta > 6.74$ (finer lattices).

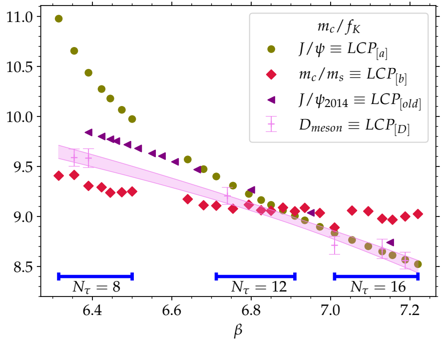
Bare charm quark mass on $\mathrm{LCP}_{[D]}$



$$am_c(\beta) = af_K(\beta)\frac{M_c^{\mathrm{RGI}}}{f_K}\left(\frac{20b_0}{\beta}\right)^{\frac{4}{9}}\left[\frac{1+\frac{10}{\beta}m_{1c}f^2(\beta)}{1+\frac{10}{\beta}dm_{1c}f^2(\beta)}\right],$$

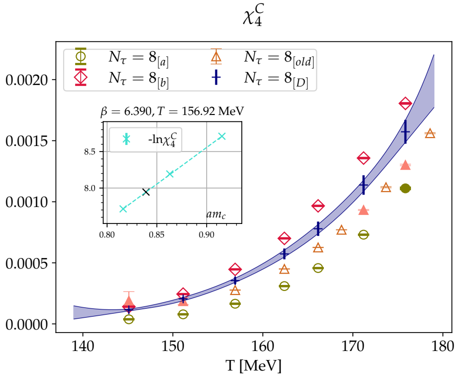
$M_c^{\mathrm{RGI}} = 1.528$ GeV, $f_K = (155.7/\sqrt{2})$ MeV FLAG 2024,
$m_{1c} = 140585.579 \pm 16567.799, dm_{1c} = 92506.328 \pm 11434.443,\ \chi^2/dof = 0.414$

Cutoff effects for different LCPs



- Cutoff effects dependent on am_c are smaller on $\mathrm{LCP}_{[D]}$ in comparison to $\mathrm{LCP}_{[a]}$ for smaller β.
- Both $\mathrm{LCP}_{[D]}$ and $\mathrm{LCP}_{[a]}$ converge in the continuum limit.
- Mistuning of am_s reflects in am_c on $\mathrm{LCP}_{[b]}$ for larger beta.

Interpolating quartic susceptibility in am_c at $N_\tau = 8$



- χ_n^C is a proxy of partial charm pressure, and at a given T, receives dominant contribution from the lightest charmed state, whose Boltzmann weight is $\propto e^{-am_c/aN_\tau}$.

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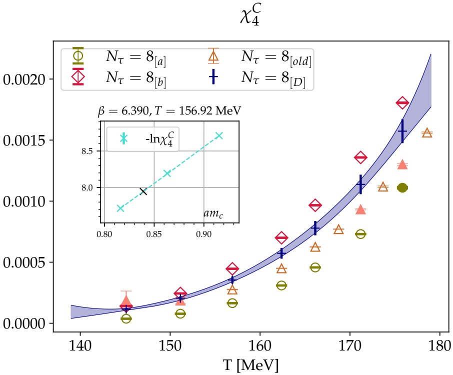

- At each T, linear interpolation of $-\ln\chi_4^C$ in am_c gives χ_4^C on LCP$_{[D]}$ – blue plus markers which incorporate bootstrap error and error from uncertainity of am_c on LCP$_{[D]}$.

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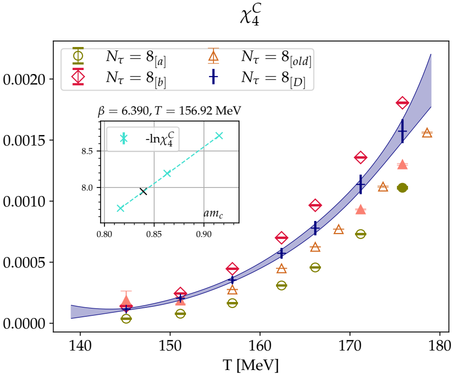
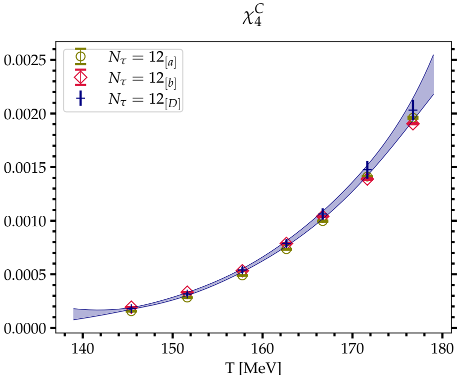


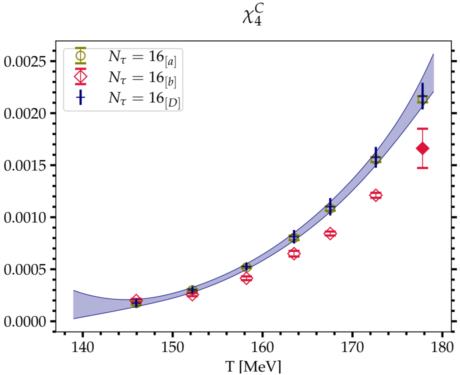
- At each T, linear interpolation of $-\ln \chi_4^C$ in am_c gives χ_4^C on LCP$_{[D]}$ – blue plus markers which incorporate bootstrap error and error from uncertainity of am_c on LCP$_{[D]}$.
- Blue band is a [2,2] Pade interpolation.

Interpolating quartic susceptibility in am_c at $N_\tau = 12$



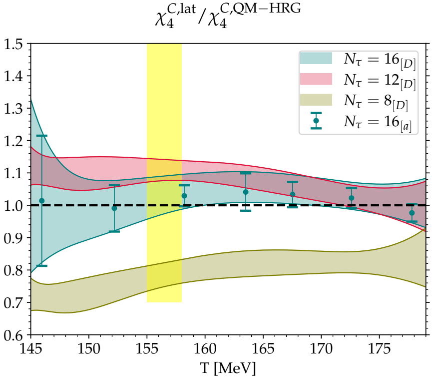
- Ordering of χ_4^C on different LCPs can a understood from the ordering of am_c values $\implies$ heavier the charmed state mass, smaller the thermodynamic contribution to the partial charm pressure.

Interpolating quartic susceptibility in am_c at $N_\tau = 16$



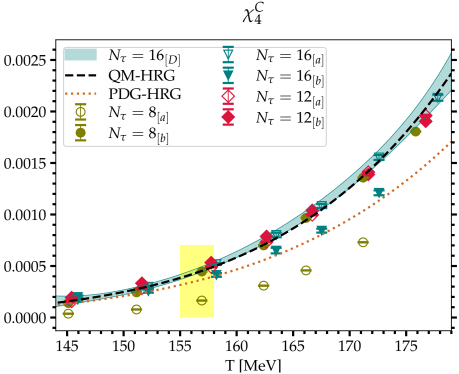
- $\text{LCP}_{[a]}$ is effectively $\text{LCP}_{[D]}$.
- mistuning of am_s also reflects in χ_4^C.

Continuum limit of quartic susceptibility



- LCP$_{[D]}$ bands for $N_\tau = 12$ and 16 overlap $\implies$ use $N_\tau = 16_{[D]}$ as the continuum estimate.

Continuum limit of quartic susceptibility



- Note: χ_4^C is not sensitive to the change in charm degrees of freedom and agreement with QM-HRG above chiral crossover is accidental.

For more details: PLB 850 (2024) 138520, arxiv:2312.12857

Statistics details

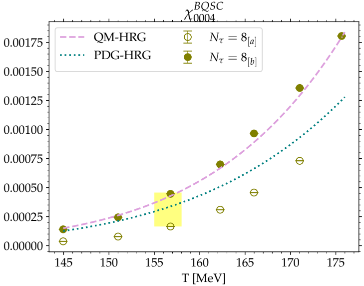
			LCP[a]		LCP[b]	
N_τ	β	T[MeV]	am_c	statistics	am_c	statistics
8	6.315	145.1	1.04112	449,689	0.892231	448,894
8	6.354	151.1	0.97025	519,953	0.857304	519,812
8	6.390	156.9	0.91534	406,878	0.816144	1,038,000
8	6.423	162.4	0.87069	661,254	0.787450	662,607
8	6.445	166.1	0.84320	505,573	0.765223	522,688
8	6.474	171.2	0.80920	229,013	0.742996	232,114
8	6.500	175.8	0.78059	–	0.723946	151,478
12	6.712	145.40	0.59316	49,589	0.574711	49,591
12	6.754	151.62	0.56328	43,367	0.549310	43,368
12	6.794	157.75	0.53656	50,352	0.530258	50,353
12	6.825	162.65	0.51694	58,547	0.511207	58,547
12	6.850	166.69	0.50176	36,801	0.498506	36,803
12	6.880	171.65	0.48426	36,076	0.485805	36,078
12	6.910	176.73	0.46751	39,079	0.469929	39,080

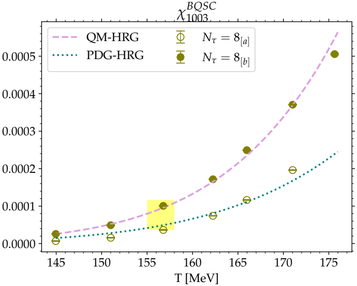
Statistics details

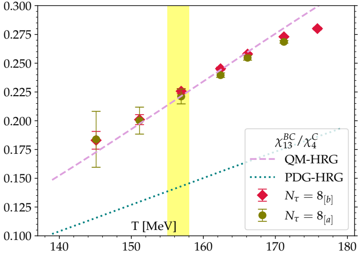
			$\text{LCP}_{[a]}$		$\text{LCP}_{[b]}$	
N_τ	β	T[MeV]	am_c	statistics	am_c	statistics
16	7.010	145.95	0.41657	13,546	0.419126	13,554
16	7.054	152.19	0.39631	13,391	0.409601	13,390
16	7.095	158.21	0.37849	14,050	0.393725	14,048
16	7.130	163.50	0.36405	6,779	0.377849	6,807
16	7.156	167.53	0.35375	7,282	0.368323	7,308
16	7.188	172.60	0.34155	7,192	0.358798	7,192
16	7.220	177.80	0.32985	3,515	0.349272	-

- Continuum limit of other charm susceptibilities?

Ratios calculated on different LCPs

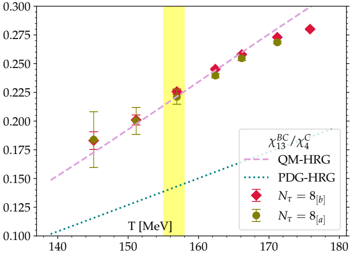


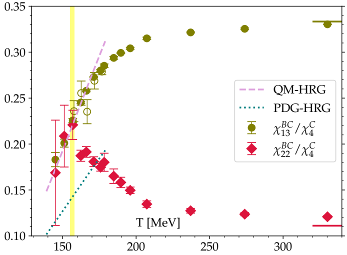




- Sensitivity to the choice of LCP cancels to a large extent in the ratios at a fixed N_τ.

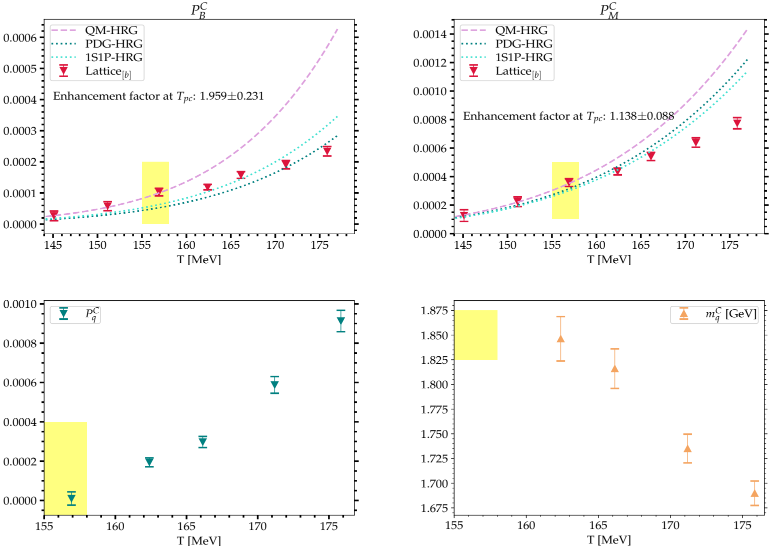
Ratios calculated using different N_τ values





- Right figure shows results for LCP$_{[b]}$. The solid symbols represent $N_\tau = 8$, and open symbols represent $N_\tau = 12$.
- Use $N_\tau = 8$ ratios and continuum χ_4^C to take the continuum limit of other charm susceptibilities.

Some continuum partial pressures



Conclusions and Summary

- Charm susceptibilities are sensitive to the choice of LCPs used to tune the bare charm quark mass.
- To reduce the cutoff effects for coarser lattices at finite temperature, choice of LCP should be motivated by the thermodynamics.
- For finer lattices, different LCPs converge.
- We quantified the cutoff effects arising due to bare charm quark mass in lattice observables at finite temperature.

Backup Slide: Hadron Resonance Gas (HRG) model

- HRG describes a non-interacting gas of hadron resonances. HRG has been found to be a good approximation to QCD results for $\mathrm{T} < \mathrm{T_{pc}}$.
- Charmed baryons and mesons contribute separately to the partition function of HRG, which in turn reflects in contributions to the pressure: $\mathrm{P_C}(\mathrm{T}, \overrightarrow{\mu})/\mathrm{T}^4 = \mathrm{M_C}(\mathrm{T}, \overrightarrow{\mu}) + \mathrm{B_C}(\mathrm{T}, \overrightarrow{\mu})$. [C. R. Allton et al., 2005]
- $$\mathrm{M_C}(\mathrm{T}, \overrightarrow{\mu}) = \frac{1}{2\pi^2} \sum_{\mathrm{i}} \mathrm{g_i} \left(\frac{\mathrm{m_i}}{\mathrm{T}}\right)^2 \mathrm{K_2}(\mathrm{m_i}/\mathrm{T}) \cosh(\mathrm{Q_i}\hat{\mu}_{\mathrm{Q}} + \mathrm{S_i}\hat{\mu}_{\mathrm{S}} + \mathrm{C_i}\hat{\mu}_{\mathrm{C}})$$

  [A. Bazavov et al., 2014]
- For Baryons the argument of $\cosh$ changes to
  $$\mathrm{B_i}\hat{\mu}_{\mathrm{B}} + \mathrm{Q_i}\hat{\mu}_{\mathrm{Q}} + \mathrm{S_i}\hat{\mu}_{\mathrm{S}} + \mathrm{C_i}\hat{\mu}_{\mathrm{C}}$$
- Boltzmann approximation is good in the charm sector not just for mesons and baryons but also for a charm-quark gas.
- $\hat{\mu}_{\mathrm{X}} = \mu/\mathrm{T}$, $\mathrm{X} \in \{\mathrm{B}, \mathrm{Q}, \mathrm{S}, \mathrm{C}\}$.

Backup slide:Generalized susceptibilities of the conserved charges

$$\mathrm{M_C(T, \vec{\mu}) = \frac{1}{2\pi^2} \sum_i g_i \left(\frac{m_i}{T}\right)^2 K_2(m_i/T) cosh(Q_i\hat{\mu}_Q + S_i\hat{\mu}_S + C_i\hat{\mu}_C)}$$

- Dimensionless generalized susceptibilities of the conserved charges using $\mathrm{P_C}$:

$$\chi^{\mathrm{BQSC}}_{\mathrm{klmn}} = \frac{1}{2\pi^2} \sum_{\mathrm{i \in C\text{-}H}} \mathrm{g_i} \left(\frac{\mathrm{m_i}}{\mathrm{T}}\right)^2 \mathrm{K_2(m_i/T)\ B^k Q^l S^m C^n}$$

- $\underbrace{\chi^{BC}_{mn}}_{\chi^{\mathrm{BQSC}}_{\mathrm{m00n}}} = \mathrm{B_{C,1} + 2^n B_{C,2} + 3^n B_{C,3} \simeq B_{C,1} = B_C, \forall (m+n) \in}$ even
- $\chi^{\mathrm{C}}_{\mathrm{m}} = \mathrm{P_C}, \forall \mathrm{m} \in$ even
- At present, we have gone upto fourth order in calculating various cumulants.

Backup slide: Intermediate T range

- Based on carrriers of C in low and high-T phase, pose a quasi-particle model consisting of non-interacting meson, baryon and quark-like states:

$$
\begin{aligned}
\mathrm{P_C}(\mathrm{T},\hat{\mu}_\mathrm{C},\hat{\mu}_\mathrm{B})/\mathrm{T}^4 = & \mathrm{P_M^C}(\mathrm{T})\cosh(\hat{\mu}_\mathrm{C}+...)+\mathrm{P_B^C}(\mathrm{T})\cosh(\hat{\mu}_\mathrm{C}+\hat{\mu}_\mathrm{B}+...) \\
& +\mathrm{P_q^C}(\mathrm{T})\cosh(\frac{2}{3}\hat{\mu}_\mathrm{Q}+\frac{1}{3}\hat{\mu}_\mathrm{B}+\hat{\mu}_\mathrm{C})
\end{aligned}
$$

[S. Mukherjee et al., 2016]

- Use quantum numbers B and C to construct partial pressures:

$$
\begin{aligned}
\mathrm{P_q^C} &= 9(\chi_{13}^{\mathrm{BC}}-\chi_{22}^{\mathrm{BC}})/2 \\
\mathrm{P_B^C} &= (3\chi_{22}^{\mathrm{BC}}-\chi_{13}^{\mathrm{BC}})/2 \\
\mathrm{P_M^C} &= \chi_4^{\mathrm{C}}+3\chi_{22}^{\mathrm{BC}}-4\chi_{13}^{\mathrm{BC}}
\end{aligned}
$$

  - Constraint on cumulants in a simple quasi-particle model:

$$\mathrm{c}=\chi_{13}^{\mathrm{BC}}+3\chi_{31}^{\mathrm{BC}}-4\chi_{22}^{\mathrm{BC}}=0$$