Spectral quantities in thermal QCD: a progress report

Gert Aarts

Swansea University
Prifysgol Abertawe

Spectral features

many questions have been/are being addressed

- hadronic phase: thermal broadening, mass shift
- QGP: deconfinement/dissolution/melting
- quarkonia survival as thermometer
- transport: conductivity/dileptons from vector current
- chiral symmetry restoration
- baryons, hyperons
- . . .

Lattice QCD

specific challenges for lattice QCD (at finite temperature)

- high precision
- dynamical quarks, $N_f = 2 + 1$
- inversion, from $G(\tau)$ to $\rho(\omega)$
- many time slices: anisotropic $\xi = a_s/a_\tau > 1$
- continuum limit, physical quark masses, large volume
- ...

Outline

- status report of FASTSUM collaboration
- outline of what we do/want/desire

new:

- towards physical light quarks
- $\mathcal{O}(\mu^2)$ corrections to mesonic correlators

everything is **preliminary**, time is scarce...

UKRI Centre for Doctoral Training in Artificial Intelligence, Machine Learning & Advanced Computing

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The **UKRI CDT in Artificial Intelligence, Machine Learning and Advanced Computing** provides 4-year, fully funded PhD opportunities across the broad areas of particle physics and astronomy, biological and health, and mathematical and computer sciences. Training in AI, high-performance computing (HPC) and high-performance data analytics (HPDA) plays an essential role, as does engagement with external partners, which include large international companies, locally based start-ups and SMEs, and government and Research Council partners.

The CDT is built upon longstanding research and training collaborations between the universities of Aberystwyth, Bangor, Bristol, Cardiff and Swansea. In addition, Supercomputing Wales and the University Computing Academies provide bespoke support via Research Software Engineers and access to HPC facilities in a coordinated fashion.

Training

The programme consists of a substantial training component in the first year, including cohort-based training in AI and computational methods, to establish a common base. Engagement with our external partners is embedded throughout and includes short-term placements in Year 1 and 2 and a 6-month placement in Year 3/4. Transferable skills training is delivered via residential meetings, at our annual CDT conference, and in cooperation with the Alan Turing Institute. More details can be found on the Training page.

Research

Our doctoral training programme is constructed around three research themes:

- T1: data from large science facilities (particle physics, astronomy, cosmology)
- T2: biological, health and clinical sciences (medical imaging, electronic health records, bioinformatics)
- T3: novel mathematical, physical, and computer science approaches (data, hardware, software, algorithms)

While the themes are diverse as academic disciplines, in our CDT they are linked through the use of AI, machine learning and advanced computing methods. Therefore, a crucial role is played by knowledge exchange across themes via cohort training, joint supervision, peer-to-peer interaction and student mentoring. Research project are embedded within one of the themes, with supervisory support across themes, to develop new synergies. More details can be found on the Research page.

Fully funded PhD positions

Fully funded PhD positions are available for students with a strong interest and aptitude in computational science and in one of our research themes. Positions are funded for 4 years, including the placements with the external partners. The CDT will recruit 5 cohorts, with a minimum of 11 PhD students per cohort. The first cohort will start in October 2019. For details on how to apply, see the Applications page.

cdt-aimlac.org

FASTSUM

GA (Swansea)
Chris Allton (Swansea)
Simon Hands (Swansea)
Benjamin Jäger (Odense)
Seyong Kim (Sejong University)
Maria-Paola Lombardo (Firenze)
Sinead Ryan (Trinity College Dublin)
Jonivar Skullerud (Maynooth)
Liang-Kai Wu (Jiangsu)
Aleksandr Nikolaev (Swansea)
Tim Burns (Swansea)

Alan Kirby (Swansea)
Sam Offler (Swansea)
Dawid Stasiak (Swansea)
Sergio Chaves (Swansea)

Jonas Glesaaen (Swansea->)
Davide de Boni (Swansea->)
Tim Harris (TCD->Mainz->Milan)
Ale Amato (Swansea->Helsinki->)
Wynne Evans (Swansea->Bern->)
Pietro Giudice (Swansea->Münster->)
Aoife Kelly (Maynooth->)
Bugra Oktay (Utah->)
Kristi Praki (Swansea->)
Don Sinclair (Argonne)

Ensembles

anisotropic lattices, towards continuum limit with physical quarks

1. continuum time limit $a_\tau \to 0$, a_s fixed, $\xi = a_s/a_\tau \to \infty$
2. continuum limit, $a_s, a_\tau \to 0$, $\xi = a_s/a_\tau$ fixed
3. physical quarks, $m_q \to m_{ud}$, m_s physical

current status:

- working on point 3, at fixed $a_\tau^{-1} \approx 6$ GeV and $\xi \approx 3.5$

these are Generation 2 ensembles

GA, Glesaaen, Jäger et al, Lattice 2018 [arXiv:1812.08151 [hep-lat]]

Ensembles

- $N_f = 2+1$ Wilson-clover fermions
  Symanzik-improved anisotropic gauge action with tree-level mean-field coefficients and a mean-field–improved Wilson clover fermion action with stout-smeared links
- tuning and ensembles at the lowest temperatures have been provided by HadSpec
- lattice details for the Generation 2 and 2L ensembles

	a_s [fm]	a_τ [fm]	a_τ^{-1} [GeV]	$\xi = a_s/a_\tau$	N_s	m_π [MeV]	$m_\pi L$
Gen 2	0.1227(8)	0.0350(2)	5.63(4)	3.5	24	384(4)	5.7
Gen 2L	0.1136(6)	0.0330(2)	5.997(34)	3.453(6)	32	236(2)	4.3

- fixed scale approach: vary temperature by varying N_τ

Ensembles

N_τ	128*	40	36	32	28	24	20	16
T [MeV]	44	141	156	176	201	235	281	352
T/T_c	0.24	0.76	0.84	0.95	1.09	1.27	1.52	1.90
N_{cfg}	139	501	501	1000	1001	1001	1000	1001

Gen 2 ensembles, lattice size $24^3 \times N_\tau$

N_τ	256*	128	64	56	48	40	36
T [MeV]	23	47	94	107	125	150	167
N_{cfg}	750	300	500	500	500	500	500
N_τ	32	28	24	20	16	12	8
T [MeV]	187	214	250	300	375	500	750
N_{cfg}	500	1000	1000	1000	1000	1000	1000

Gen 2L ensembles, lattice size $32^3 \times N_\tau$

the lower temperatures with $N_{\text{cfg}} = 500$ are currently upgraded to 1000

Observables

Gen 2:

- bottomonium
- conductivity/diffusion coefficient
- D mesons
- baryons/hyperons
- finite μ corrections (Liang-Kai Wu, Aleksandr Nikolaev – in progress)

- -

Gen 2L:

- bottomonium (Seyong Kim – in progress)
- mesons (Sergio Chaves – in progress)
- (charmed) baryons (Ben Jäger, Dawid Stasiak, Tim Burns – in progress)
- transport
- finite μ corrections
- ...

Outline

- comparing Gen 2 and Gen 2L: transition temperatures
- $\mathcal{O}(\mu^2)$ corrections to mesonic correlators

multi-year project, with essential contributions by

- Jonas Glesaaen (especially code development)
- Ben Jäger (especially code development, simulations)
- Liang-Kai Wu (simulations)
- Aleksandr Nikolaev (analysis, simulations, theory)
- . . .

code: modification of OpenQCD

J. Glesaaen & B. Jäger, openQCD-FASTSUM, doi.org/10.5281/zenodo.2216356

J. Glesaaen, openqcd-hadspec, doi.org/10.5281/zenodo.2217028

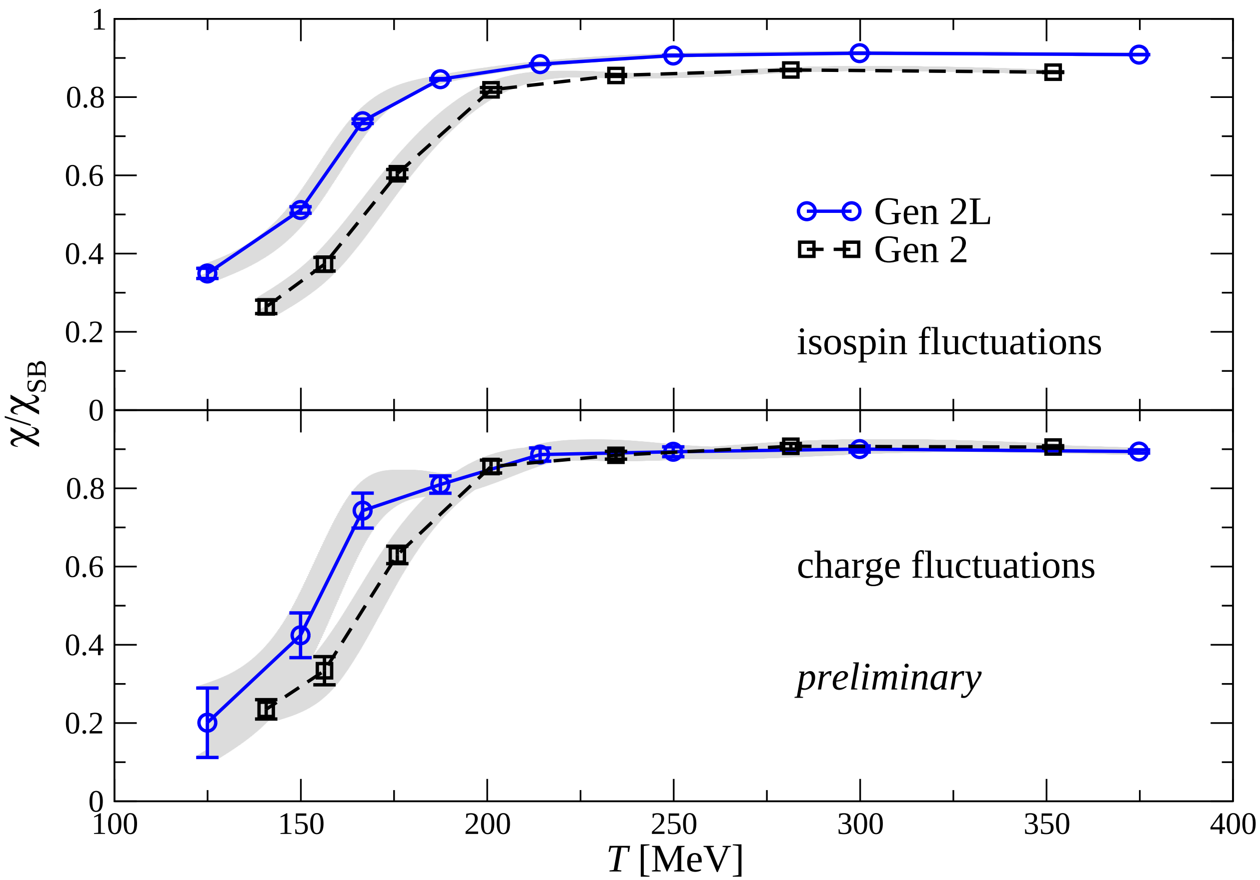
Towards physical pion mass

- most thermodynamic studies uses staggered fermions (Budapest-Wuppertal, Bielefeld-BNL, Hot QCD)
- Wilson fermions used less, more expensive
- some exceptions: WHOT QCD `Ejiri et al`
  tmfT (twisted mass) `Lombardo, Ilgenfritz et al`

hence a study of properties of the thermal crossover with Wilson fermion is still interesting

- transition temperature depends on observable
- T_c denotes pseudo-critical temperature for given observable
- expectation: shift of T_c's to lower values as m_π is reduced

Isospin and charge fluctuations



normalised with massless, lattice Stefan-Boltzmann result

shift of T_c : $T_{\text{infl}} \simeq 169$ MeV (Gen 2) $\simeq 155$ MeV (Gen 2L)

arXiv:1812.08151 [hep-lat]

Parity doubling in the baryon spectrum

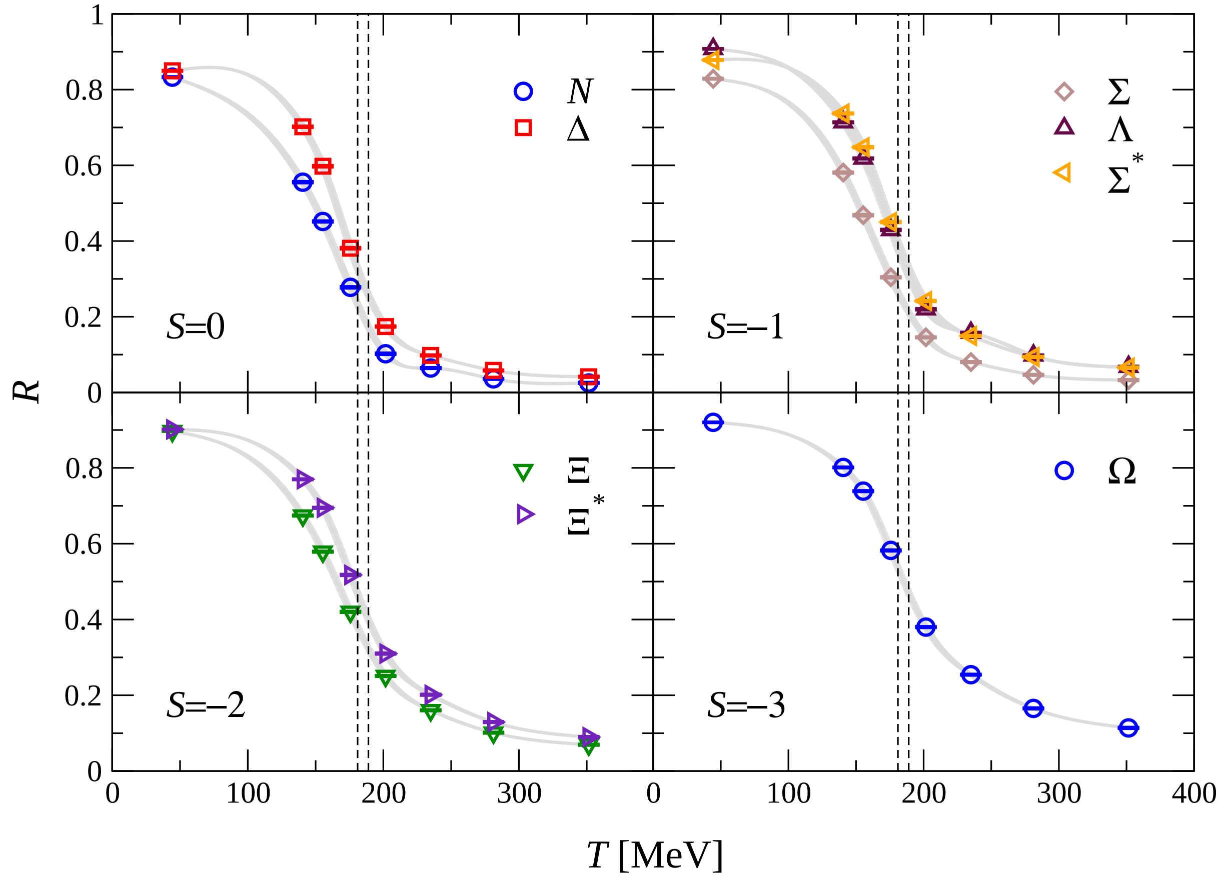
- chiral symmetry restoration: parity doubling
- positive and negative parity states become degenerate
- Gen 2: hyperons arXiv:1812.07393 [hep-lat]
- measure degeneracy directly in correlators

$$R(\tau) = \frac{G_+(\tau) - G_+(1/T - \tau)}{G_+(\tau) + G_+(1/T - \tau)},$$

- parity doubling: $G_+(\tau) = G_+(1/T - \tau) = -G_-(\tau) \Rightarrow R(\tau) = 0$
- no parity doubling, with $m_- \gg m_+ \Rightarrow R(\tau) = 1$
- quasi-order parameter

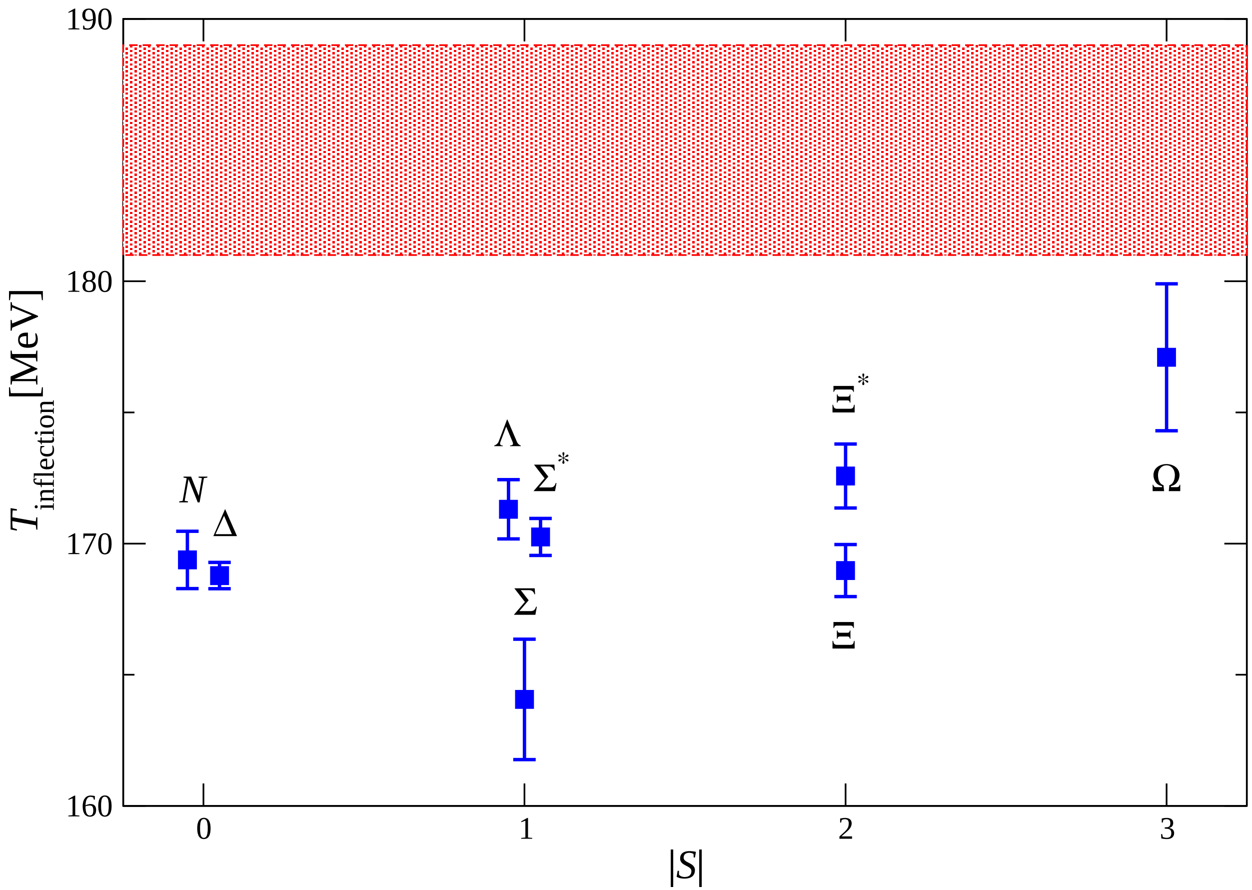
$$0 \leq R = \frac{\sum_n R(\tau_n)/\sigma^2(\tau_n)}{\sum_n 1/\sigma^2(\tau_n)} \leq 1$$

Parity doubling in the baryon spectrum



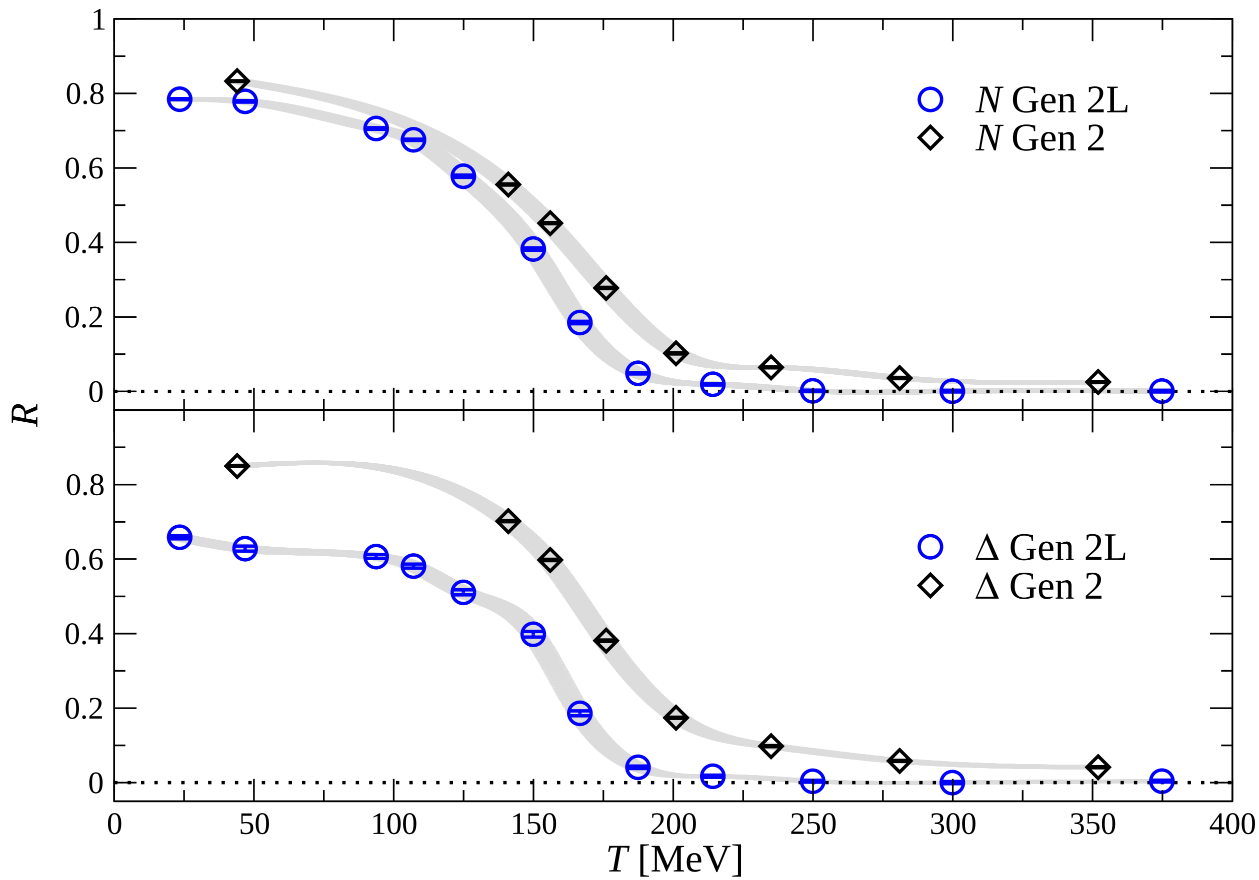
- R from (close to) 1 to (close) 0
- strange quark mass dependence at high T
- vertical lines: $T_c = 185(4)$ MeV from Polyakov loop

Parity doubling: transition



- hashed region: T_c from renormalised Polyakov loop
- inflection-point temperatures somewhat lower
- potential strangeness dependence

Parity doubling: Gen 2 vs Gen 2L



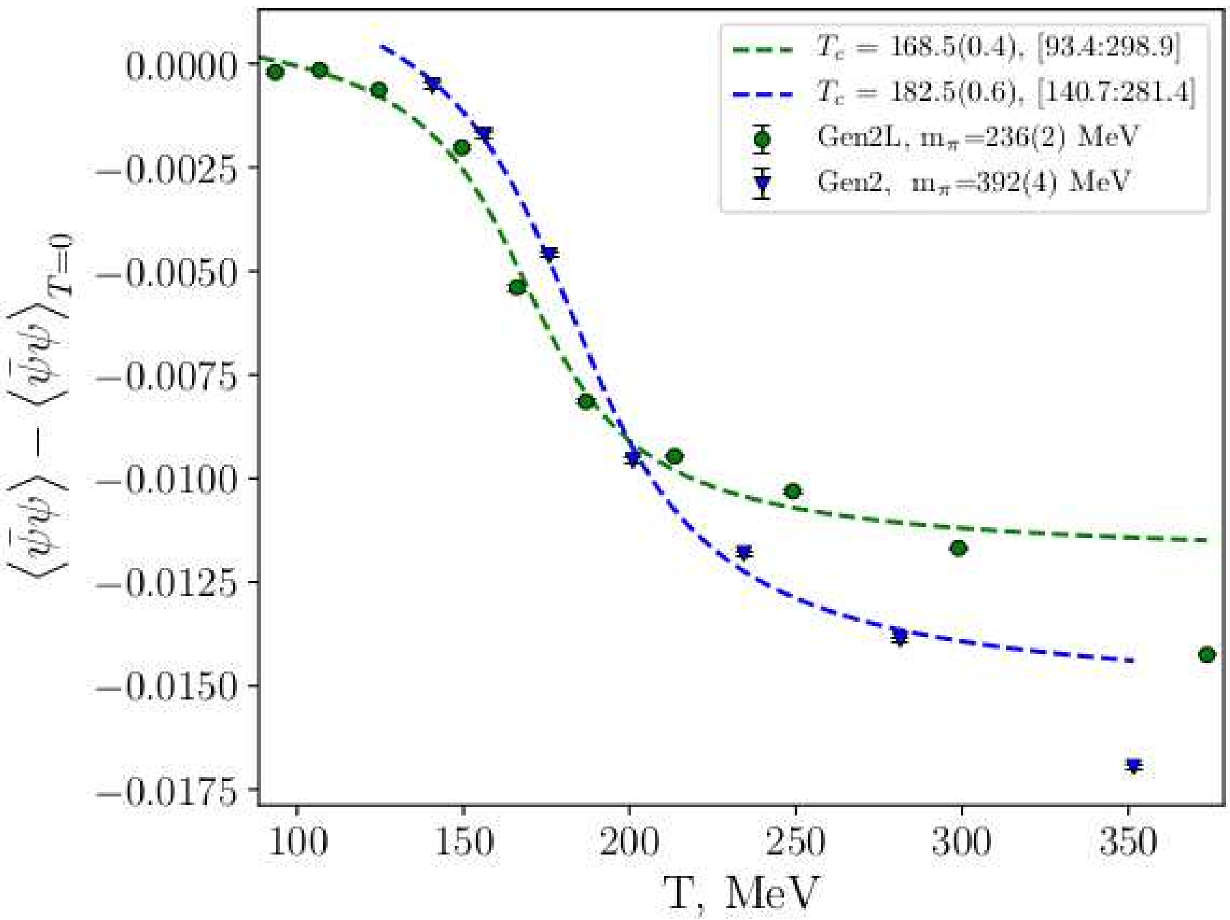
shift of T_c : $T_{\text{infl}} \simeq 169$ MeV (Gen 2) $\simeq 159$ MeV (Gen 2L)

- R closer to 0 for Gen 2L at high T
- analysis of hyperons on Gen 2L is in progress

Chiral condensate

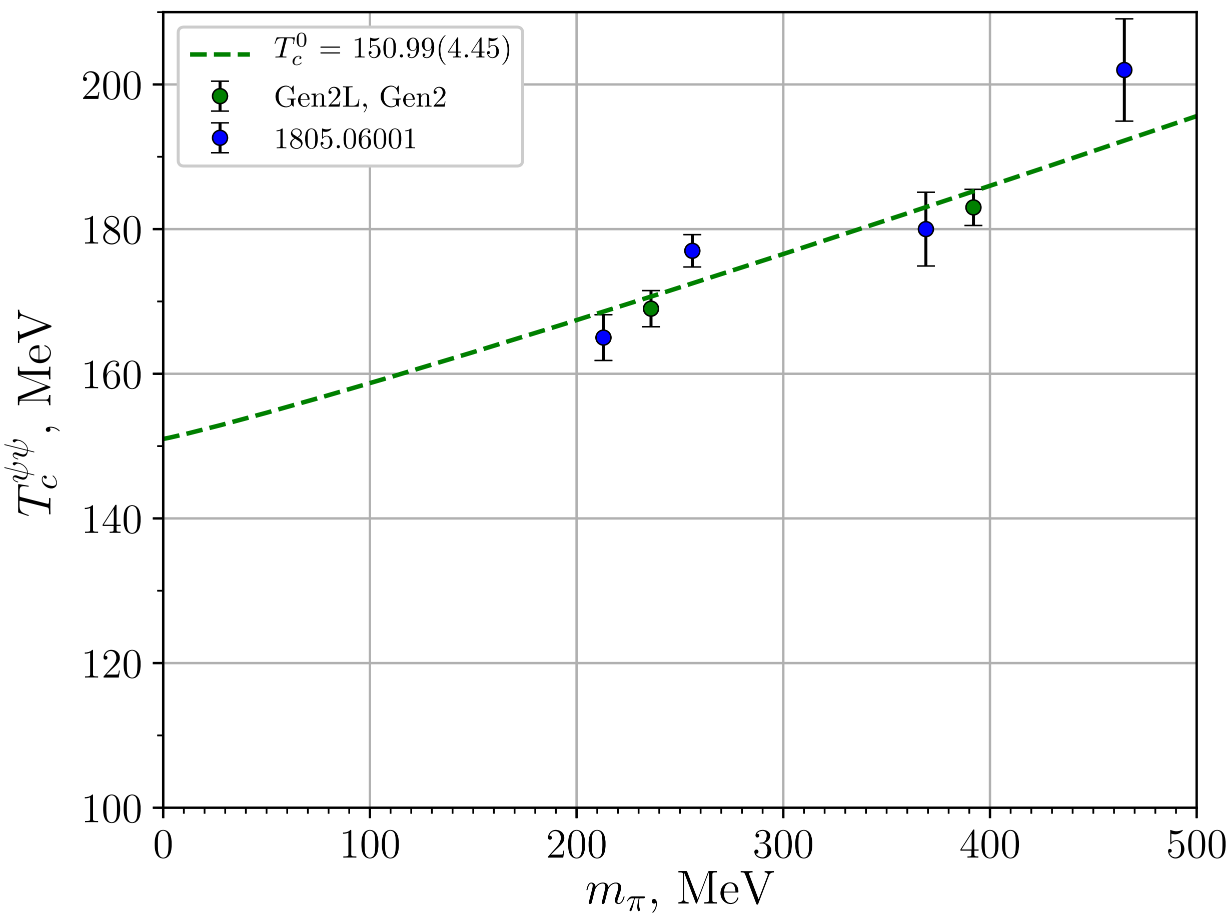
fixed scale approach

additive $+$ multiplicative renormalisation are T independent



Chiral condensate

T_c from inflection point, compare with twisted mass fermions 1805.06001 Lombardo et al



consistency, towards physical masses with Wilson fermions

interval

Finite μ corrections

- direct simulations have to cope with sign problem
- Taylor expansion in μ/T widely used to probe $\mu > 0$ region
- typically used for
  - thermodynamics
  - higher-order susceptibilities
  - curvature of the crossover line

in this talk

- corrections to spectrum at $\mu \neq 0$
- see pioneering paper by QCD-TARO

  `Choe, de Forcrand, Stamatescu et al, hep-lat/0107002`

Finite μ corrections

apply Taylor series to mesonic correlators:

- expand both determinant and propagator
- $\mathcal{O}(\mu)$ term vanishes
- $\mathcal{O}(\mu^2)$ term is nontrivial
- expansion of det: disconnected diagrams $\Rightarrow$ expensive

important contributions by Davide de Boni (theory), Jonas Glesaaen, Ben Jäger (coding), Liang-Kai Wu (simulations), Aleksandr Nikolaev (analysis)

- OpenQCD-FASTSUM code essential
- everything is preliminary !

Derivation: short-hand notation

- write $Z = \langle\!\langle \det \rangle\!\rangle$, brackets denote gluonic averaging
- two-point correlator of mesonic operators: $J = \bar{\psi}\Gamma\psi$

$$G(x) = \frac{\langle\!\langle \det g(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} \qquad\qquad g(x) = \mathrm{tr}\, S(x)\Gamma S(-x)\Gamma^\dagger$$

- first μ derivative vanishes at $\mu = 0$

$$G'(x) = \frac{\langle\!\langle \det' g(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} + \frac{\langle\!\langle \det g'(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} - \frac{\langle\!\langle \det g(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle}\frac{\langle\!\langle \det' \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle}$$

- second derivative

$$\begin{aligned} G''(x) = {} & \frac{\langle\!\langle \det'' g(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} + 2\frac{\langle\!\langle \det' g'(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} - 2\frac{\langle\!\langle \det' g(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle}\frac{\langle\!\langle \det' \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} - \frac{\langle\!\langle \det g(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle}\frac{\langle\!\langle \det'' \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} \\ & -2\frac{\langle\!\langle \det g'(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle}\frac{\langle\!\langle \det' \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} + 2\frac{\langle\!\langle \det g(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle}\left(\frac{\langle\!\langle \det' \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle}\right)^2 + \frac{\langle\!\langle \det g''(x) \rangle\!\rangle}{\langle\!\langle \det \rangle\!\rangle} \end{aligned}$$

Derivation

- in terms of proper brackets: $\langle O \rangle = \langle\langle \det O \rangle\rangle / \langle\langle \det \rangle\rangle$
- second derivative: reorganise terms

$$
\begin{aligned}
G''(x) = & \left\langle \frac{\det''}{\det} g(x) \right\rangle - \left\langle \frac{\det''}{\det} \right\rangle \langle g(x) \rangle \\
& +2 \left\langle \frac{\det'}{\det} g'(x) \right\rangle - 2 \left\langle \frac{\det'}{\det} \right\rangle \langle g'(x) \rangle \\
& -2 \left(\left\langle \frac{\det'}{\det} g(x) \right\rangle - \left\langle \frac{\det'}{\det} \right\rangle \langle g(x) \rangle \right) \left\langle \frac{\det'}{\det} \right\rangle \\
& + \langle g''(x) \rangle
\end{aligned}
$$

with $\det = e^{\mathrm{Tr}\,\ln M} \quad \Rightarrow \quad \det' / \det = \mathrm{Tr}\ M^{-1} M'$, etc

- first three lines are disconnected contributions
- at $\mu = 0$: $\langle \det' / \det \rangle \sim \langle n_q \rangle = 0$
- expensive to compute, vanish as $g \to 0$, i.e. $T \to \infty$

Finite μ corrections

at $T \to \infty$, only $\langle g''(x) \rangle$ contributes

- free quarks, with μ-dependent propagators
- do analytical calculation, in continuum and on lattice

follow GA & Martínez Resco, 2005

propagators $\quad S(\tau, \mathbf{k}) = \gamma_4 S_4(\tau, \mathbf{k}) + \gamma_i S_i(\tau, \mathbf{k}) + \mathbb{1} S_u(\tau, \mathbf{k})$

with
$$S_4(\tau, \mathbf{k}) = \frac{1}{2}\left[f_-(\tau, \omega_\mathbf{k}) + b_+(\tau, \omega_\mathbf{k})\right]$$
$$S_i(\tau, \mathbf{k}) = \frac{-ik_i}{2\omega_\mathbf{k}}\left[f_-(\tau, \omega_\mathbf{k}) - b_+(\tau, \omega_\mathbf{k})\right]$$
$$S_u(\tau, \mathbf{k}) = \frac{m}{2\omega_\mathbf{k}}\left[f_-(\tau, \omega_\mathbf{k}) - b_+(\tau, \omega_\mathbf{k})\right]$$

$$f_\pm(\tau, \omega_\mathbf{k}) = \left[1 - n_F(\omega_\mathbf{k} \pm \mu)\right] e^{-(\omega_\mathbf{k} \pm \mu)\tau}$$
$$b_\pm(\tau, \omega_\mathbf{k}) = \left[1 - n_F(\omega_\mathbf{k} \pm \mu)\right] e^{-(\omega_\mathbf{k} \pm \mu)(1/T - \tau)} = n_F(\omega_\mathbf{k} \pm \mu) e^{(\omega_\mathbf{k} \pm \mu)\tau}$$

Finite μ corrections

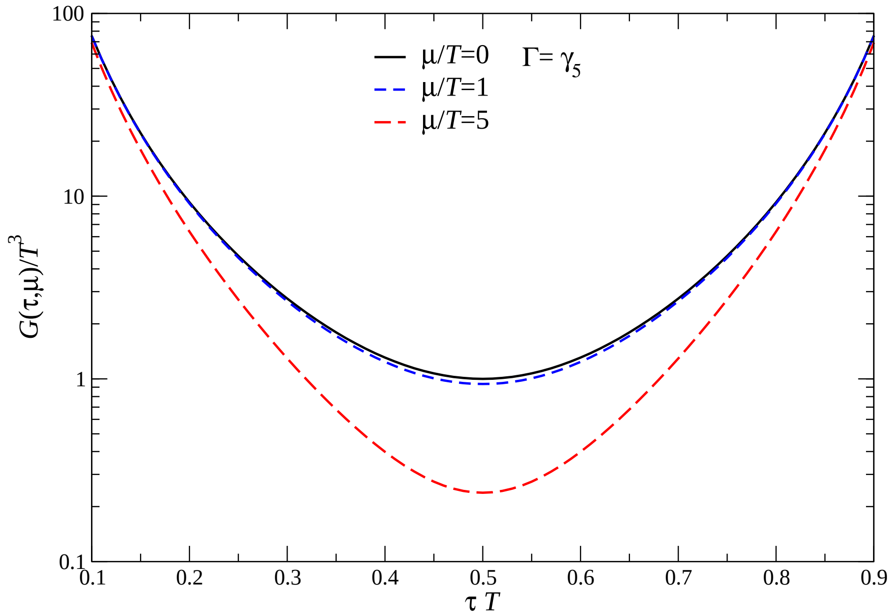
- mesonic correlator in different channels H

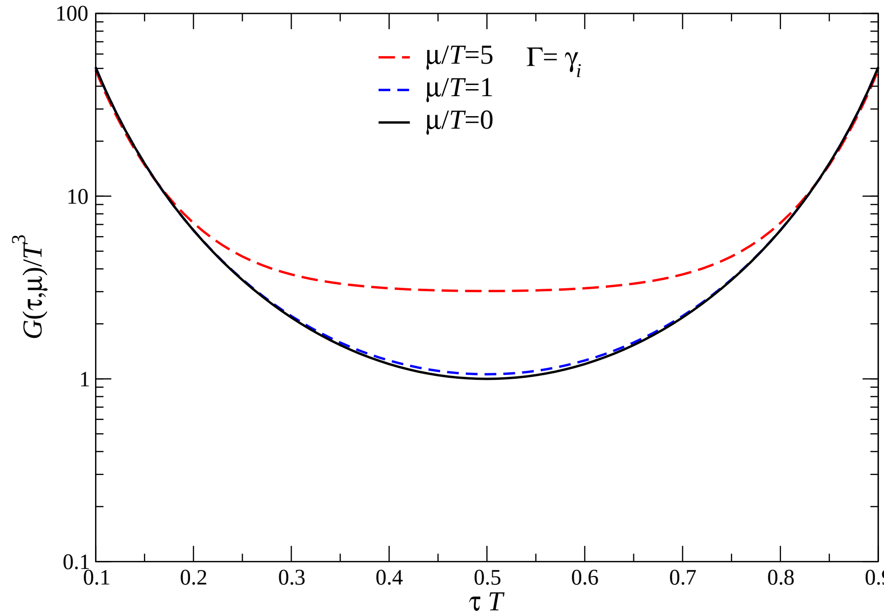
$$G_H(\tau,\mathbf{0}) = N_c \int_{\mathbf{k}} \Bigg\{ \left(a_H^{(1)} - a_H^{(2)} \frac{k^2}{\omega_{\mathbf{k}}^2} - a_H^{(3)} \frac{m^2}{\omega_{\mathbf{k}}^2} \right)$$
$$\Big([1 - n_F(\omega_{\mathbf{k}} + \mu)] \, [1 - n_F(\omega_{\mathbf{k}} - \mu)] \, e^{-2\omega_{\mathbf{k}}\tau} + n_F(\omega_{\mathbf{k}} + \mu) n_F(\omega_{\mathbf{k}} - \mu) e^{2\omega_{\mathbf{k}}\tau} \Big)$$
$$+ \left(a_H^{(1)} + a_H^{(2)} \frac{k^2}{\omega_{\mathbf{k}}^2} + a_H^{(3)} \frac{m^2}{\omega_{\mathbf{k}}^2} \right)$$
$$\Big([1 - n_F(\omega_{\mathbf{k}} - \mu)] \, n_F(\omega_{\mathbf{k}} - \mu) + [1 - n_F(\omega_{\mathbf{k}} + \mu)] \, n_F(\omega_{\mathbf{k}} + \mu) \Big) \Bigg\}$$

- coefficients $a_H^{(i)}$ depend on channel
- second contribution is τ-independent
- evaluate integral analytically in massless case

Massless quarks at high T

- $G(\tau,\mu)/T^3$ on a logarithmic scale vs τT





$\Gamma_H = \gamma_5$ $\qquad\qquad$ $\Gamma_H = \gamma_i$

- note opposite effect of increasing μ:

  pseudoscalar/vector correlator is reduced/enhanced

Massless quarks at high T

- second-order correction

$$T^2 \frac{\partial^2}{\partial\mu^2} G_H(\tau, \mathbf{0})\Big|_{m=\mu=0} = \frac{N_c T^3}{\pi^2} \left[a_H^{(1)} + a_H^{(2)} - \frac{1}{12} \left(a_H^{(1)} - a_H^{(2)} \right) h(u) \right]$$

with

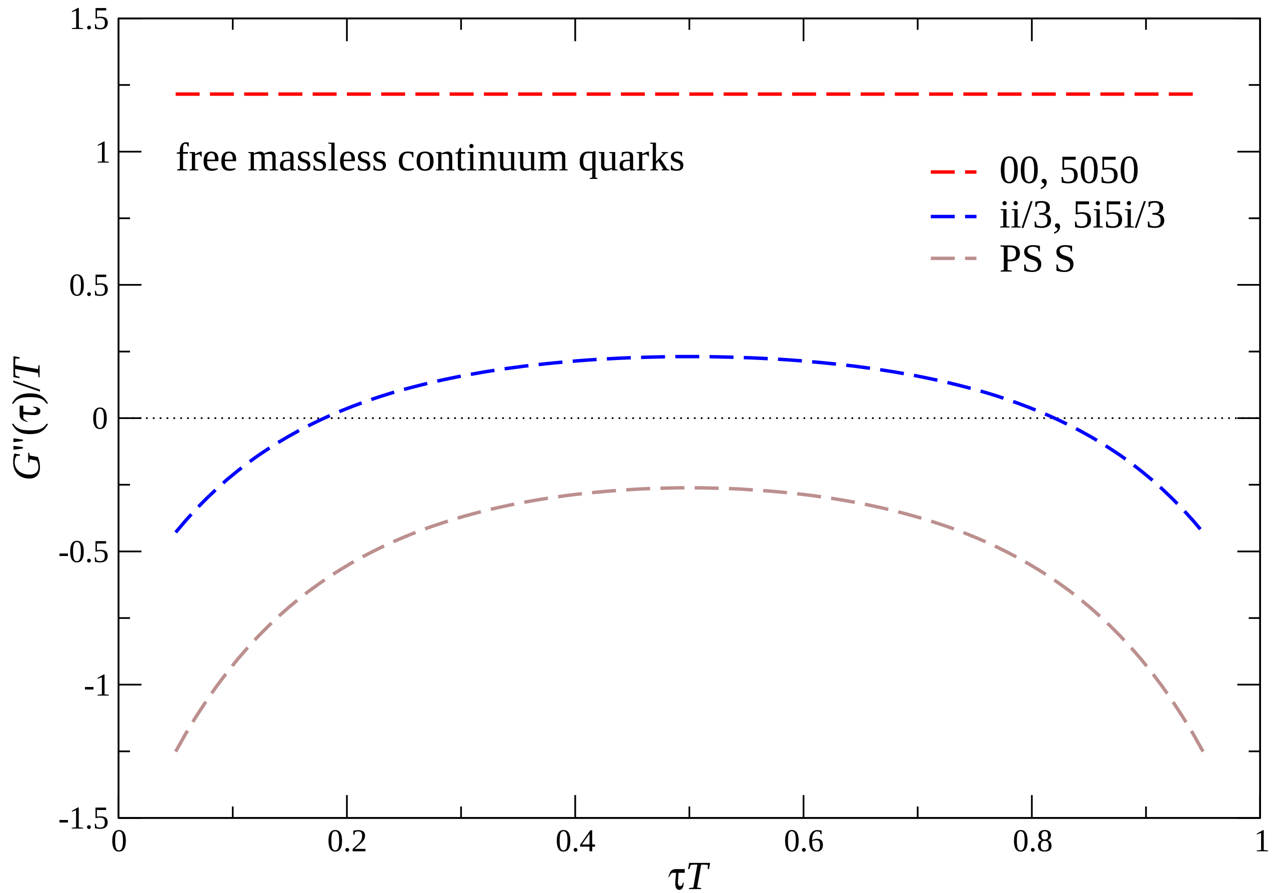
$$h(u) = \frac{3u(\pi^2 - u^2 - 2) + u(\pi^2 - u^2 + 6)\cos(2u) - 2(\pi^2 - 3u^2)\sin(2u)}{\sin^3(u)}$$

and $u = 2\pi T(\tau - 1/2T)$, $-\pi < u < \pi$

- constant shift depends on channel
- τ dependence is identical – contained in $h(u)$

Massless quarks at high T

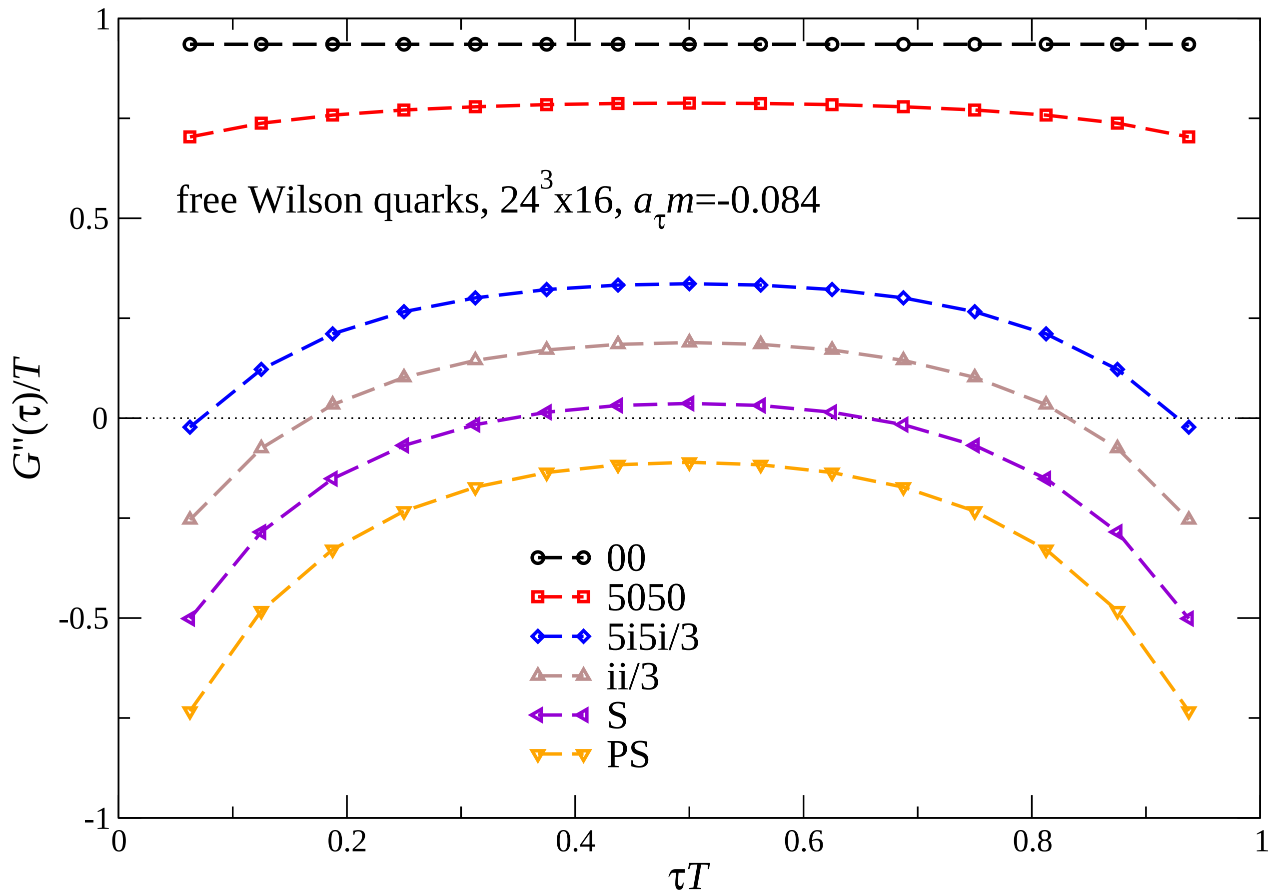
- second-order correction only



- in (axial-)vector channel correction crosses zero $\Rightarrow$ non-monotonic correction

Free lattice quarks at high T

- second-order correction only



- massive Wilson quarks, with Gen 2 bare mass and anisotropy

Finite μ corrections

let's now go to simulations: Gen 2 lattices, $24^3 \times N_\tau$

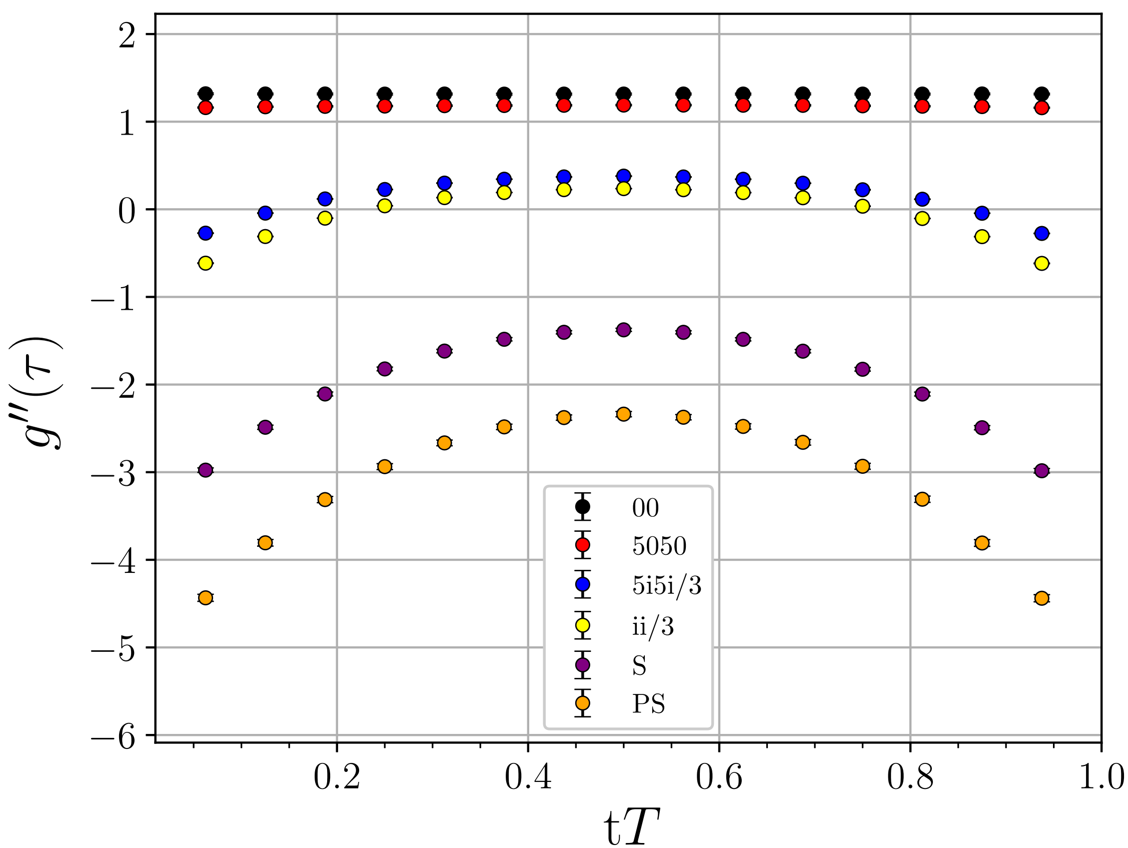
N_τ	128*	40	36	32	28	24	20	16
T [MeV]	44	141	156	176	201	235	281	352
T/T_c	0.24	0.76	0.84	0.95	1.09	1.27	1.52	1.90
$N_{\rm cfg}$	139	501	501	1000	1001	1001	1000	1001

first:

- results at the higher temperatures
- connected contributions

Simulations

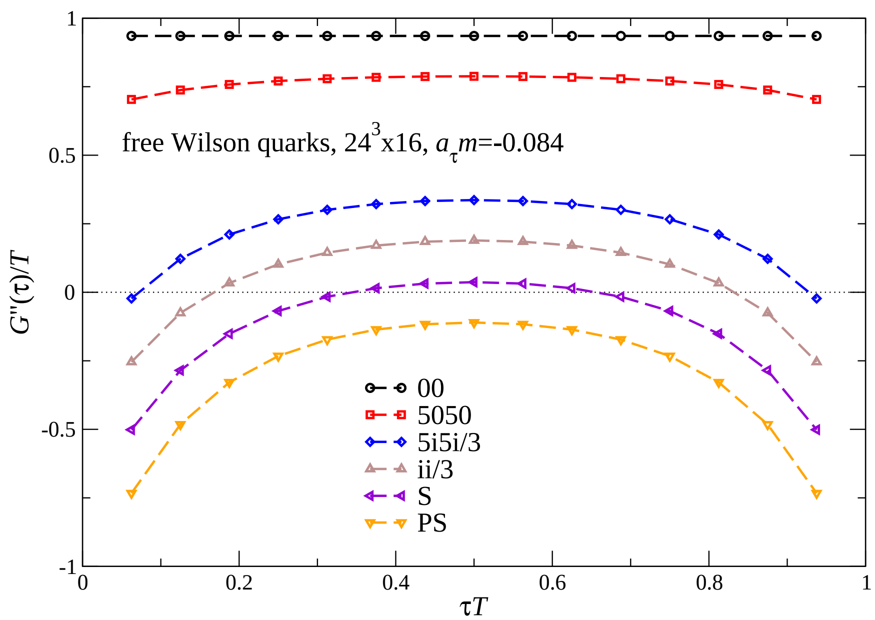
- second-order connected correction only



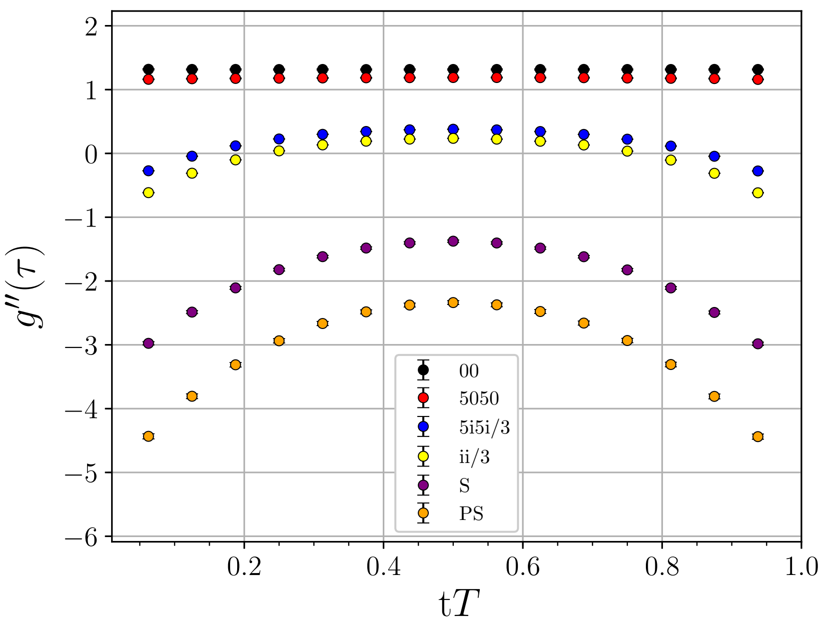
- highest temperature, $N_\tau = 16$

Comparison

- second-order connected correction only



free

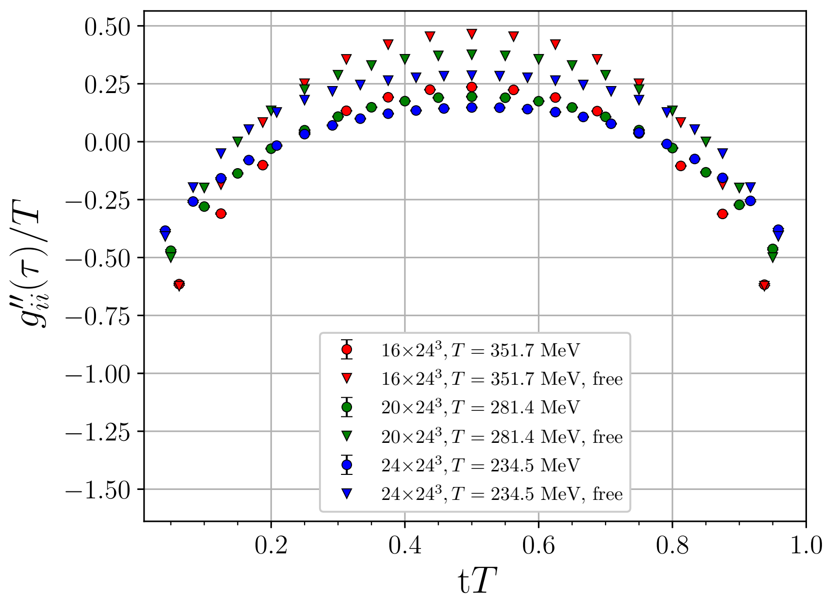


interacting

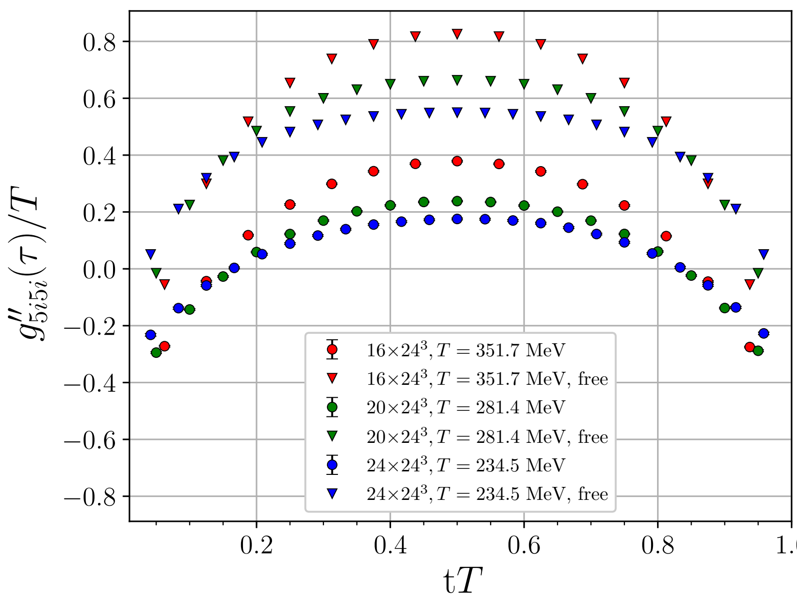
- similar qualitative behaviour
- multiplicative renormalisation, interactions

Temperature dependence

- second-order connected correction only
- highest temperatures, $N_\tau = 16, 20, 24$



vector

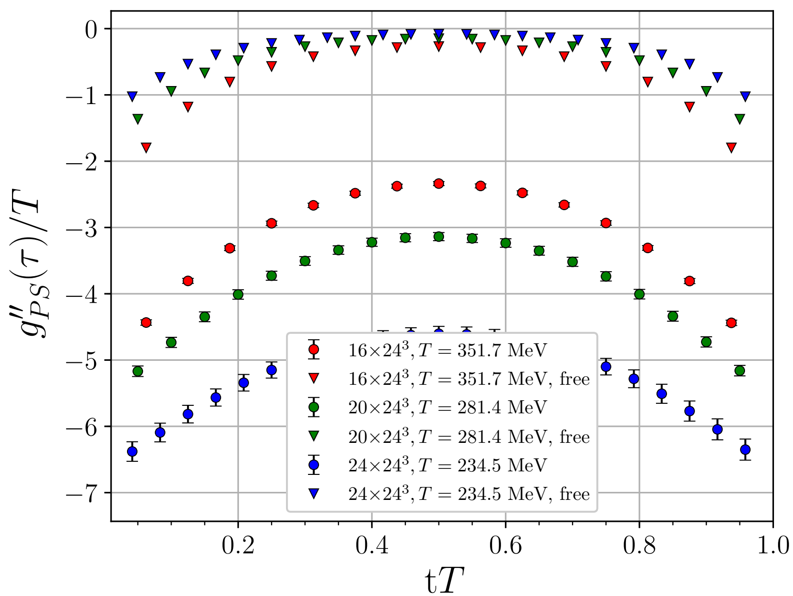


axial-vector

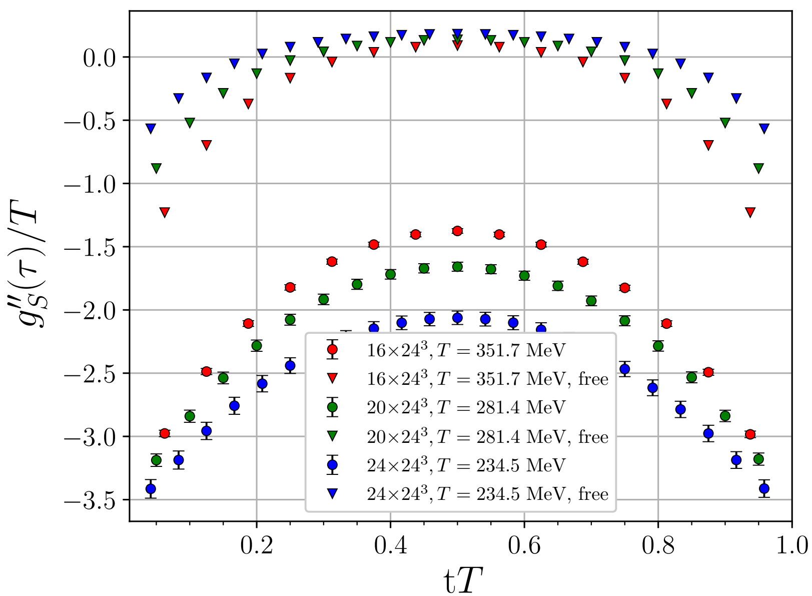
- free (triangle) compared to interacting (circles)

Temperature dependence

- second-order connected correction only
- highest temperatures, $N_\tau = 16, 20, 24$



pseudo-scalar

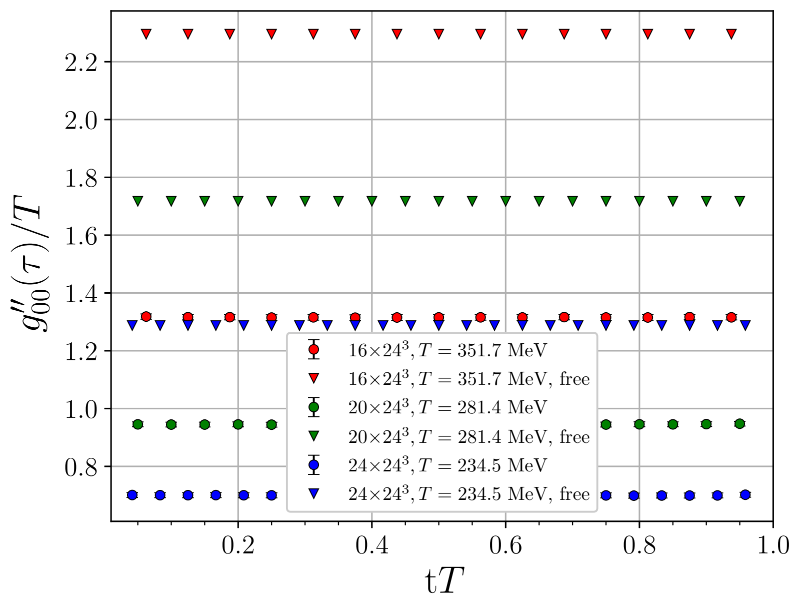


scalar

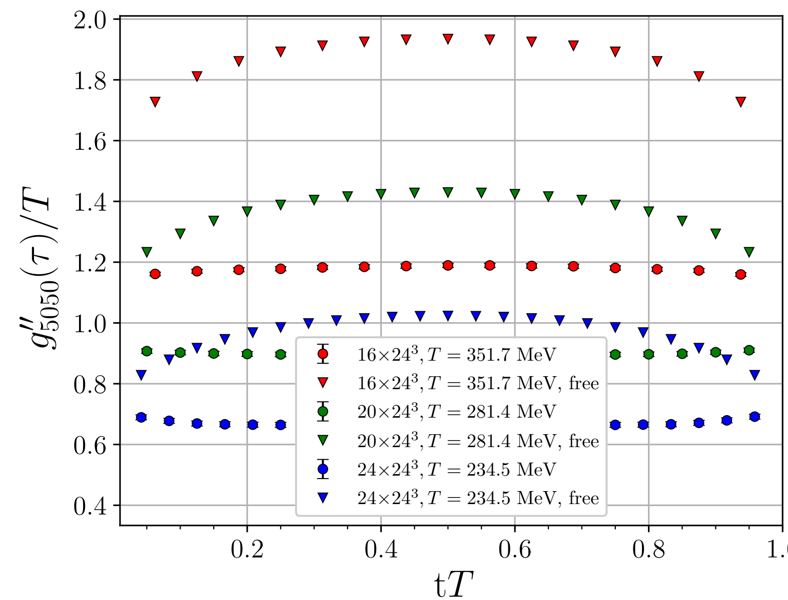
- free (triangle) compared to interacting (circles)

Temperature dependence

- second-order connected correction only
- highest temperatures, $N_\tau = 16, 20, 24$



vector charge

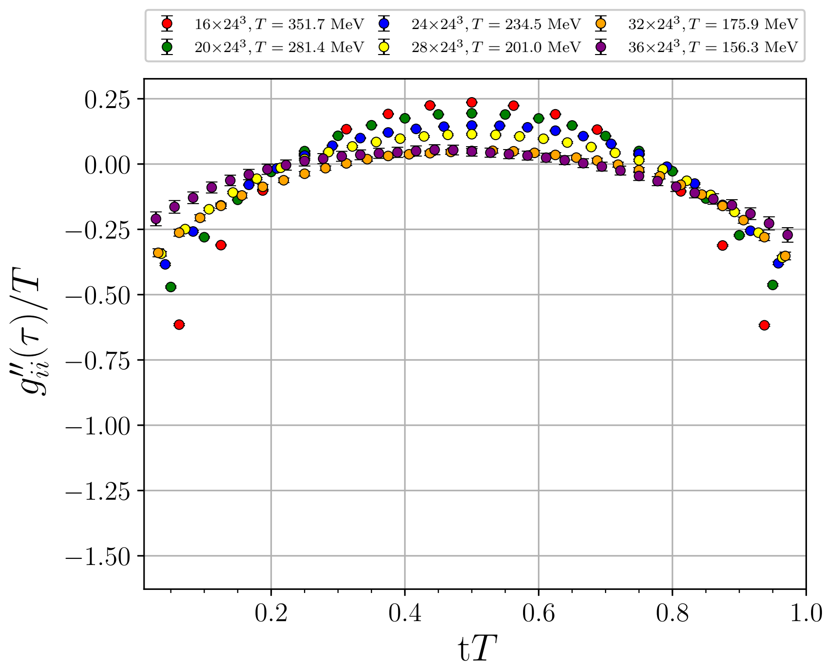


axial charge

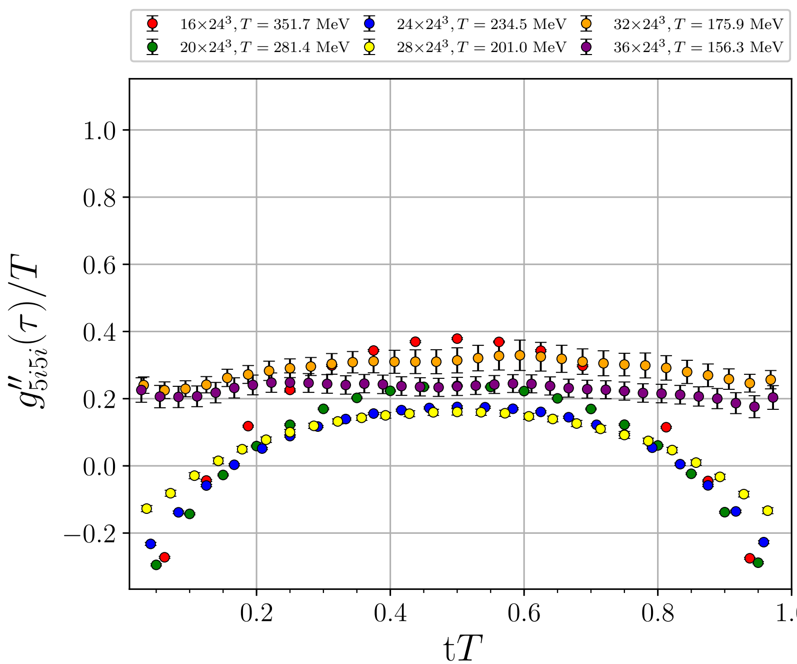
- free (triangle) compared to interacting (circles)

Full temperature dependence

- second-order connected correction only
- many temperatures, $N_\tau = 16, 20, 24, 28 \mid 32, 36$



vector

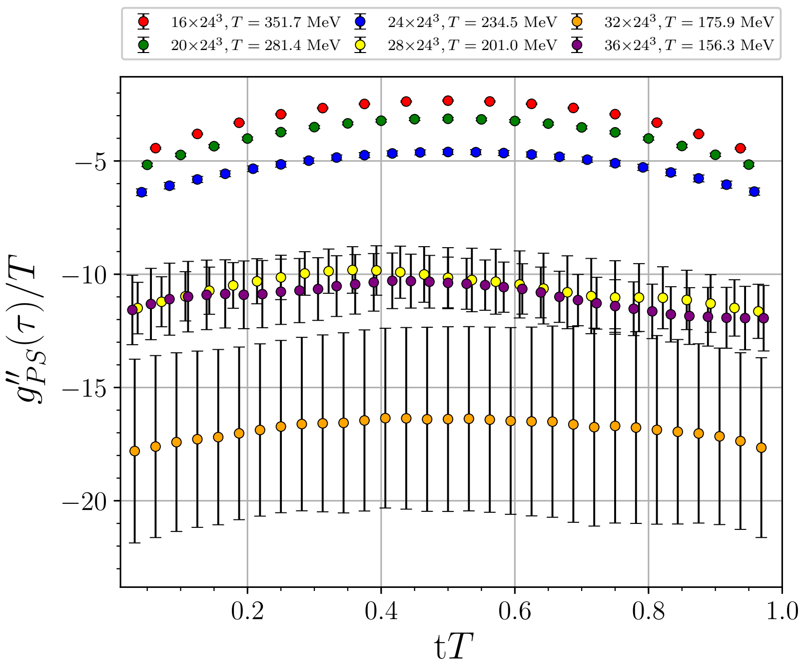


axial-vector

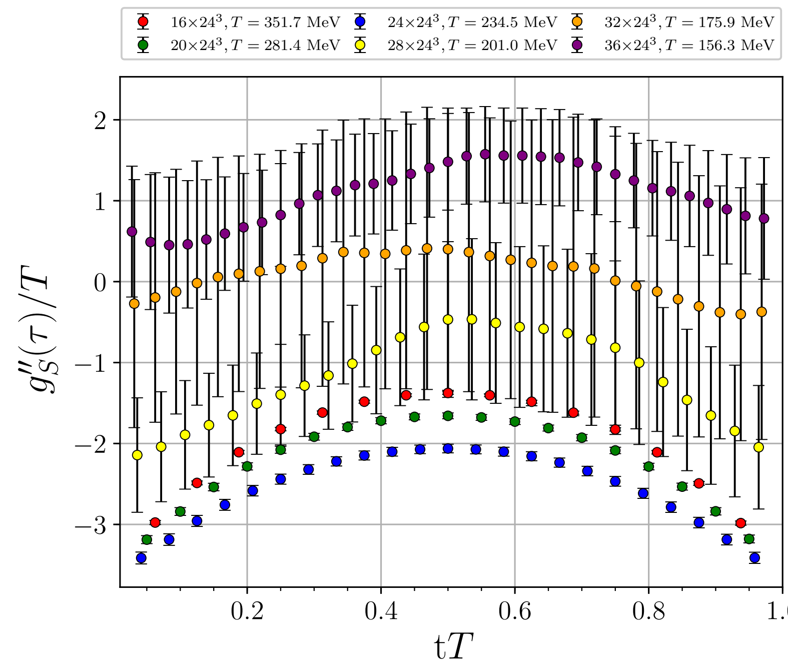
- clear change in signal when entering confined phase

Full temperature dependence

- second-order connected correction only
- many temperatures, $N_\tau = 16, 20, 24, 28 \mid 32, 36$



pseudo-scalar

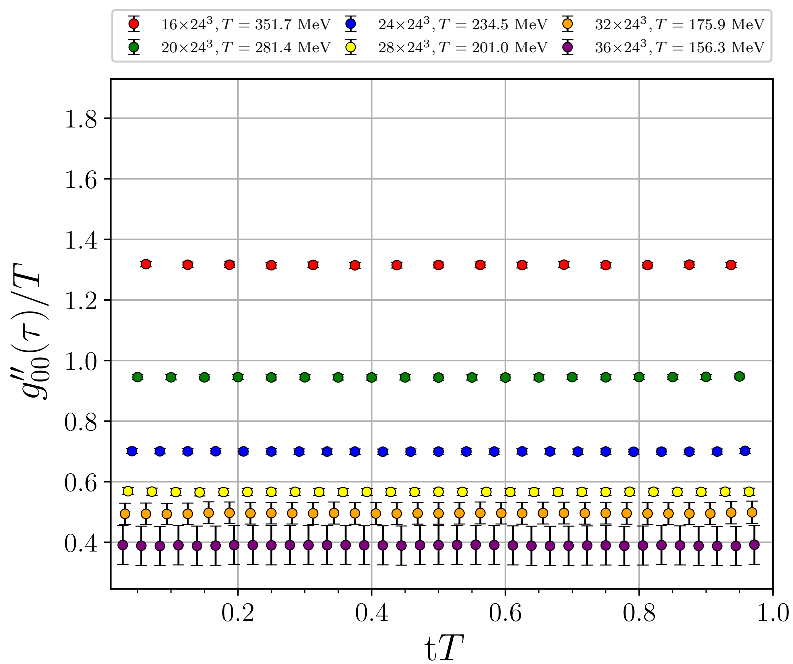


scalar

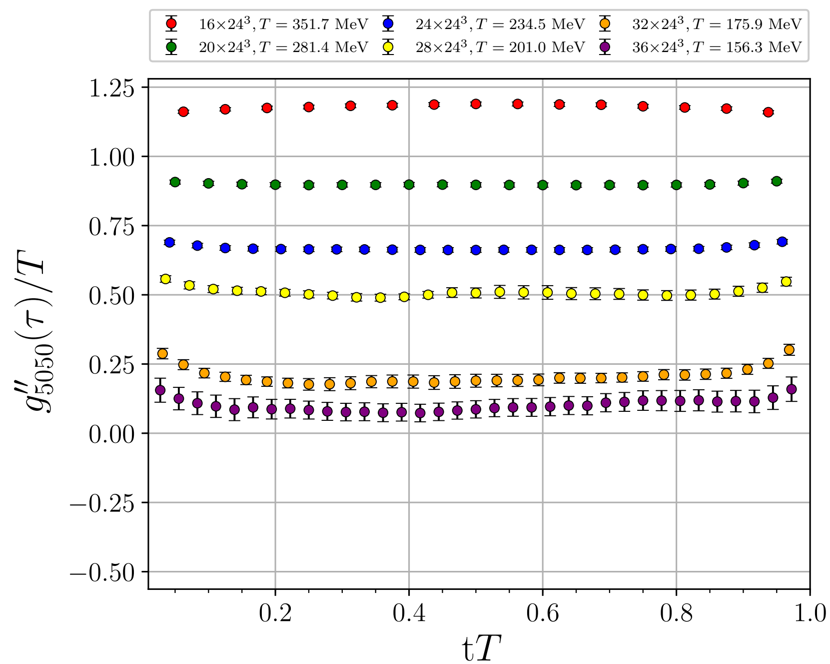
- clear change in signal when entering confined phase

Full temperature dependence

- second-order connected correction only
- many temperatures, $N_\tau = 16, 20, 24, 28 \mid 32, 36$



vector charge



axial charge

- clear change in signal when entering confined phase

A surprising cosh fit

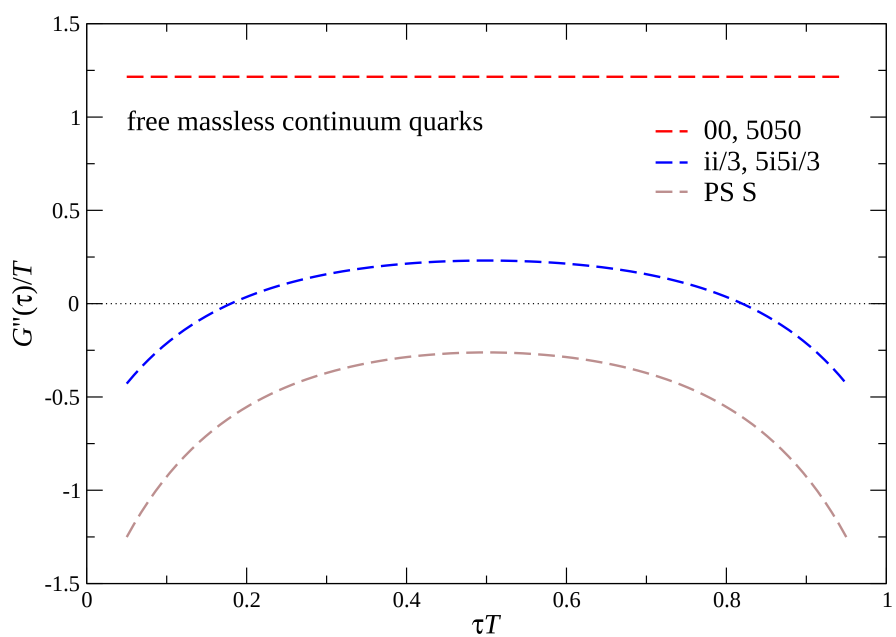
- recall analytic massless continuum expression

$$T^2 \frac{\partial^2}{\partial \mu^2} G_H(\tau, \mathbf{0})\Big|_{m=\mu=0} = \frac{N_c T^3}{\pi^2} \left[a_H^{(1)} + a_H^{(2)} - \frac{1}{12} \left(a_H^{(1)} - a_H^{(2)} \right) h(u) \right]$$

with

$$h(u) = \frac{3u(\pi^2 - u^2 - 2) + u(\pi^2 - u^2 + 6)\cos(2u) - 2(\pi^2 - 3u^2)\sin(2u)}{\sin^3(u)}$$

and $u = 2\pi T(\tau - 1/2T)$

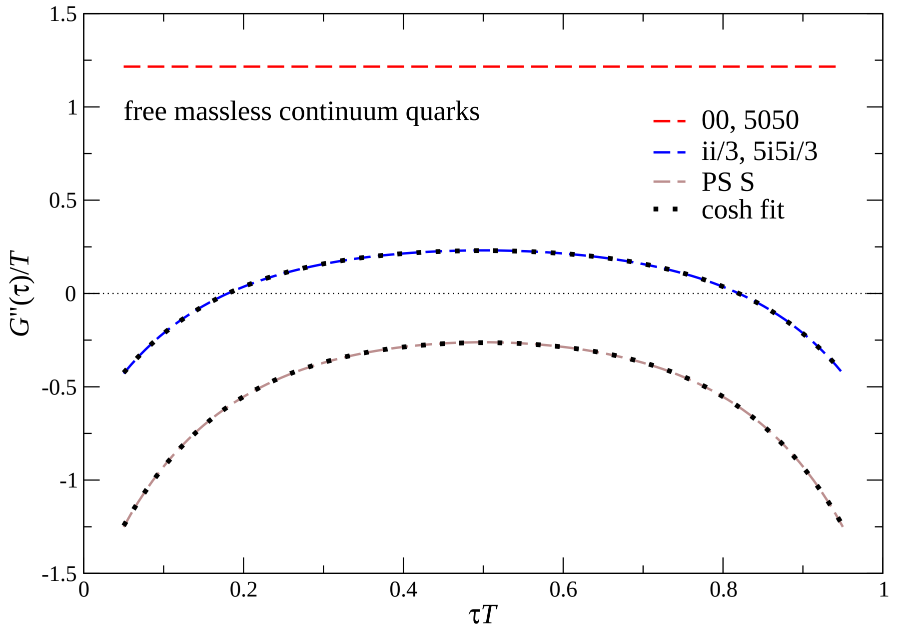


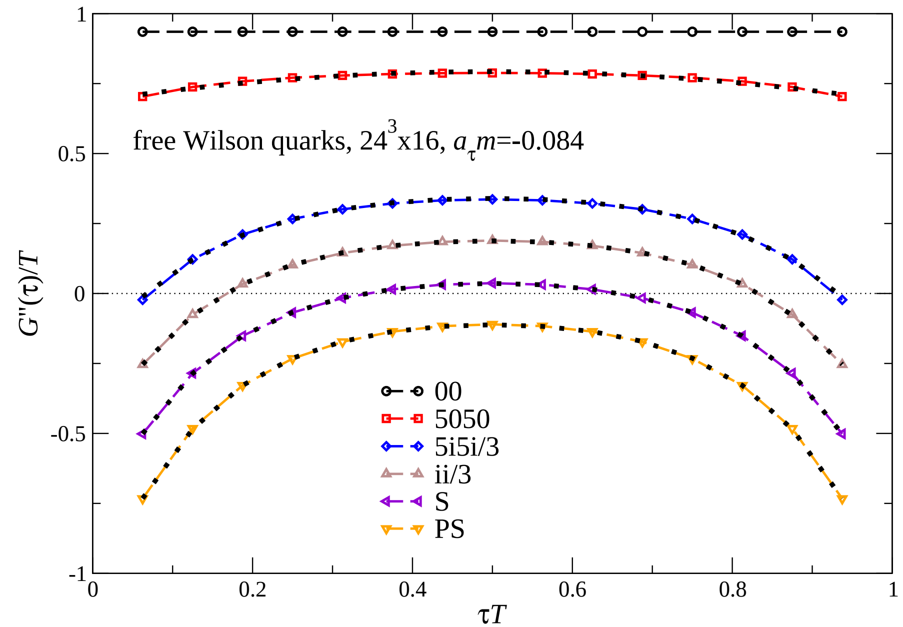
A surprising cosh fit

- very well described by fit

$$G''(\tau)/T = c_0 + c_1 \cosh[c_2(\tau T - 1/2)]$$

both in continuum and on lattice





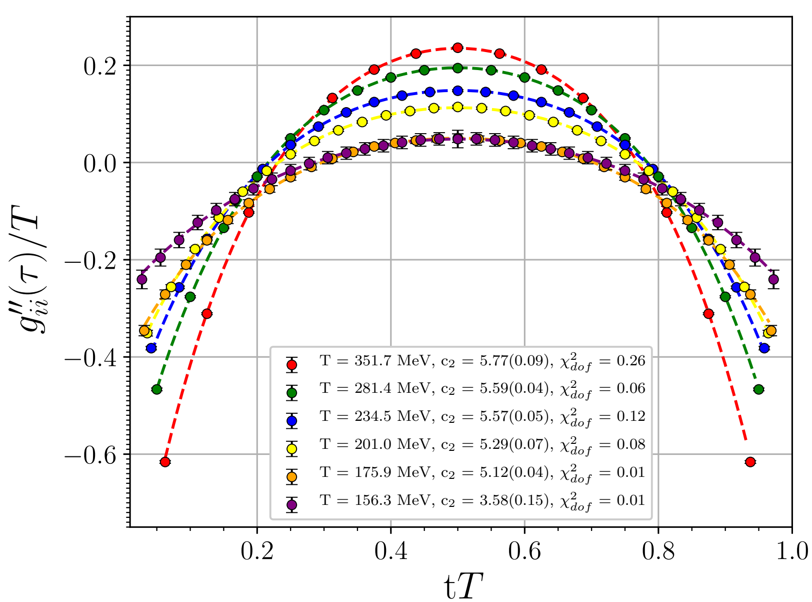
continuum, $c2 \sim 7$ lattice, $c_2 \sim 7.4$

approximately same coefficient in all channels

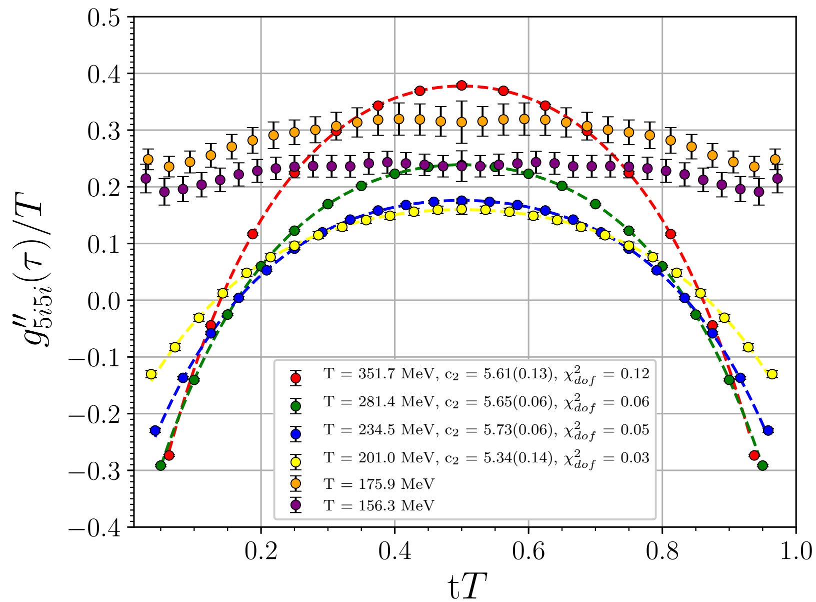
A surprising cosh fit

- connected part in interacting theory at high T very well described by fit

$$G''(\tau)/T = c_0 + c_1 \cosh[c_2(\tau T - 1/2)]$$



vector

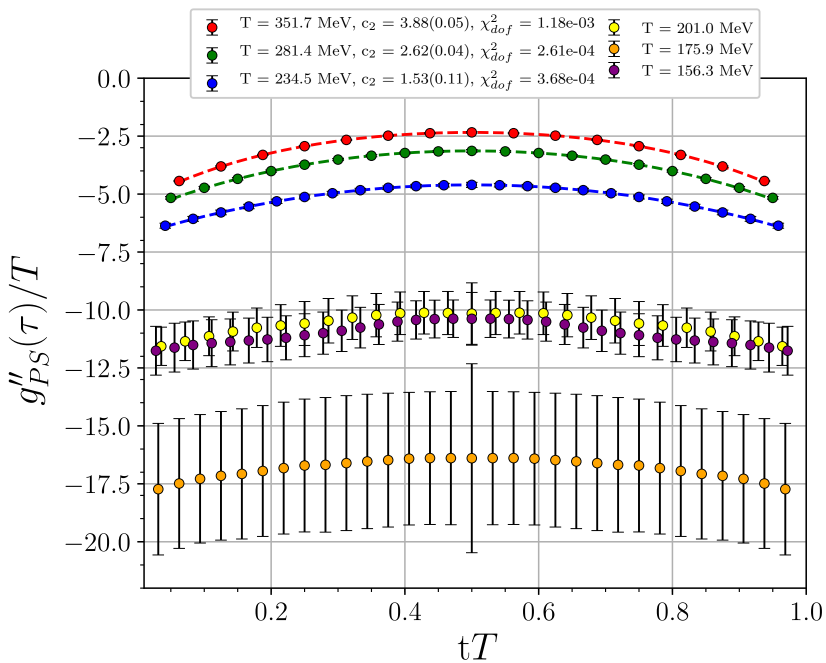


axial-vector

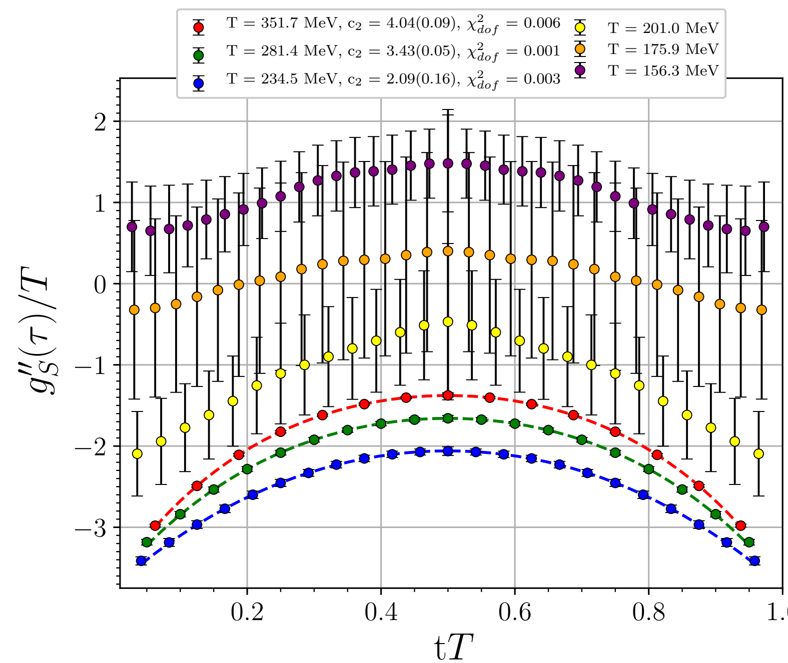
A surprising cosh fit

- connected part in interacting theory at high T very well described by fit

$$G''(\tau)/T = c_0 + c_1 \cosh[c_2(\tau T - 1/2)]$$



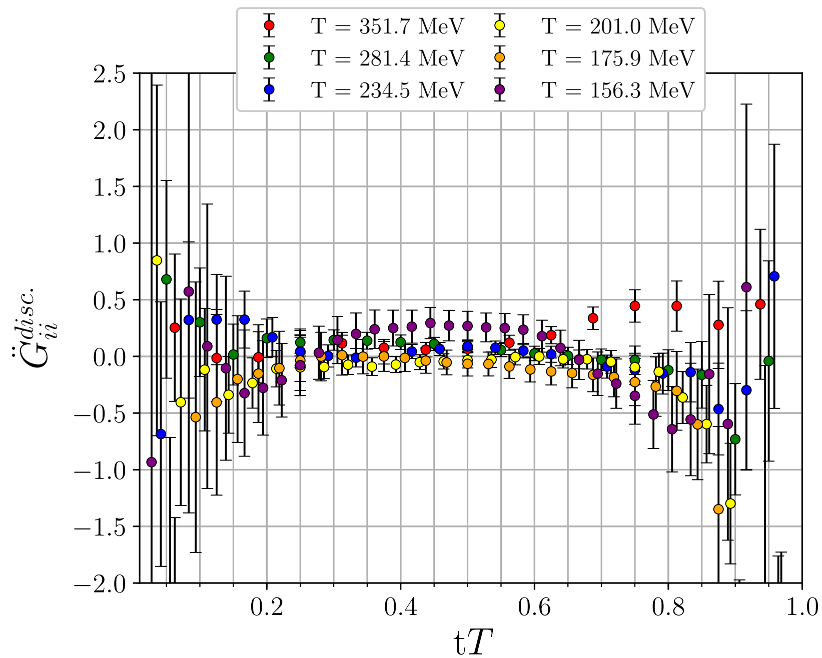
pseudo-scalar



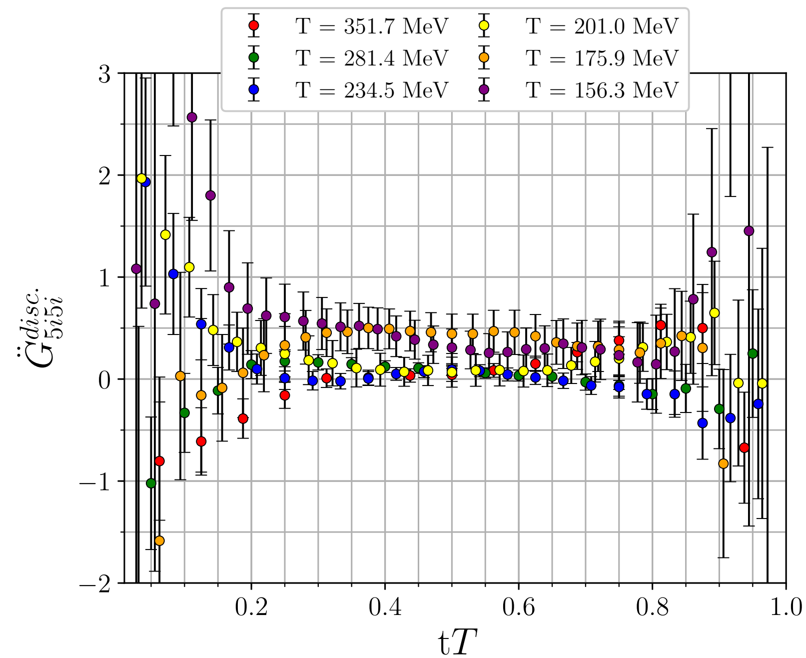
scalar

Disconnected contributions

- disconnected parts vanish in absence of interactions
- very noisy, stochastic estimators, multiple sources



vector

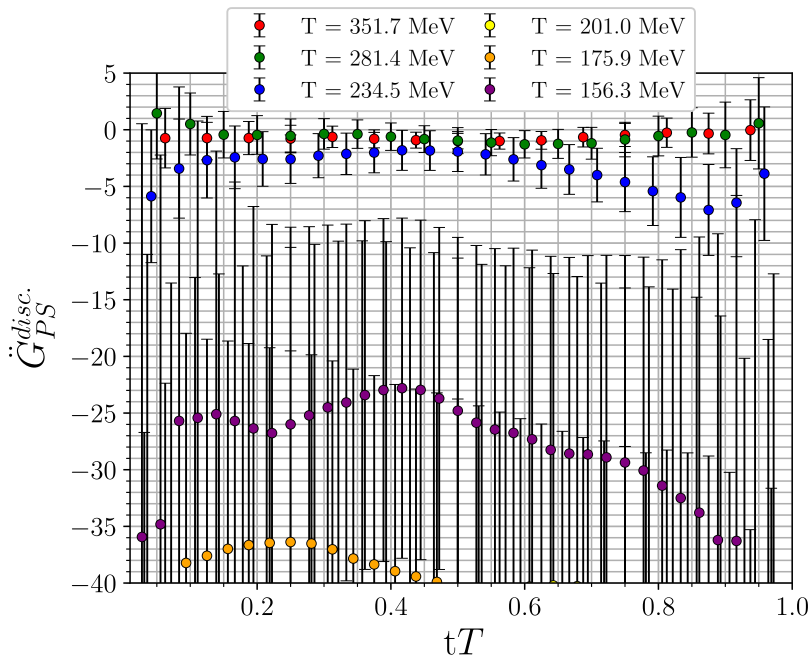


axial-vector

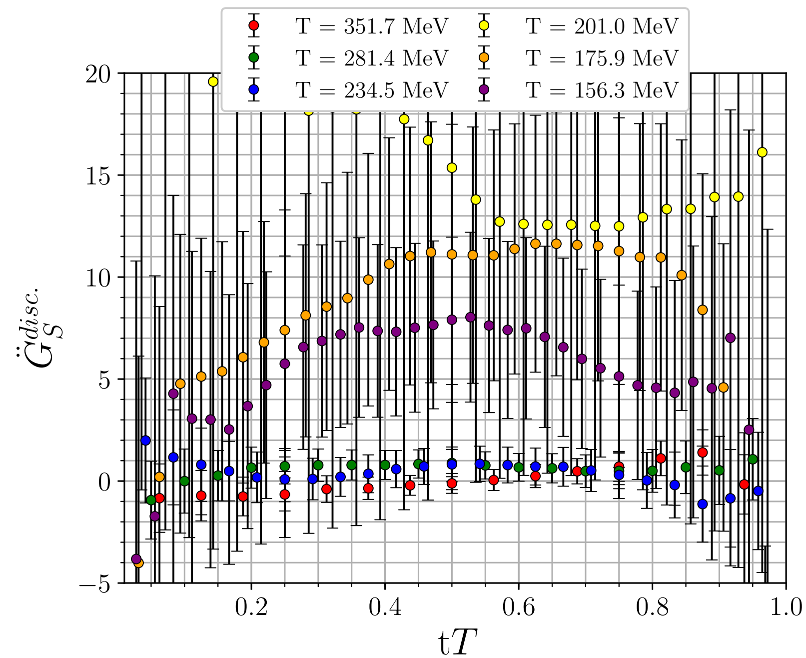
- some control at high T

Disconnected contributions

- disconnected parts vanish in absence of interactions
- very noisy, stochastic estimators, multiple sources



pseudo-scalar

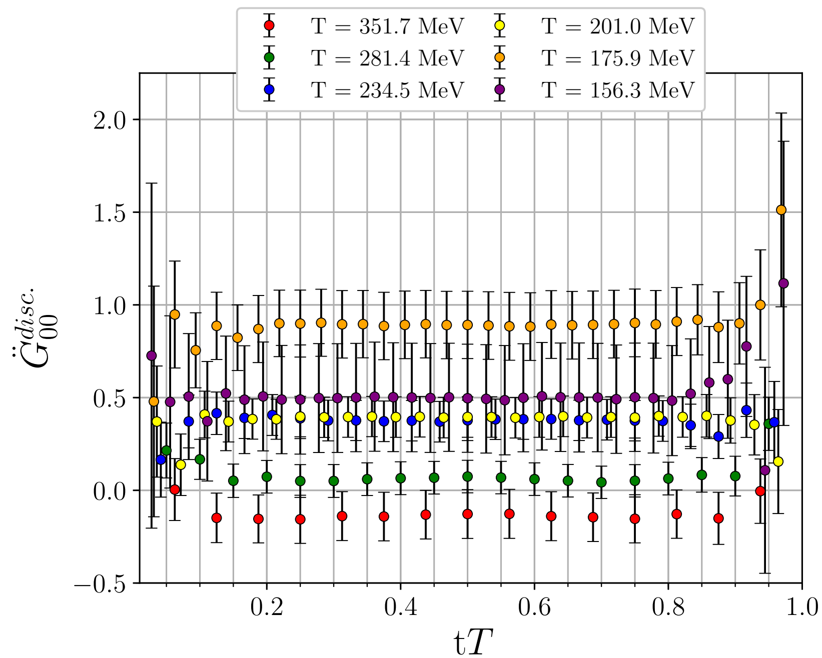


scalar

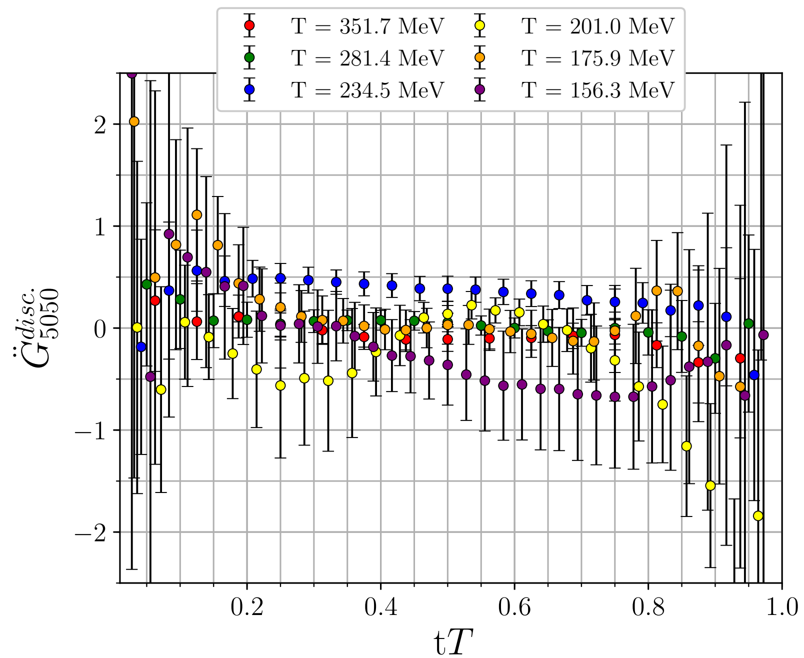
- some control at high T, no control at low T

Disconnected contributions

- disconnected parts vanish in absence of interactions
- very noisy, stochastic estimators, multiple sources



charge



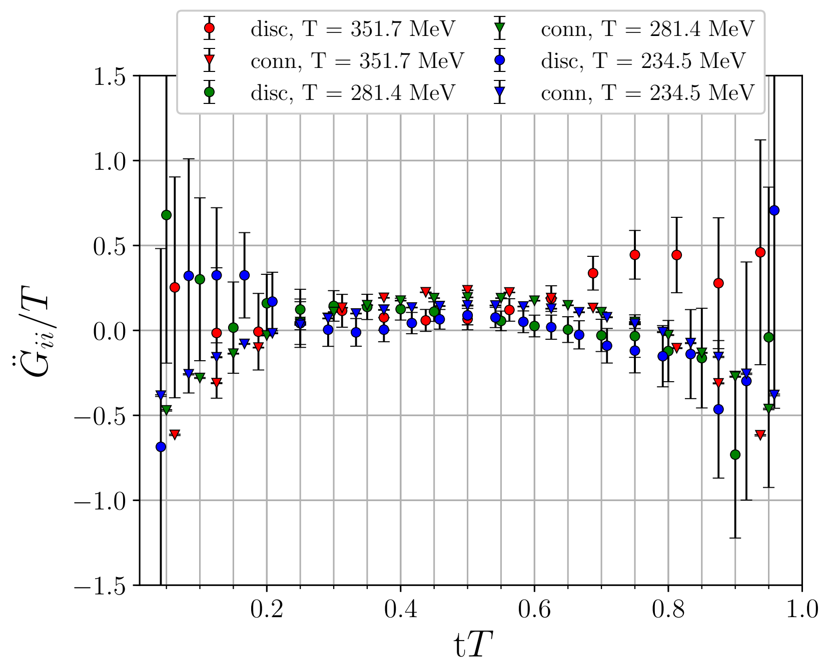
axial charge

- some control at high T, no control at low T

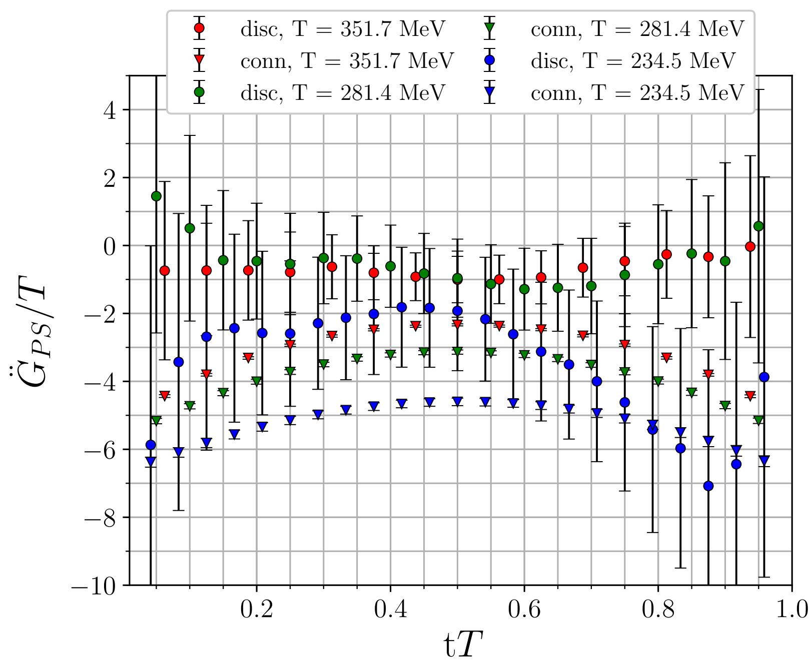
Disconnected contributions

- disconnected parts (circles) of same order as connected parts (triangles) at high T ... sometimes ...

  in vector channel, not in pseudoscalar channel



vector



pseudoscalar

- more control at high T and especially low T needed

Summary

- spectral features in thermal QCD
- FASTSUM anisotropic ensembles: lighter quarks
- properties of the chiral crossover with Wilson fermions
- nonzero chemical potential:
  - corrections to mesonic correlators
  - high temperature: anchored by noninteracting results
  - transition visible from deconfined to confined phase
  - disconnected contributions noisier as the temperature is reduced
  - more work needed
  - future baryonic correlators: linear correction in μ