A guide to lattice QCD thermodynamics

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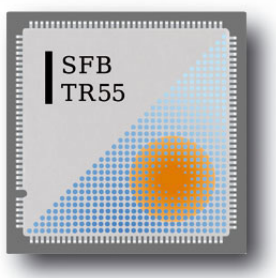
University of Wuppertal

Wigner Institute, Budapest, Dec 3, 2018
"Zimanyi School" Workshop



Outline

1. What does lattice QCD do?
2. Should I believe lattice results?
3. What can lattice calculate?
   - Low hanging fruits:
     Transition temperature, equation of state
   - Expensive goods
     Fluctuations of conserved charges
   - Mission: impossible (?)
     Finite density, (real time spectral functions, viscosity)

This is just a selection of topics lattice QCD addresses.

Wednesday: lattice QCD session with the most challenging problems.

Lattice QCD is numerical technique to solve this theory:

$$\mathcal{L}_{QCD} = -\frac{1}{4} F^a_{\mu\nu} F^{a,\mu\nu} + \sum_{q=u,d,s,c} \bar{\psi}_q [i\gamma^\mu D_\mu - m_q]\psi_q \tag{1}$$

where F and D are defined as

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^b_\mu A^c_\nu \tag{2}$$

$$D_\mu \psi = \left(\partial_\mu - igT^a A^a_\mu\right)\psi \tag{3}$$

The dynamics of gauge fields is described by the term

$$\begin{aligned} -\frac{1}{4} F^a_{\mu\nu} F^{a,\mu\nu} = & -\frac{1}{4}(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu)(\partial_\mu A^a_\nu - \partial_\nu A^a_\mu) \\ & -g f^{abc} \partial_\mu A^a_\nu A^{b,\mu} A^{c,\nu} \\ & -\frac{g^2}{4} f^{abc} f^{ade} A^b_\mu A^c_\nu A^{d,\mu} A^{e,\nu} \end{aligned} \tag{4}$$

Parameters: quark masses: $m_u = m_d$ and m_s, coupling constant g.

Often neglected: α_{QED}, $m_u - m_d$ and $1/m_c$, but we are working on it

Where does temperature and chemical potential come in?

Quantum fields at finite temperature

QFT is defined by a Hamiltonian $\hat{H}$ with eigenvalues E_i. At a temperature T the partition function reads:

$$Z = \sum_i e^{-E_i/T} = \mathrm{Tr}\, e^{-\hat{H}/T} \tag{5}$$

Trace means that we have to sum (integrate) in some basis, e.g. position

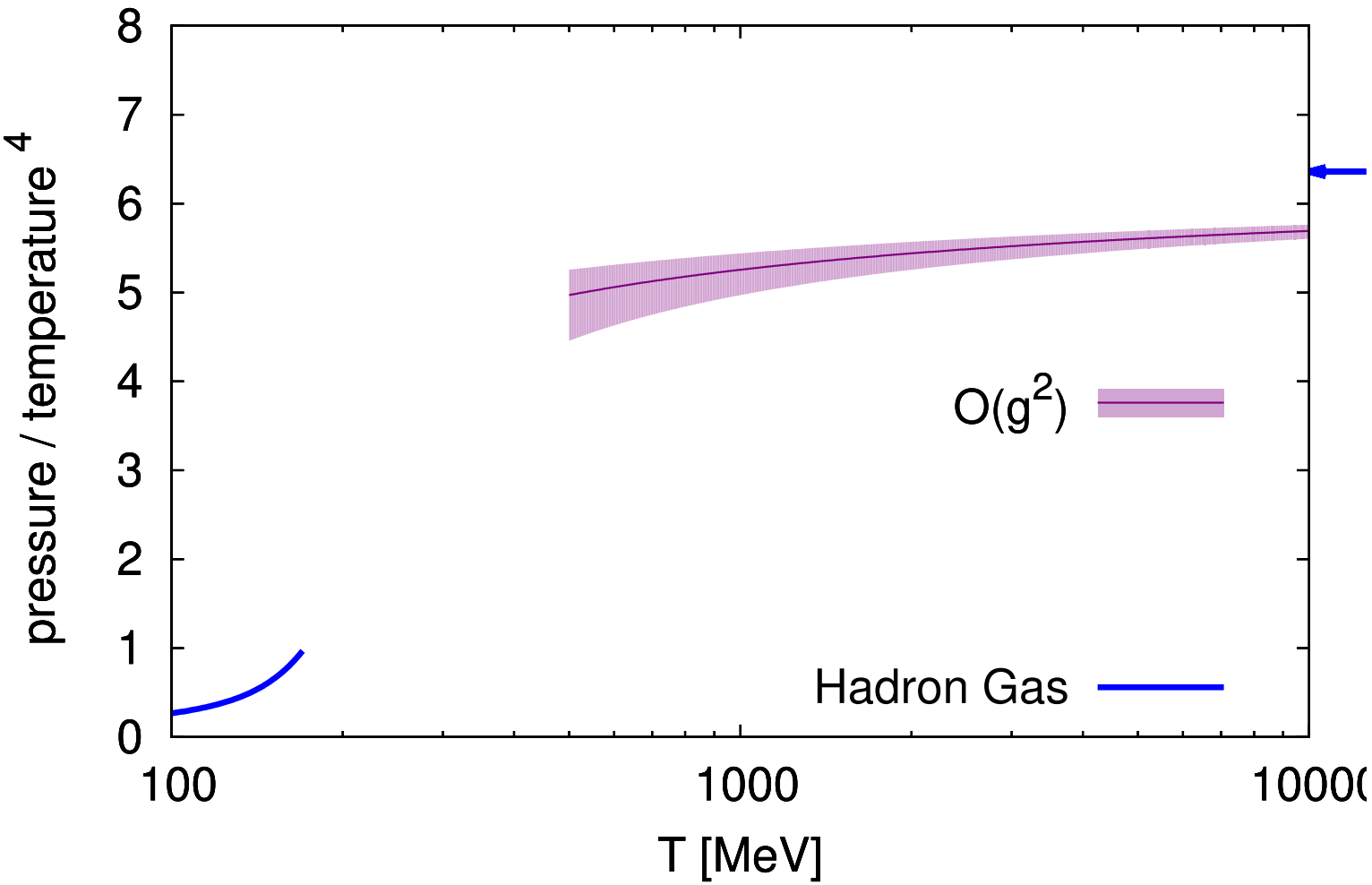
$$Z = \int d\phi^{(0)} \left\langle \phi^{(0)} \right| e^{-\hat{H}/T} \left| \phi^{(0)} \right\rangle \tag{6}$$

$$Z \sim \int D \prod_j e^{-\delta\tau \sum_i \left[\left(\frac{d\phi^{(j)}}{\delta\tau} \right)^2 + V(\phi^{(j)}) \right]} = \int D\phi e^{-\int_0^{1/T} \mathcal{L}_E(\phi)} \tag{7}$$

Thus, the finite temperature quantum system is automatically a Euclidean system with periodic (antiperiodic) boundaries for bosonic (fermionic) fields.

Most basic observable: $F = -T \log Z = -pV$

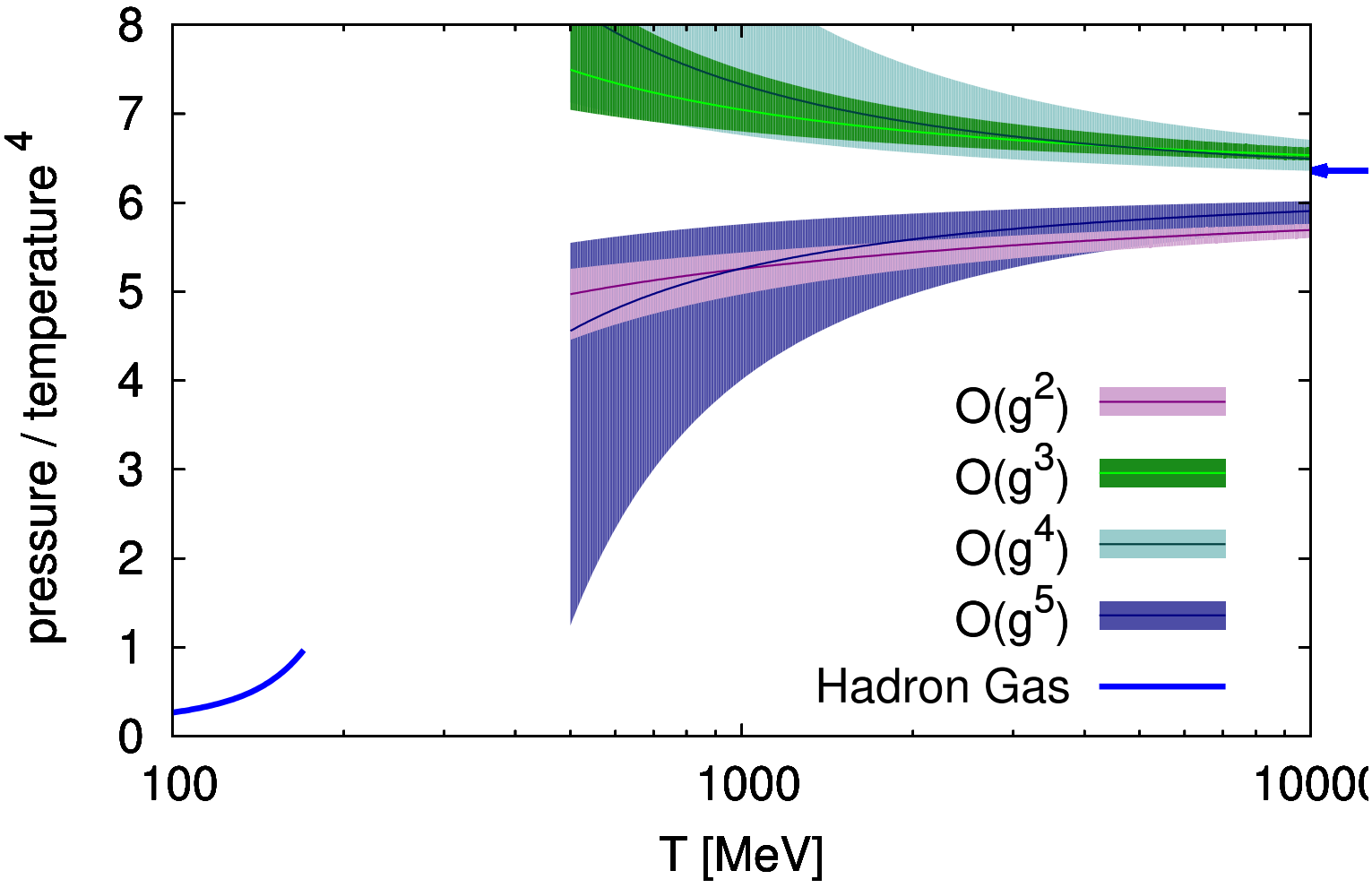
The QCD free energy



Hadron Gas: sum of the free energy of the known hadrons

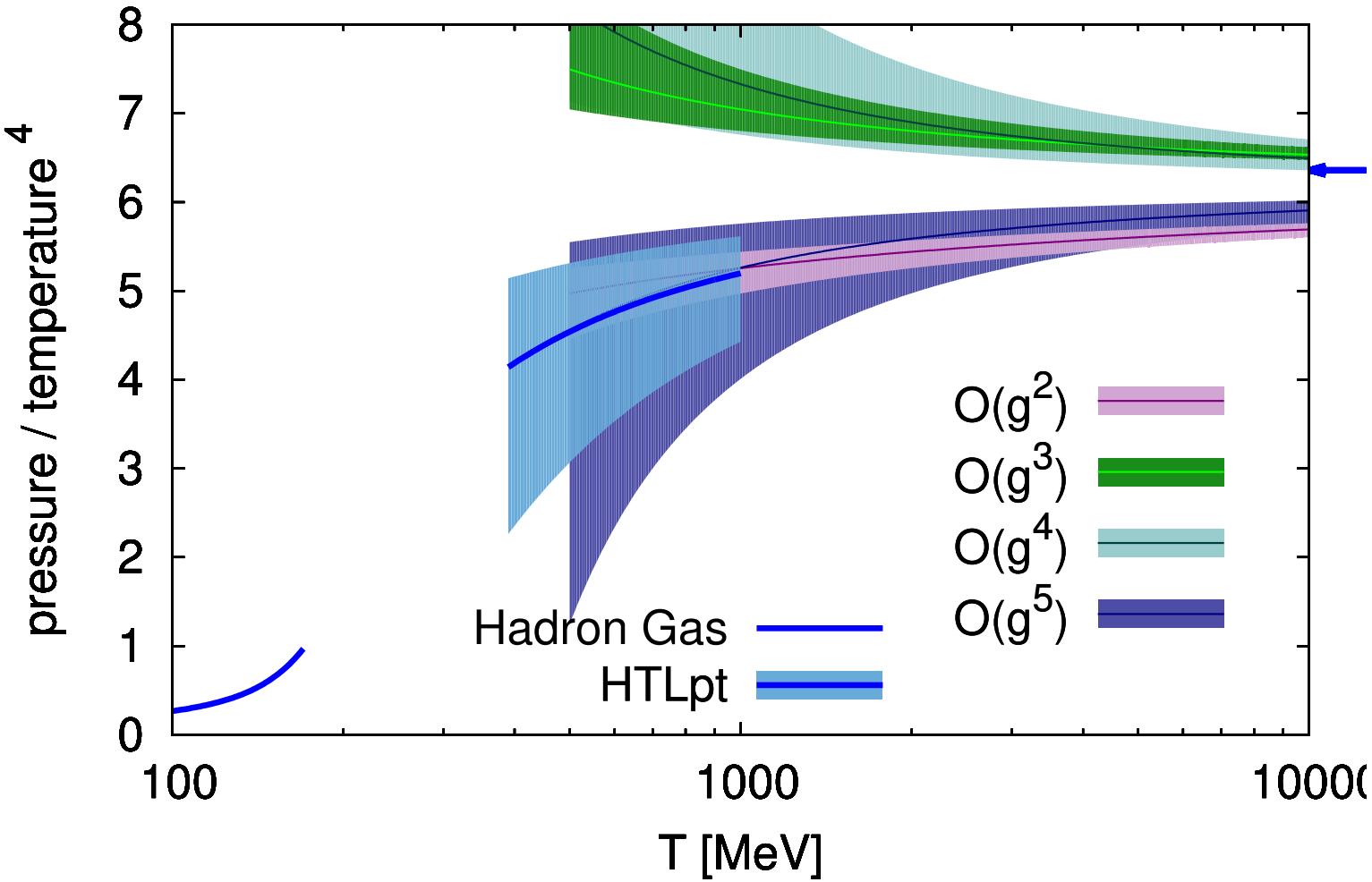
Stefan-Boltmann limit: $\frac{\pi^2}{90} \cdot 8 \cdot 2 + \frac{6\pi^2}{60} N_f$

The QCD free energy



Perturbation theory gives in principle correct results at high temperature, where the coupling is small, yet it converges very slowly.

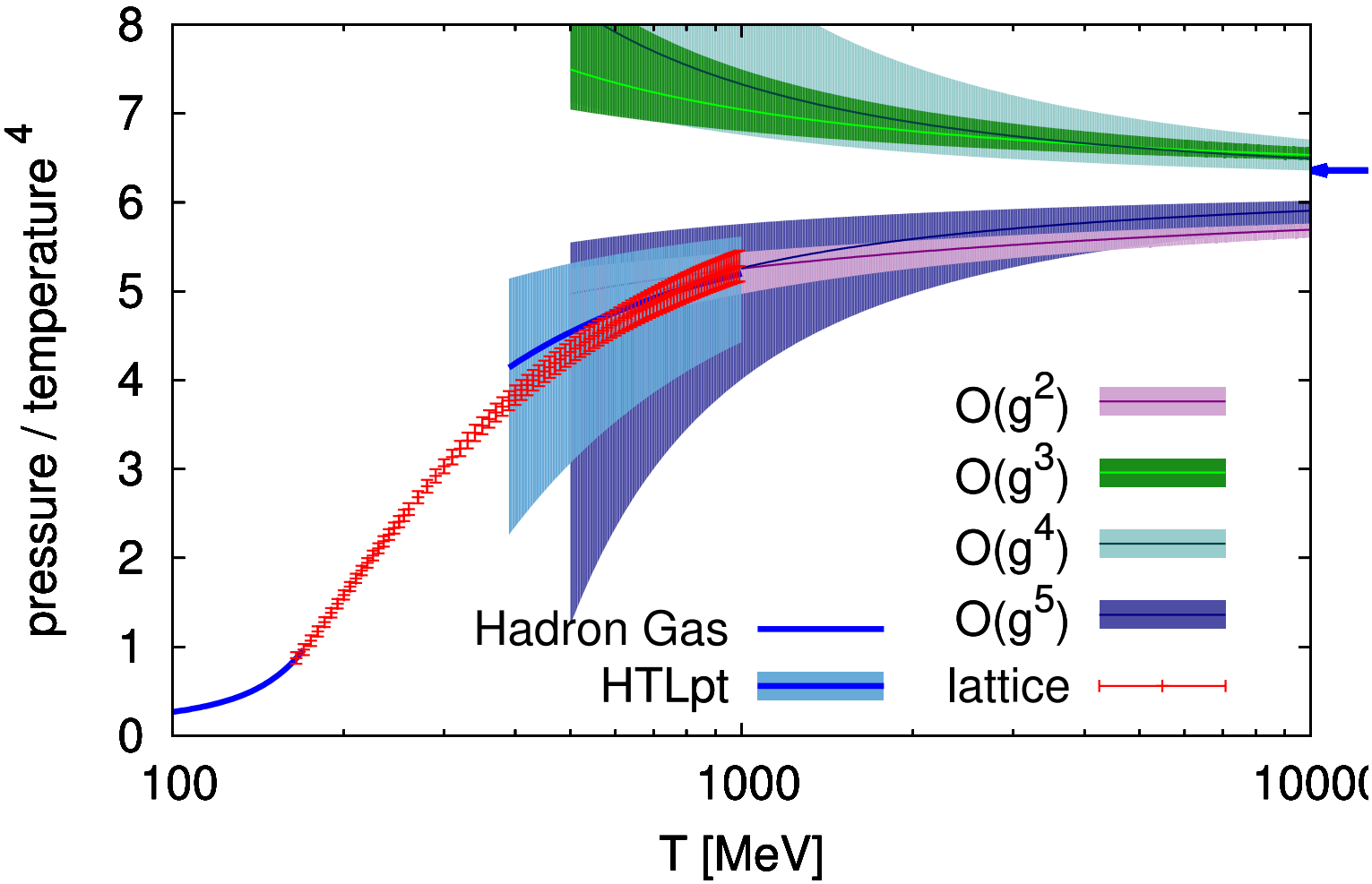
The QCD free energy



HTL pertubation theory shifts the center of the expansion and convergens better. [Braaten & Pisarski 1989]

Here we show the state of the art NNLO result. [Andersen 2011]

The QCD free energy

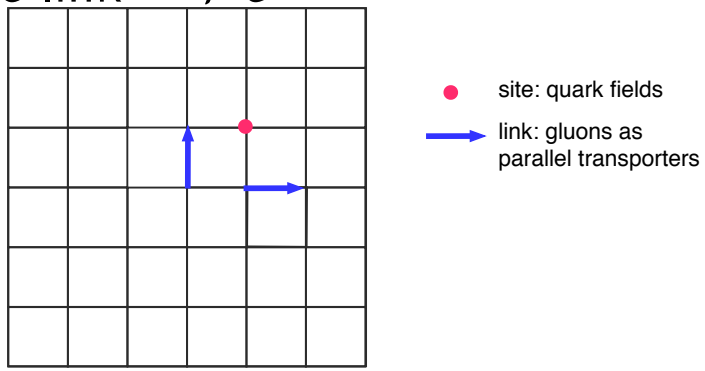


Lattice QCD simulations build a bridge between the two phases. [WB 2016]
Restoration of the chiral symmetry: Transition is crossover at 155 MeV

[WB 2006]

What is a lattice simulation?

The update algorithm solves the path integral of discretized QCD.
Gauge configuration: One set of parallel transporters: one SU(3) matrix on each lattice link $= \mathcal{P} e^{\int d\vec{x}\vec{A}}$



Each gauge configuration has a well defined probability that matches its the path integral **after the fermions are integrated out**.

$$Z = \int DAD\bar{\psi}D\psi e^{-S_{\mathrm{QCD}}(A,\bar{\phi},\phi)} = \int DAe^{-S_{\mathrm{eff}}(A)} \tag{8}$$

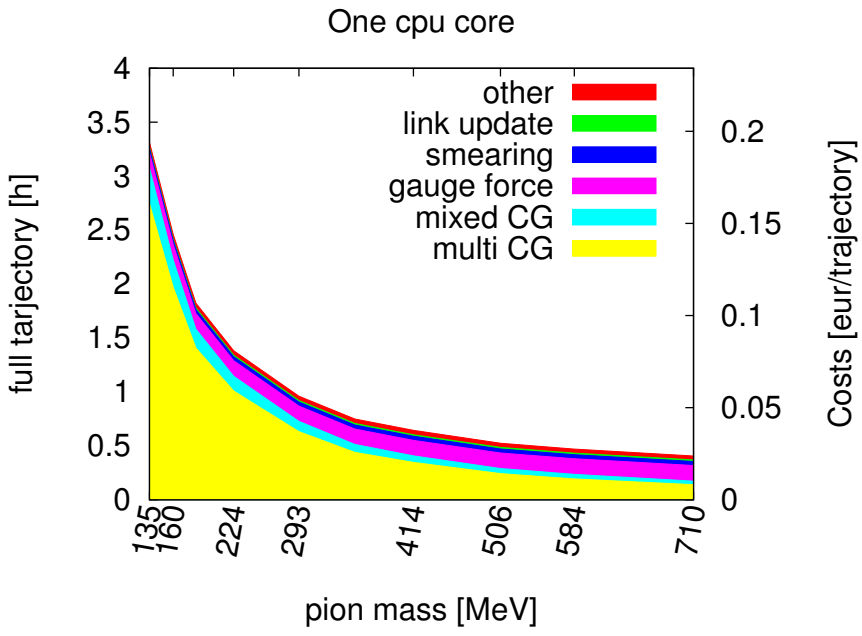
This effective action is not local. The Monte Carlo update is highly sophisticated. It requires the iterative solution of the Dirac equation:

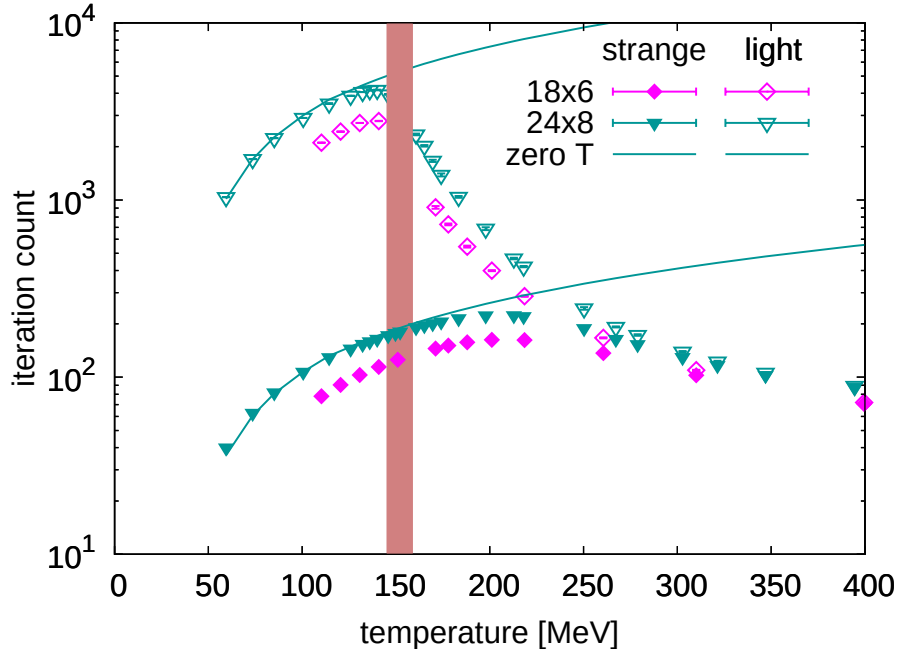
$$(\gamma^{\mu}(\partial_{\mu} + gA_{\mu}) + m)\psi = \eta \qquad \psi =? \tag{9}$$

This is the most time consuming task in a simulation.

Challenges of lattice QCD – costs

Costs are rising with smaller pion mass (iteration count, volume)
Costs are rising with lattice spacing (more sites, renormalization, autocorrelation, iteration count):
Costs peak in the transition regime.





Today, 1000 configurations on a $64^3 \times 16$ lattice cost about 1 million core hours.

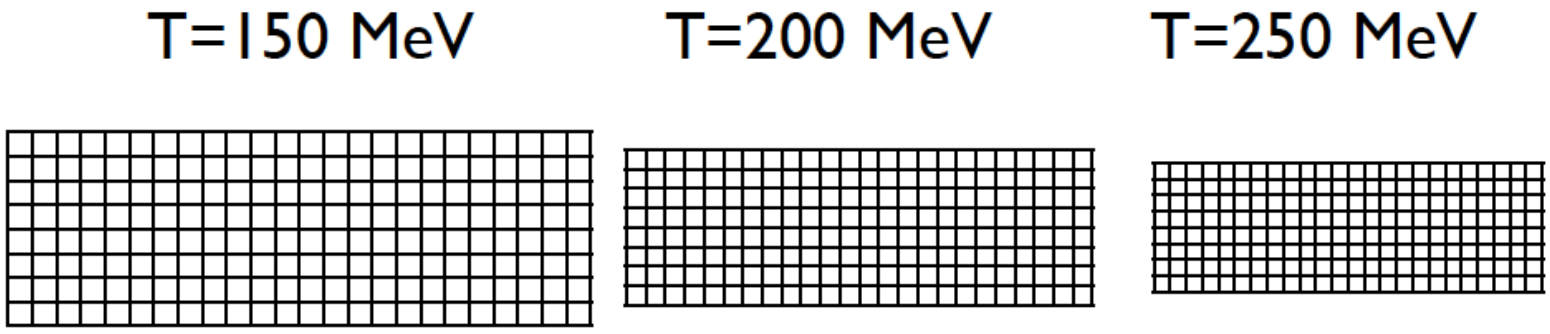
Traditional supercomputer: 1 million core hours = cca 30 k€, 15 tons CO_2
GPU based supercomputer: 1 million core hours = cca 10 k€, 6 tons CO_2

JUQUEEN supercomputer at FZ-Jülich

458,752 cores, 5.9 Petaflops

How do we set the parameters

Temperature: the 4th Euclidean direction's length is $aN_t = 1/T$.



The geometry is typically kept constant. As the Euclidean time direction $1/T$ shrinks, the whole lattice shinks. T is tuned through a.

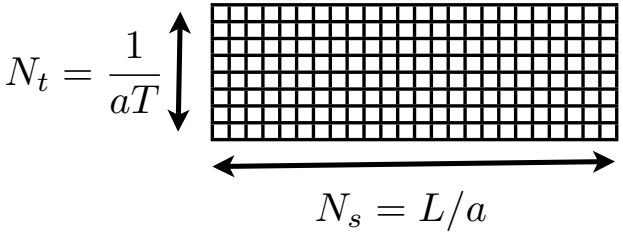
In lattice QCD the lattice spacing is not an external parameter. We have to measure a mass (e.g. aM_Ω) to find out.

We have to give g^2 on the scale of the lattice spacing.
High temperature $\rightarrow$ fine lattice $\rightarrow$ small coupling.

For each coupling we have to tune the masses such, that at very low temperature the experimental hadron spectrum is recovered. Then we do a finite temperature simulation with the same renormalized mass parameters.

Thermodynamics on the lattice

Lattice action is the used to discretize QCD on a space-time grid.

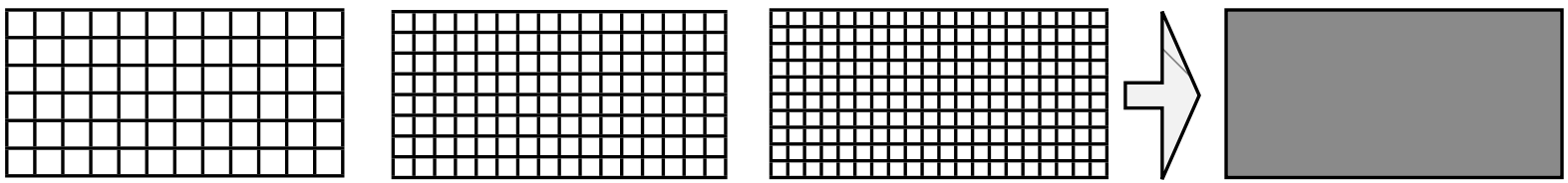


We solve the path integral for the fermions first, and simulate the resulting effective gauge action.

Typical lattice spacings in fermi

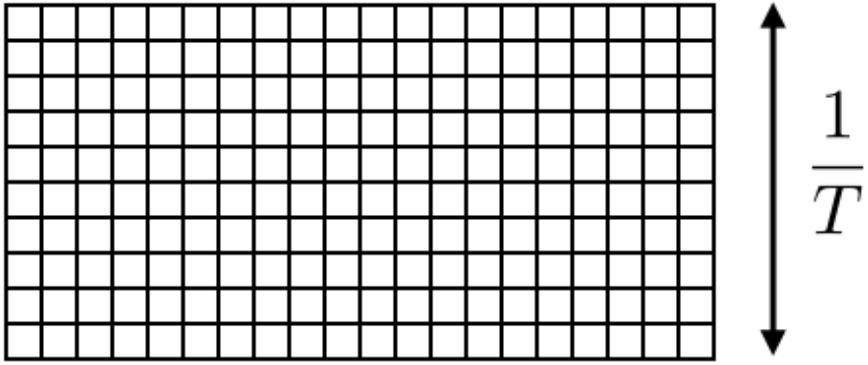
	Nt				
T	6	8	10	12	16
150	0,219	0,164	0,132	0,11	0,082
300	0,11	0,082	0,066	0,055	0,041
600	0,055	0,041	0,033	0,027	0,021
1000	0,033	0,025	0,02	0,016	0,012

Continuum limit:

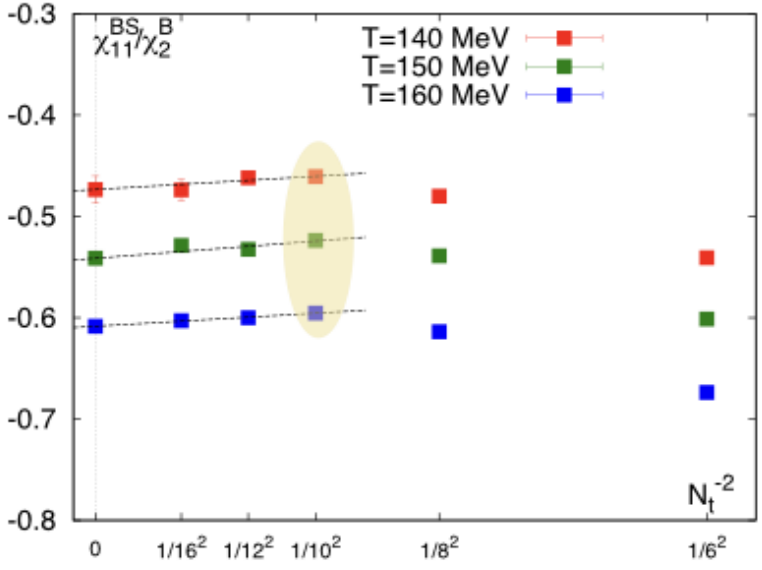


Most observables scale as $X = X_0 + X_1/N_t^2 + \ldots$.

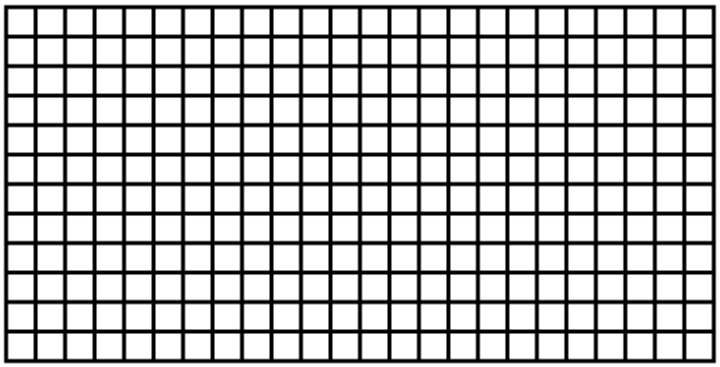
N_t=10



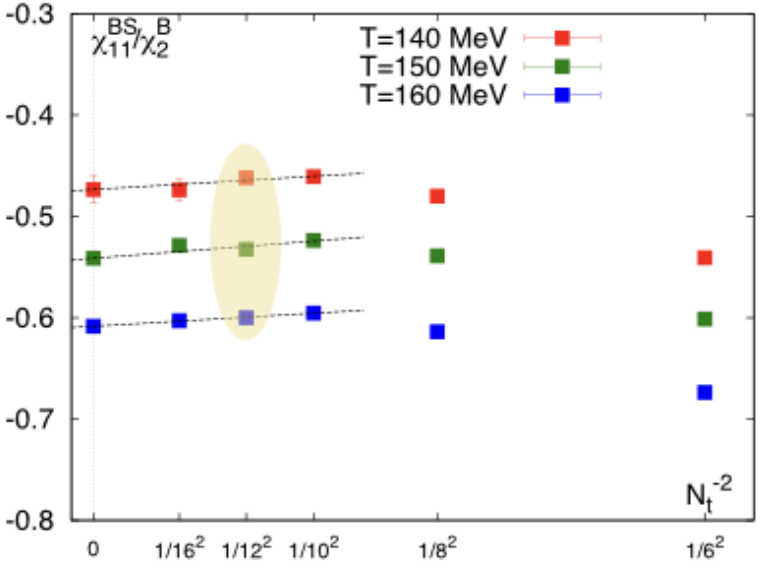
$$\frac{1}{T}$$


-0.3
-0.4
-0.5
-0.6
-0.7
-0.8
χ_{11}^{BS}/χ_2^B
T=140 MeV
T=150 MeV
T=160 MeV
N_t^{-2}
0
1/16^2
1/12^2
1/10^2
1/8^2
1/6^2

N_t=12



$$\frac{1}{T}$$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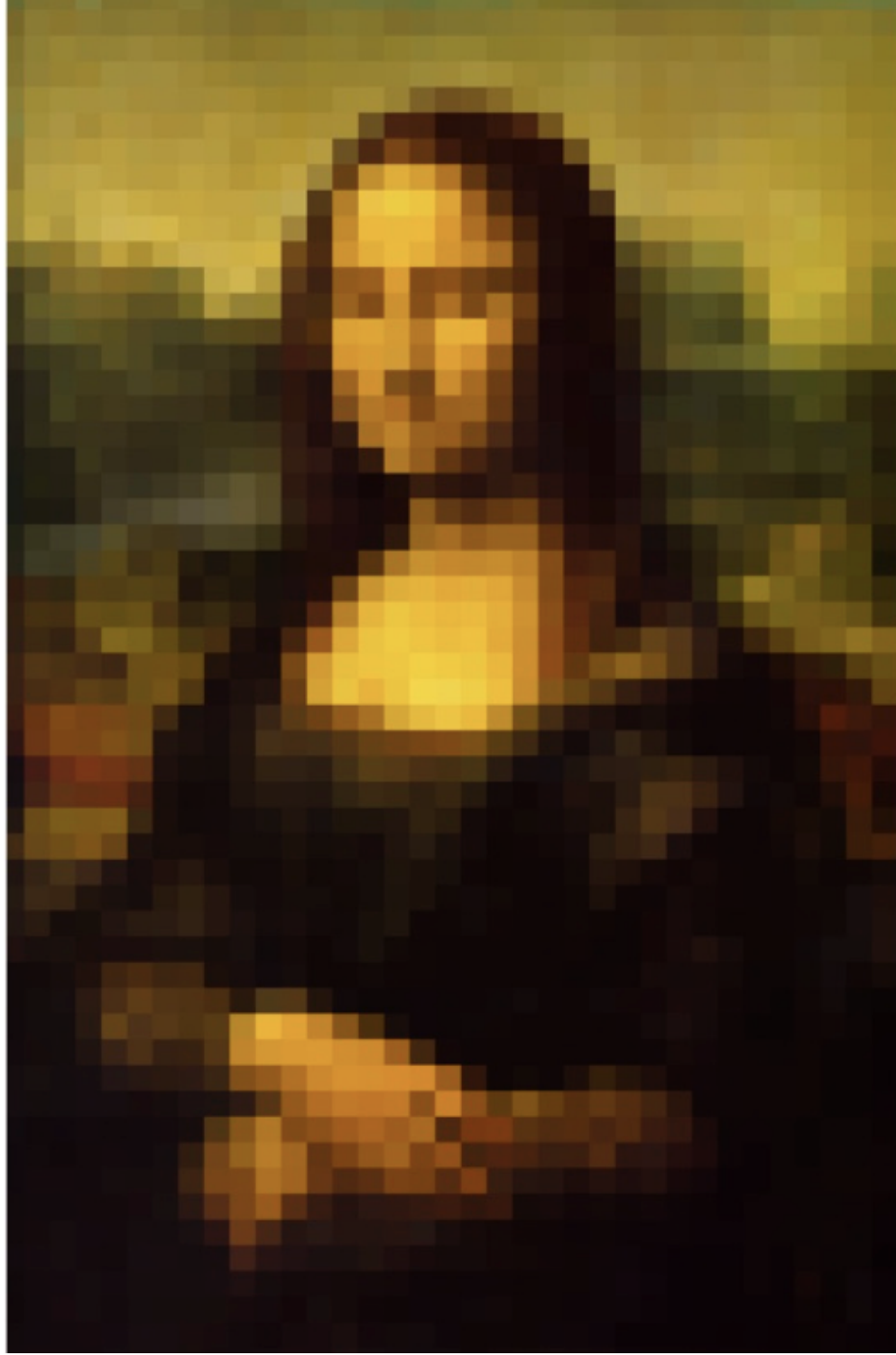
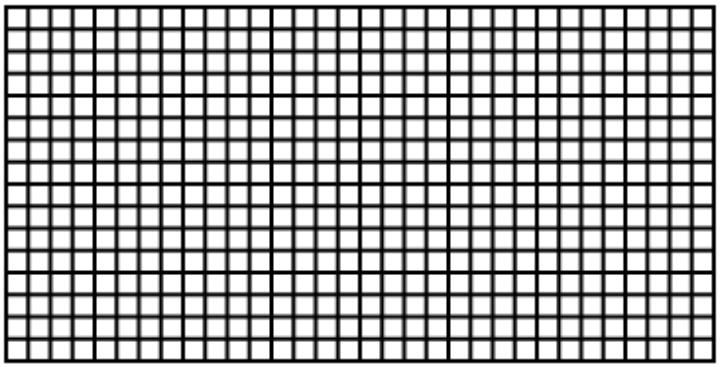
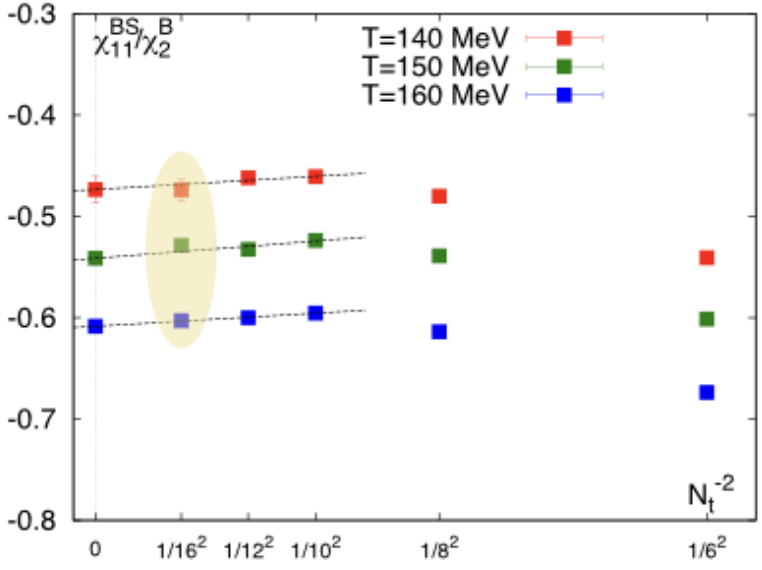


N_t=16



$\frac{1}{T}$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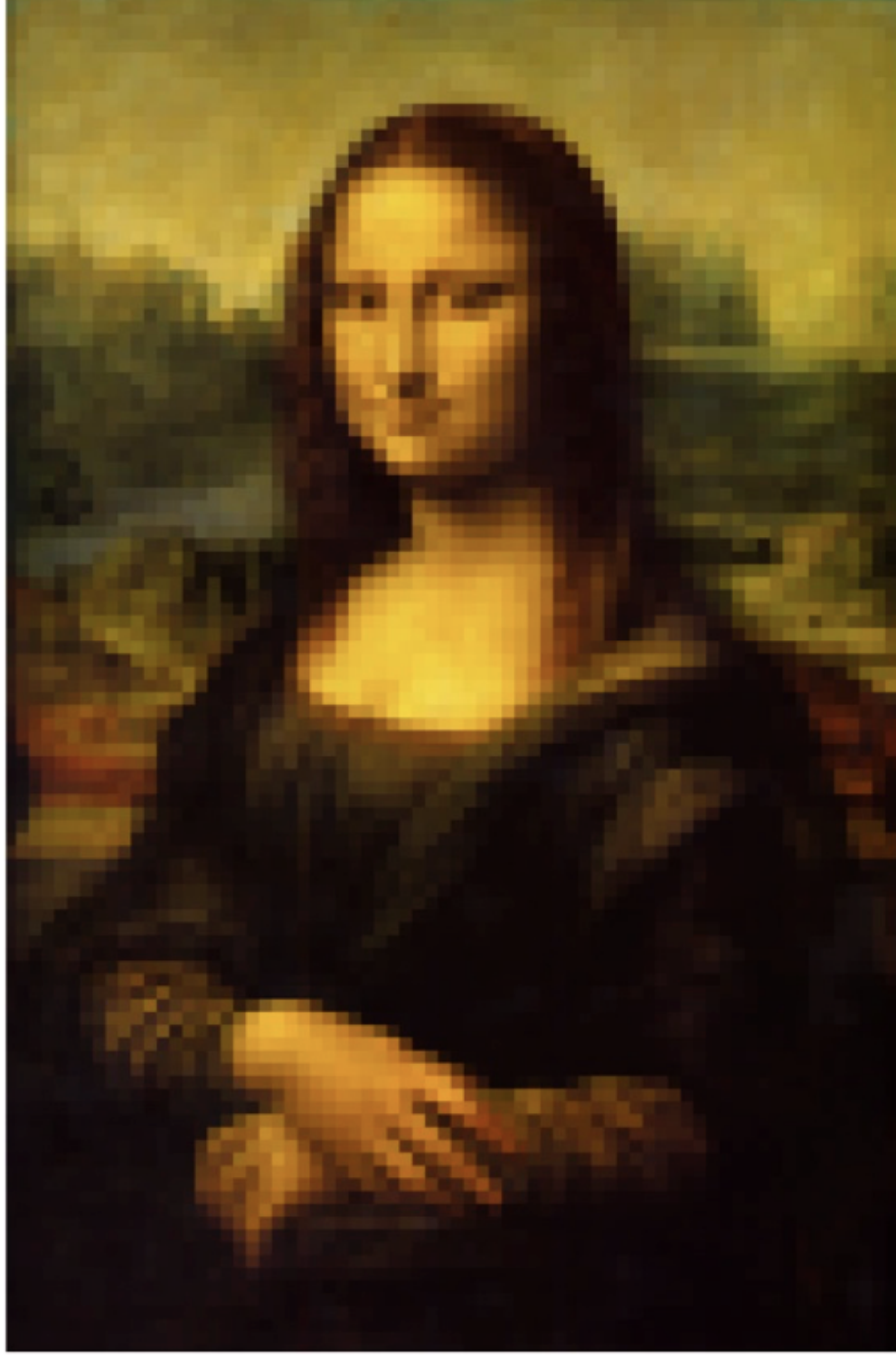
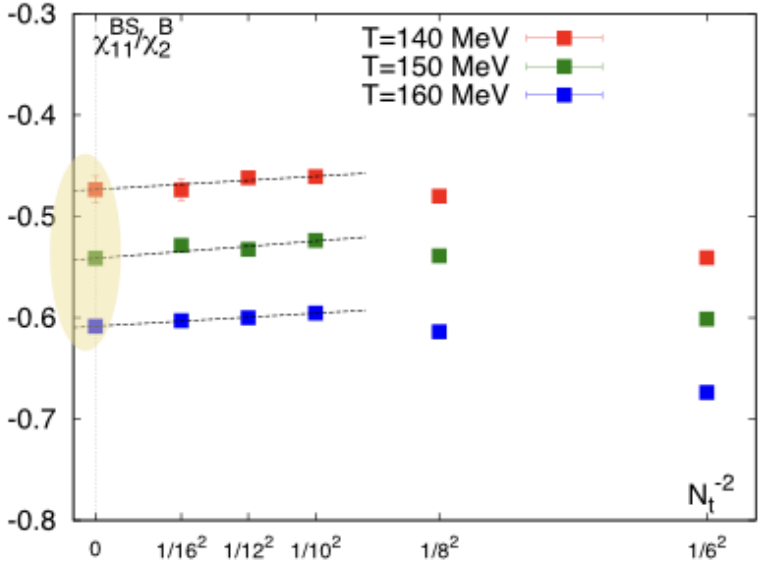
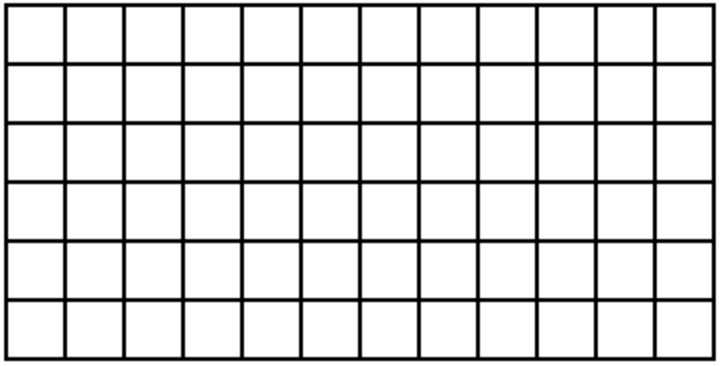


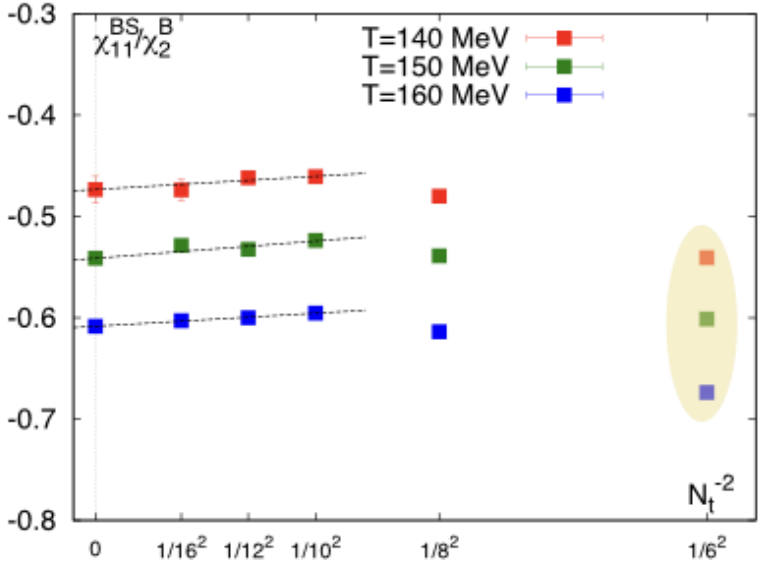
continuum limit



N_t=6



$$\frac{1}{T}$$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T=150 MeV
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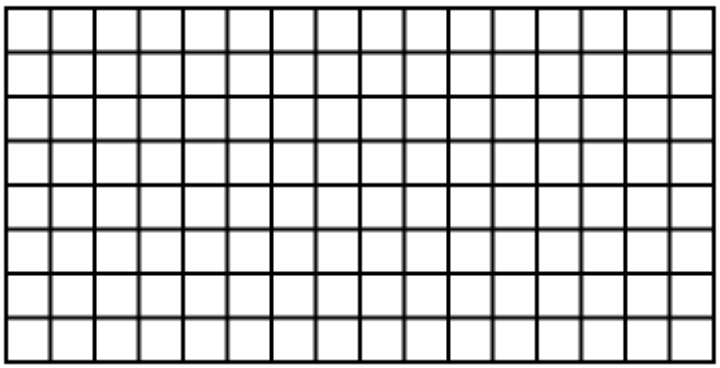
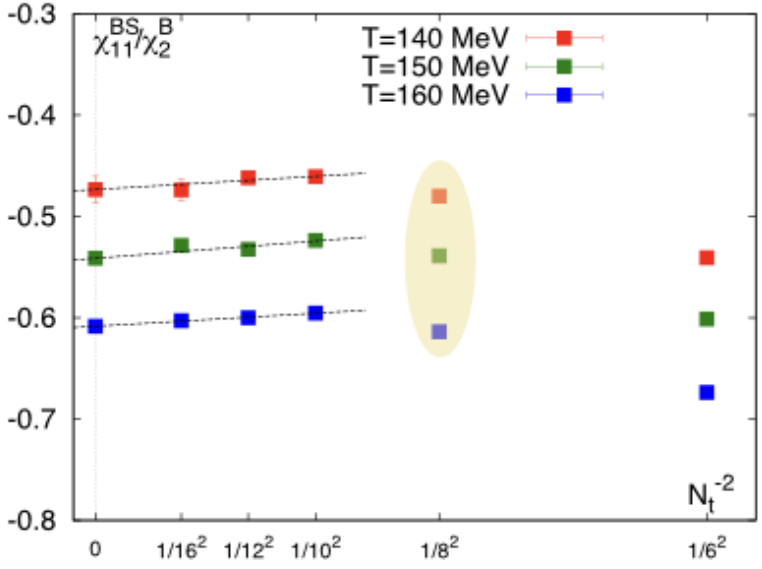
-0.4
-0.5
-0.6
-0.7
-0.8
0
1/16²
1/12²
1/10²
1/8²
1/6²
N_t^{-2}

N_t=8



$\frac{1}{T}$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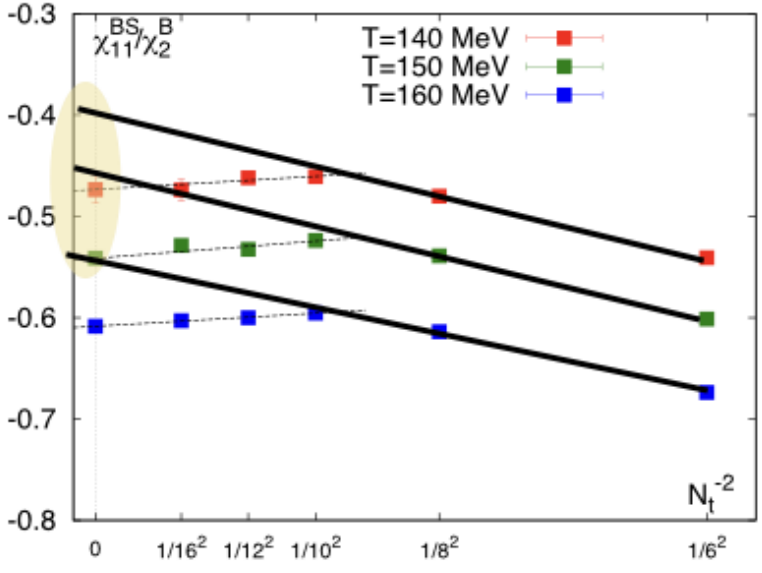
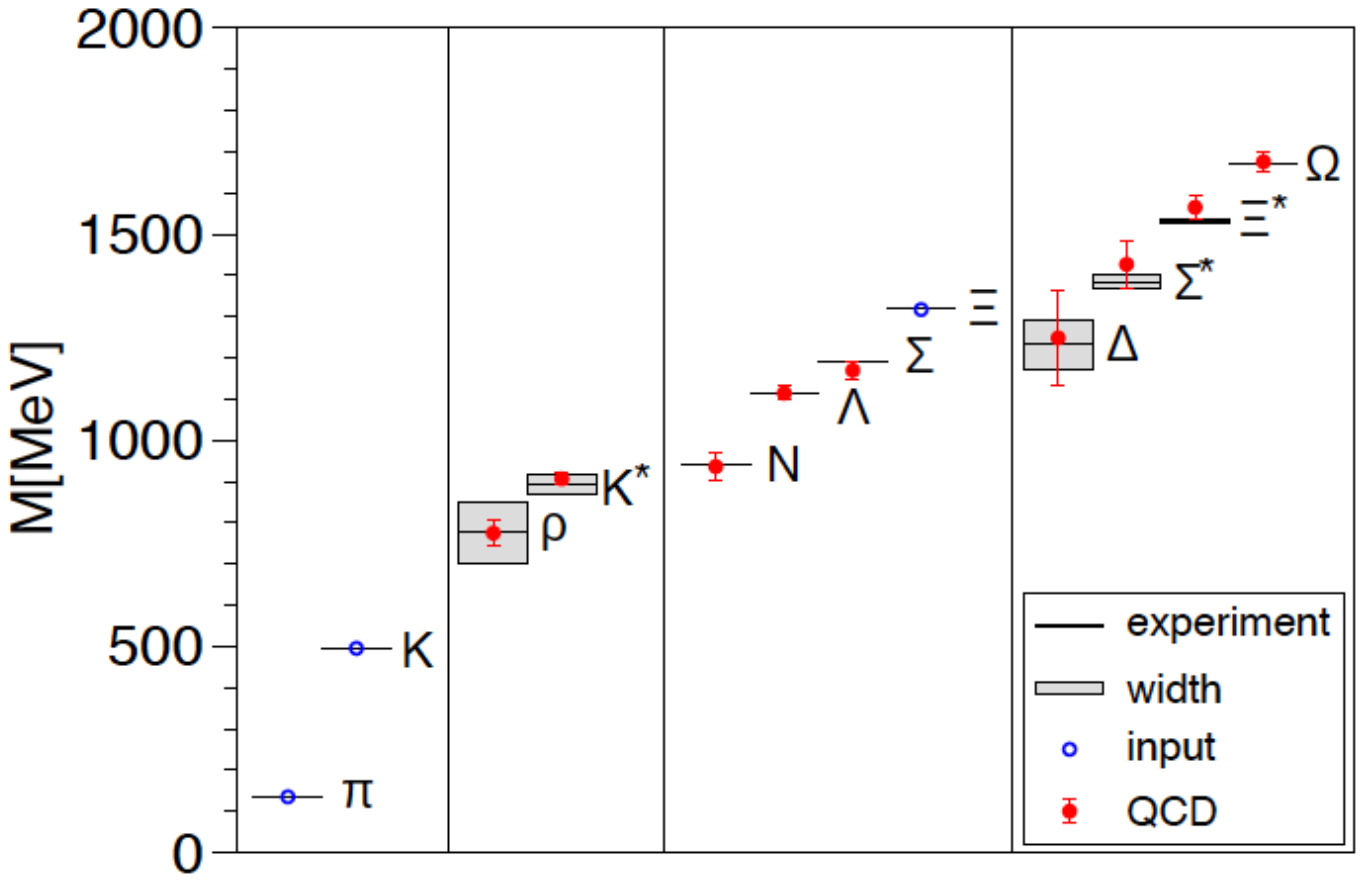
False continuum limit

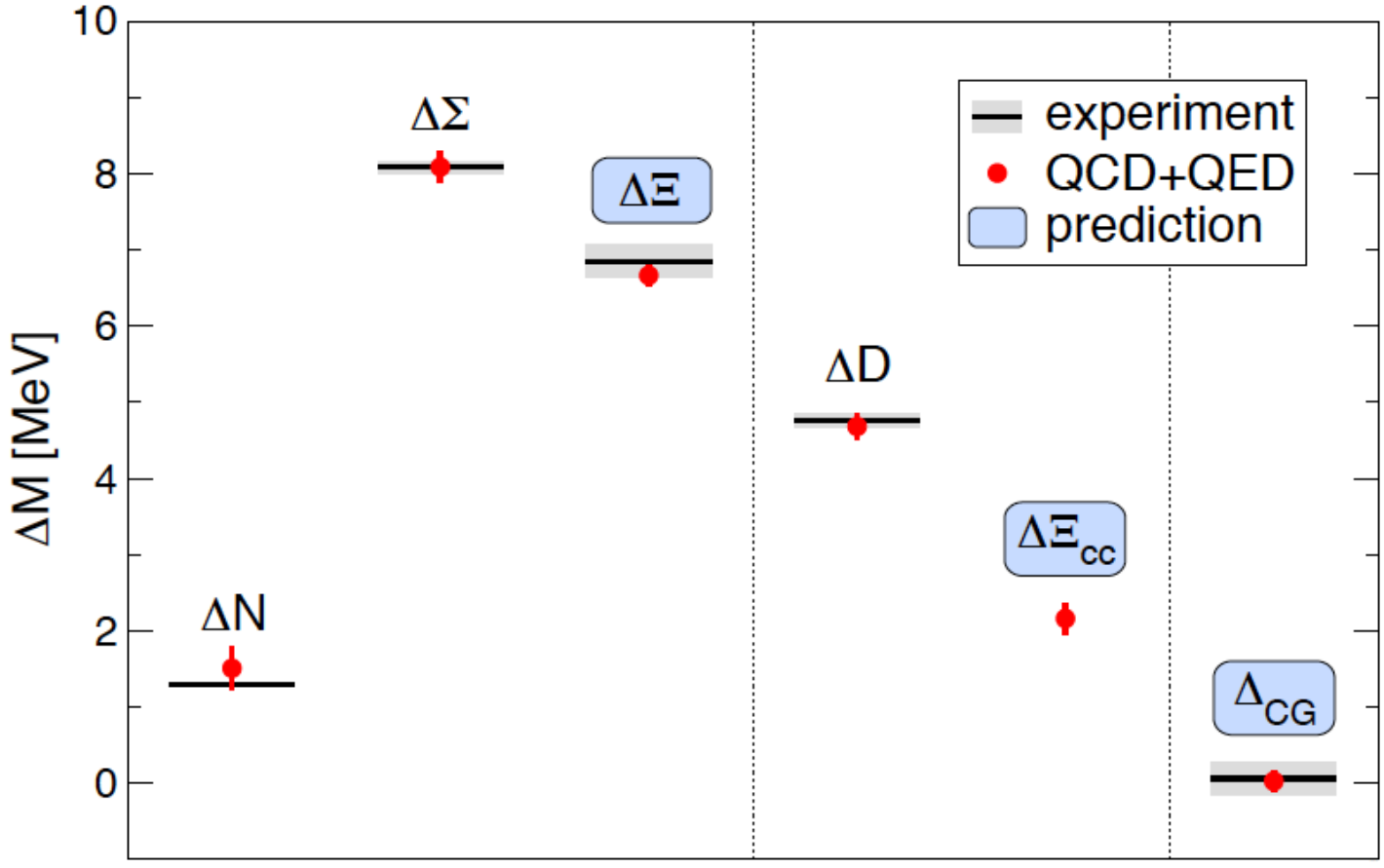


Spectrum of light hadrons

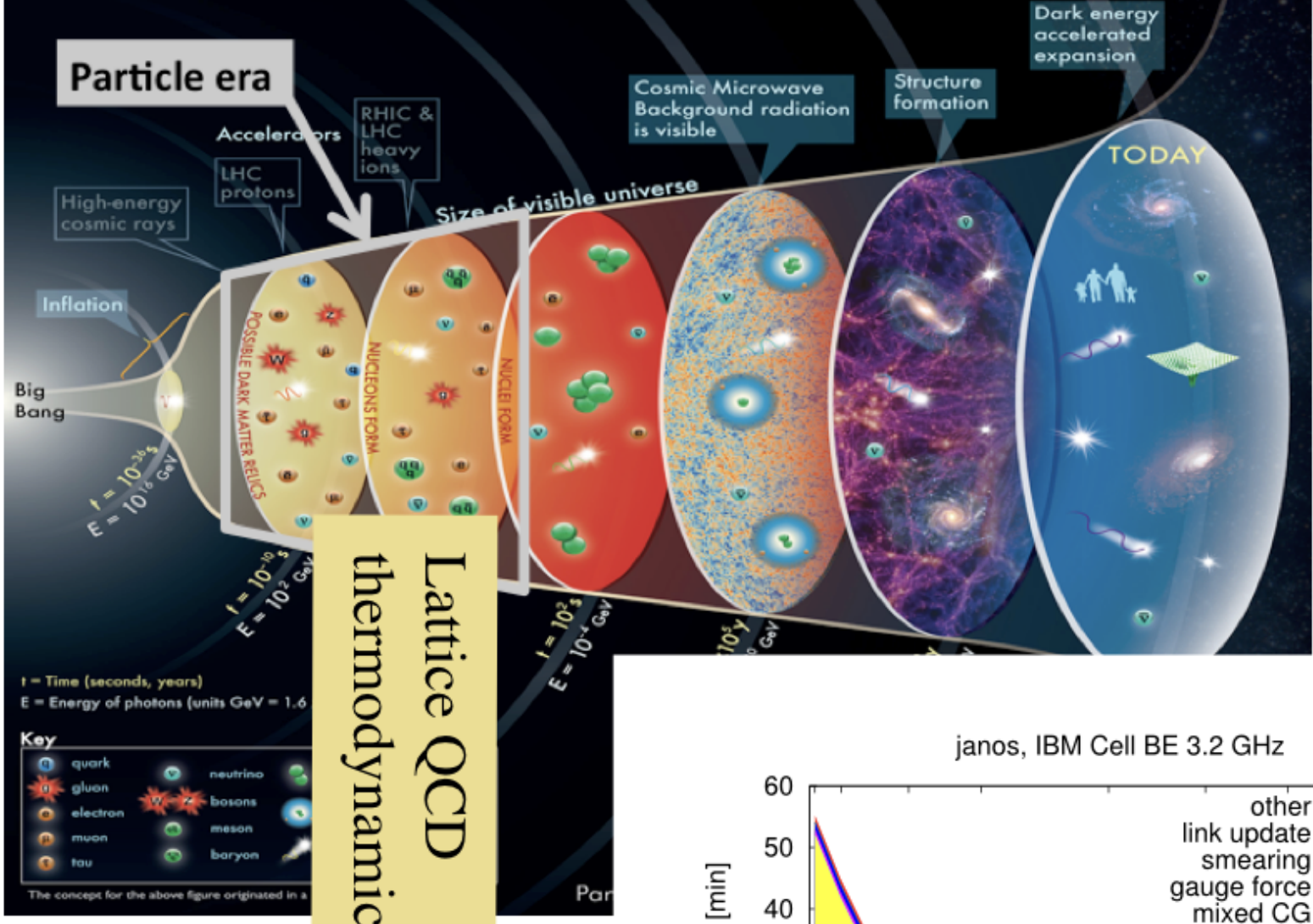


[Budapest–Marseille–Wuppertal Science 322 (2008) 1224]

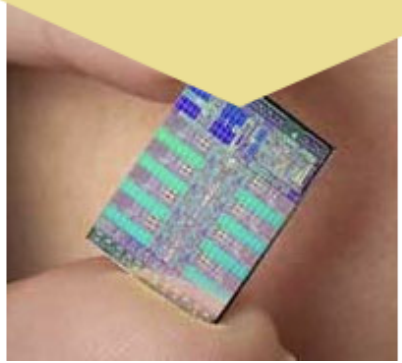
Electromagnetic and strong isospin breaking effects in the spectrum

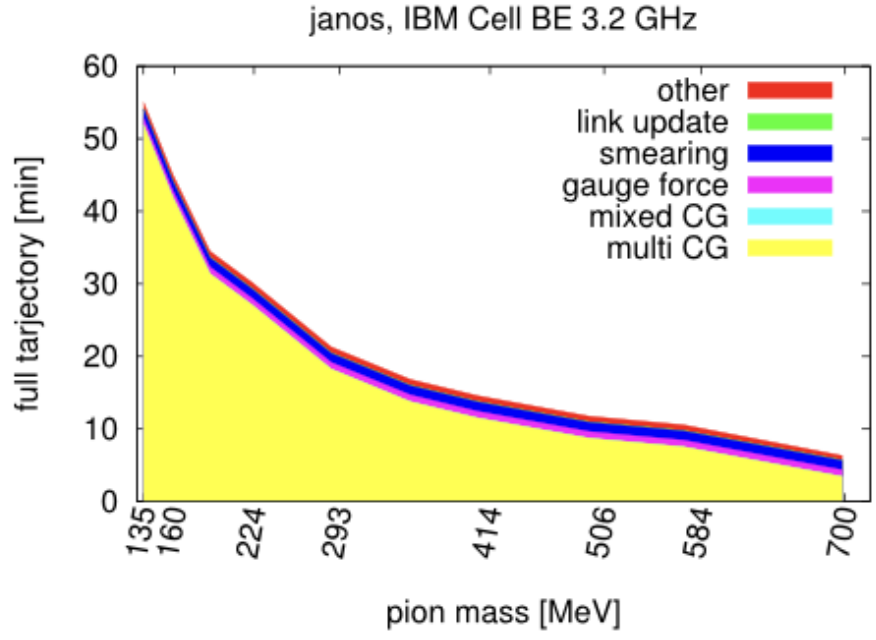


[Budapest–Marseille–Wuppertal Science 347 (2015) 1452]



Lattice QCD thermodynamics

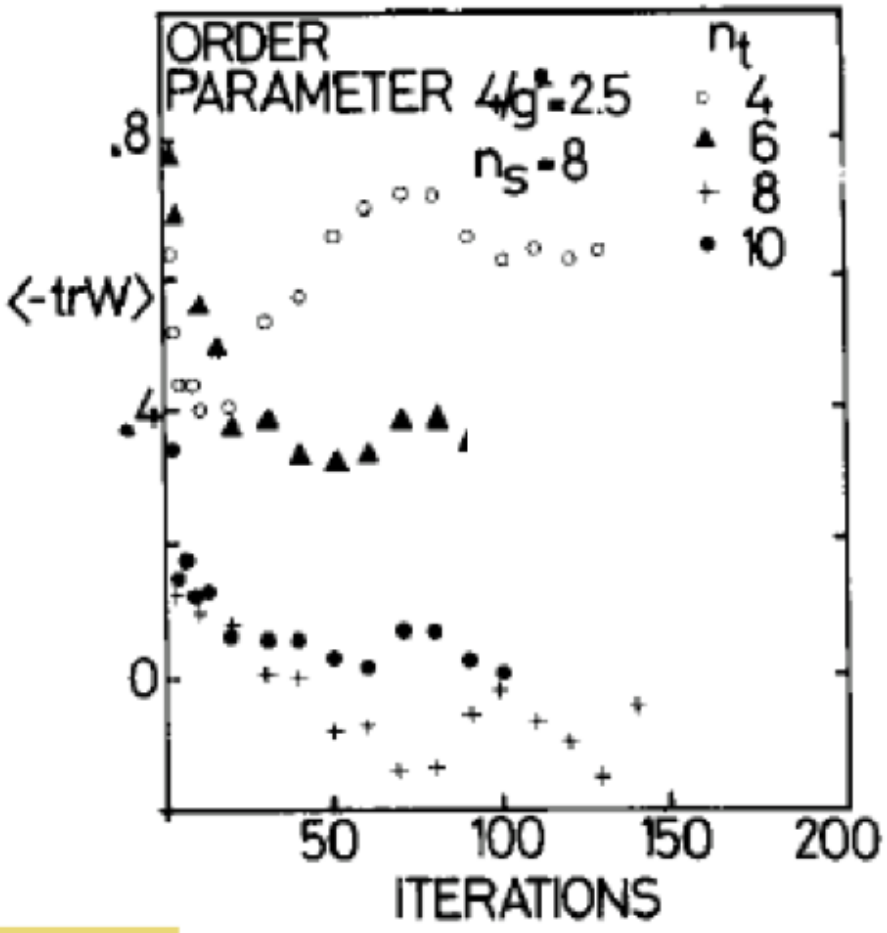




The story begins in 1981 …

$\frac{1}{T_{\text{hot}}}$

$\frac{1}{T_{\text{cold}}}$



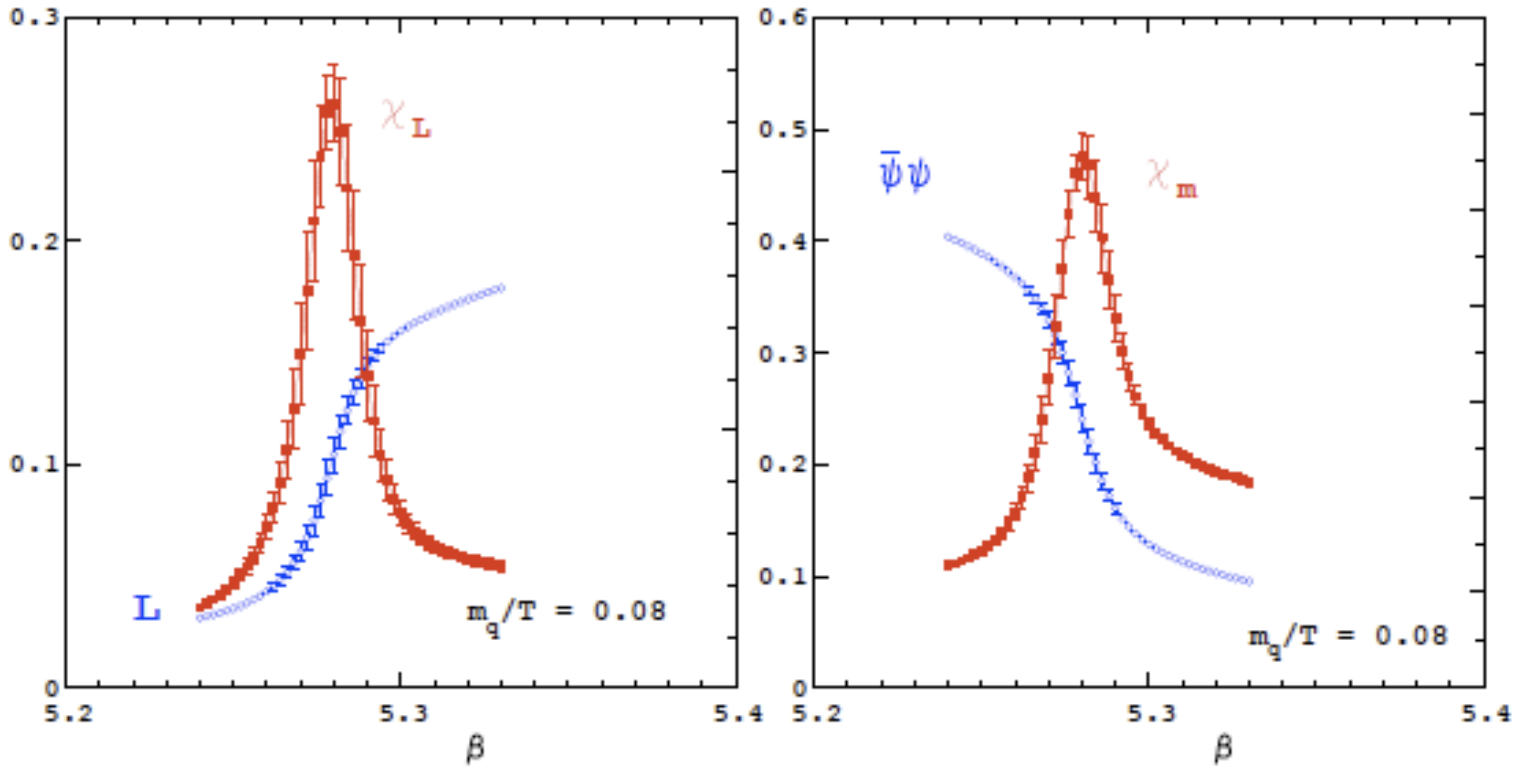
Deconfinement

Confinement

First numerical evidence for the QCD transition

[Kuti, Polonyi, Szlachanyi **Phys Lett B 98, 199** (1981)]
[McLerran, Svetitsky **Phys Lett B 98, 195** (1981)]

The Polyakov loop and its susceptibiltiy (left),
The chiral condensate and its susceptibiltiy (right):



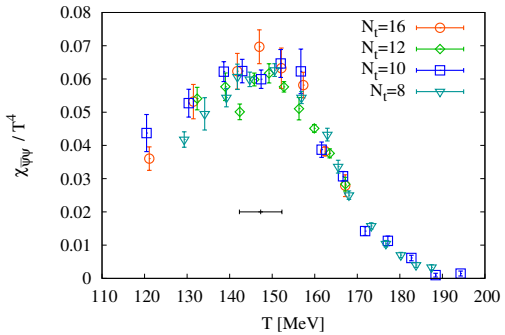
[(Karsch hep-lat/0106019; Schladming 2001)]

Observables

Chiral susceptibility:

$$\chi_{\bar{\psi}\psi} = \frac{T}{V}\frac{\partial^2 \ln Z}{\partial (m_q)^2}$$

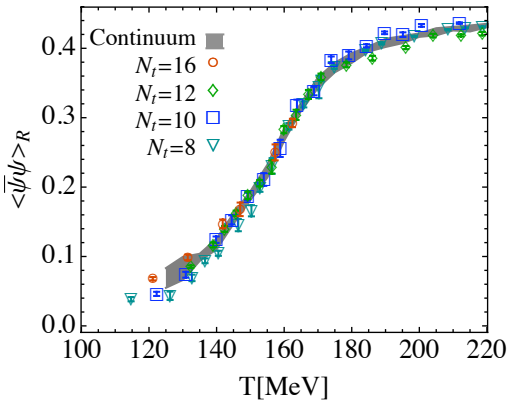
$$\chi^r_{\bar{\psi}\psi} = \left(\chi_{\bar{\psi}\psi}(T,\beta) - \chi_{\bar{\psi}\psi}(0,\beta)\right)\frac{m_l^2}{m_\pi^4}$$



Chiral condensate:

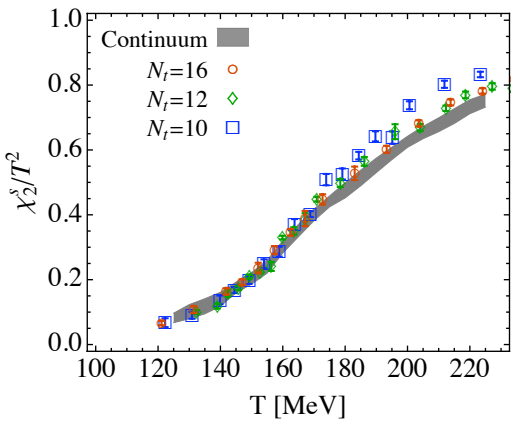
$$\langle\bar{\psi}\psi\rangle = \frac{T}{V}\frac{\partial \ln Z}{\partial m_q}$$

$$\langle\bar{\psi}\psi\rangle^r = -\left(\langle\bar{\psi}\psi\rangle(T,\beta) - \langle\bar{\psi}\psi\rangle(0,\beta)\right)\frac{m_l}{m_\pi^4}$$



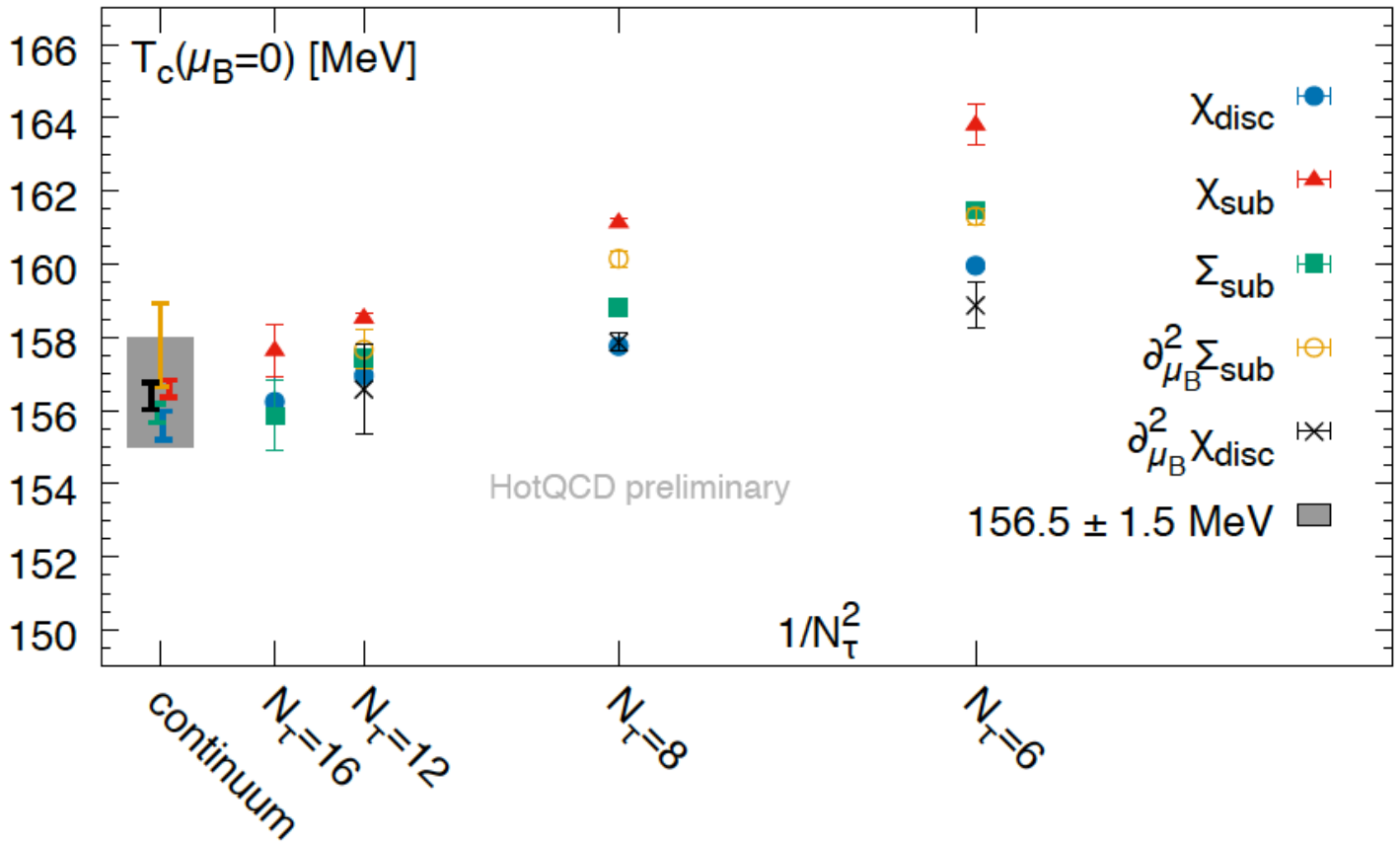
Strangeness susceptibility:

$$\chi ss = \frac{T}{V}\frac{\partial^2 \ln Z}{\partial (\mu_s)^2}$$



[WB arXiv:1005.3508]

Transition temperature, re-calculated in 2018

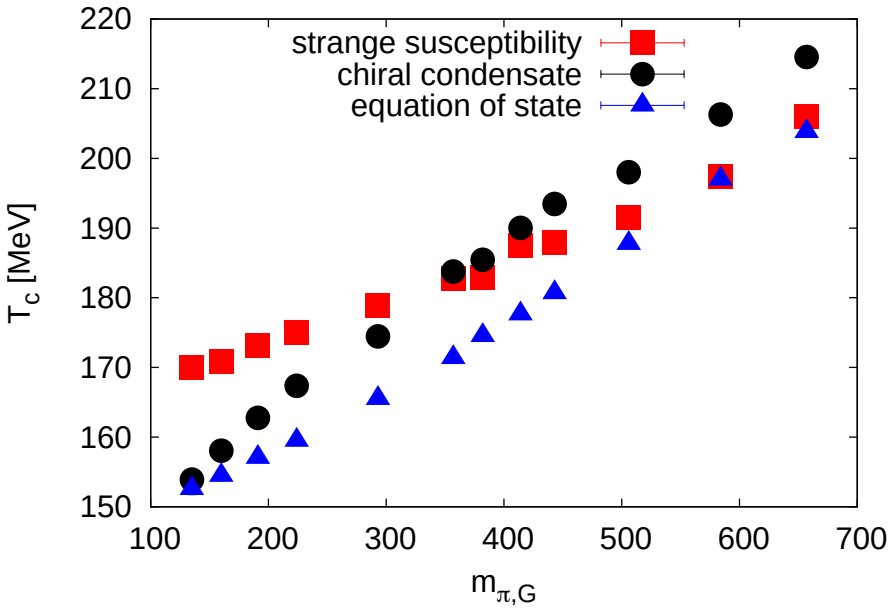


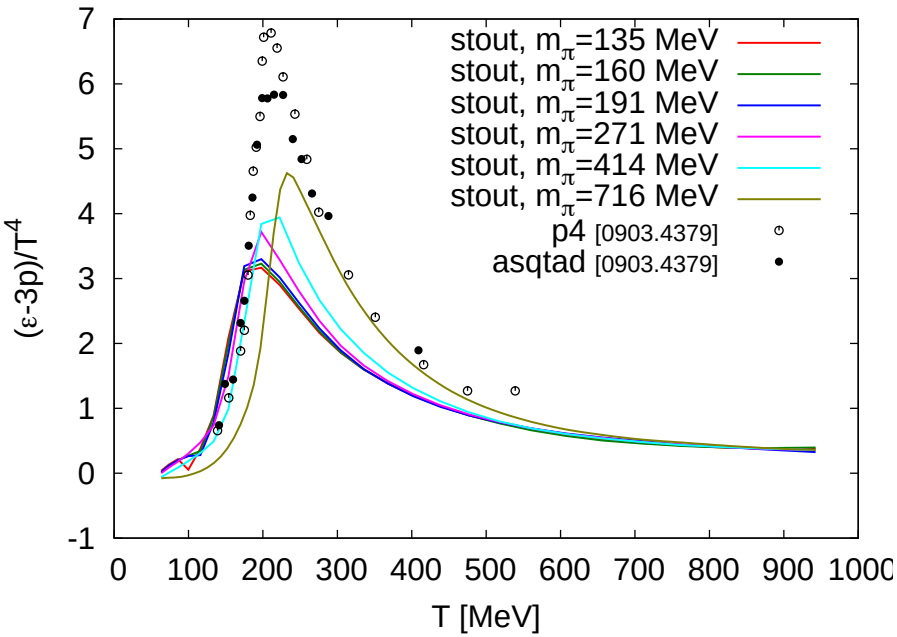
[Presented by Patrick Steinbrecher (HotQCD) at the Quark Matter 2018]

Pion mass dependence

Why do "physical quark masses" matter?

Thermodynamics is quite sensitive to the pion mass.





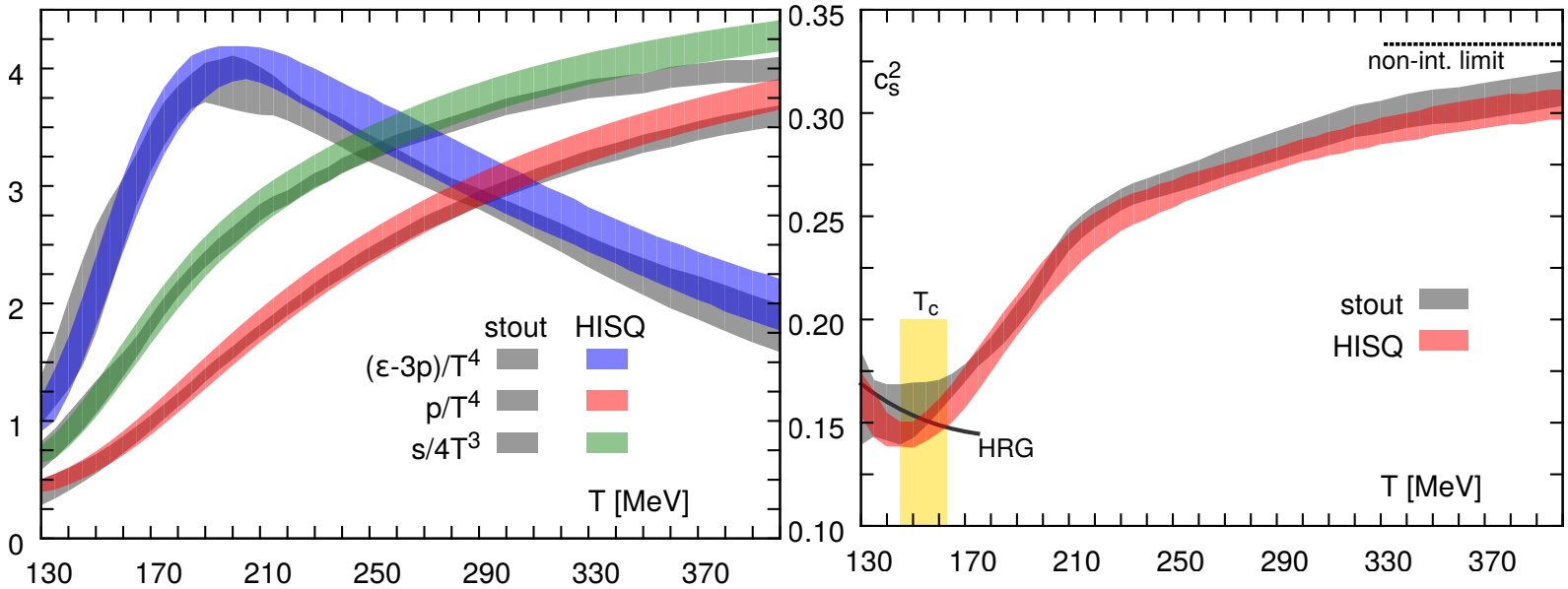
This is a result of an unpublished exploratory study from 2010, by the Wuppertal-Budapest group

$$\frac{p(T)}{T^4} = -\frac{F(T)}{VT^4}; \qquad \frac{\epsilon - 3p}{T^4} = T\frac{d}{dT}\frac{p(T)}{T^4} \tag{10}$$

In a 1st order transition $p(T)$ is continuous, $\epsilon(T)$ (and $\epsilon - 3p$) jumps.

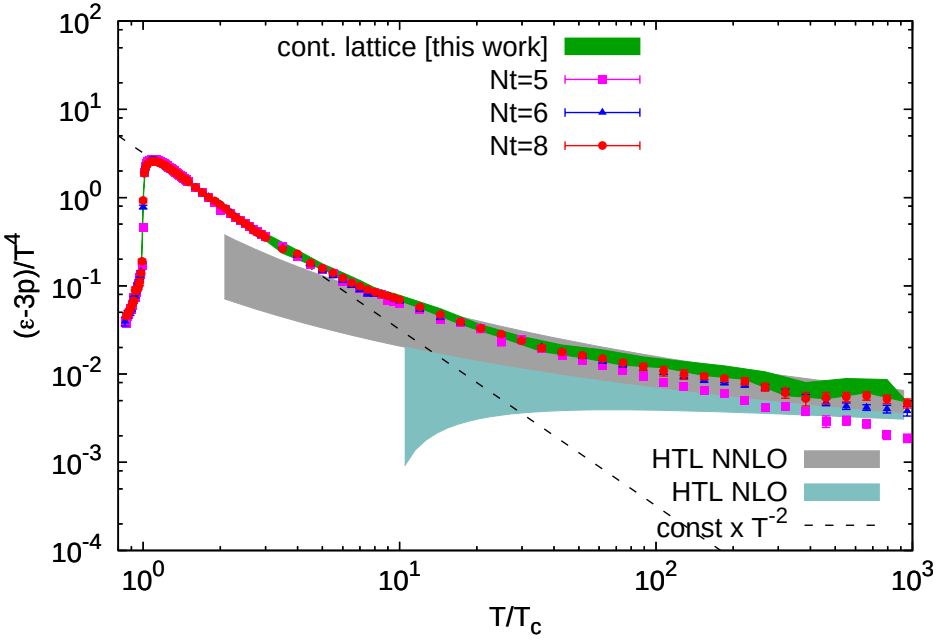
Equation of state with up,down and strange quarks

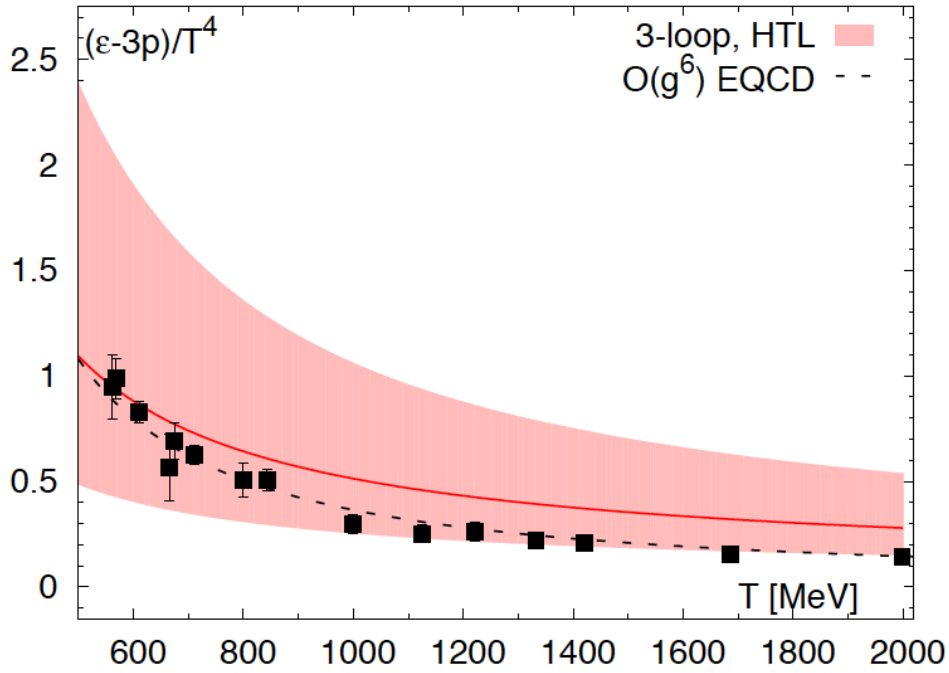
stout result: Wuppertal-Budapest group [1309.5258]
HISQ result: Bielefeld-Brookhaven group [1407.6397]



Around the transition temperature $(\epsilon - 3p)/T^4$ has a steepest point, the speed-of-sound has a minimum

Equation of state at perturbative temperatures





SU3 theory: [Wuppertal-Budapest JHEP 1207 (2012) 056]

2+1 flavars: [Bazavov-Petreczky-Weber PRD97 (2018) 1]

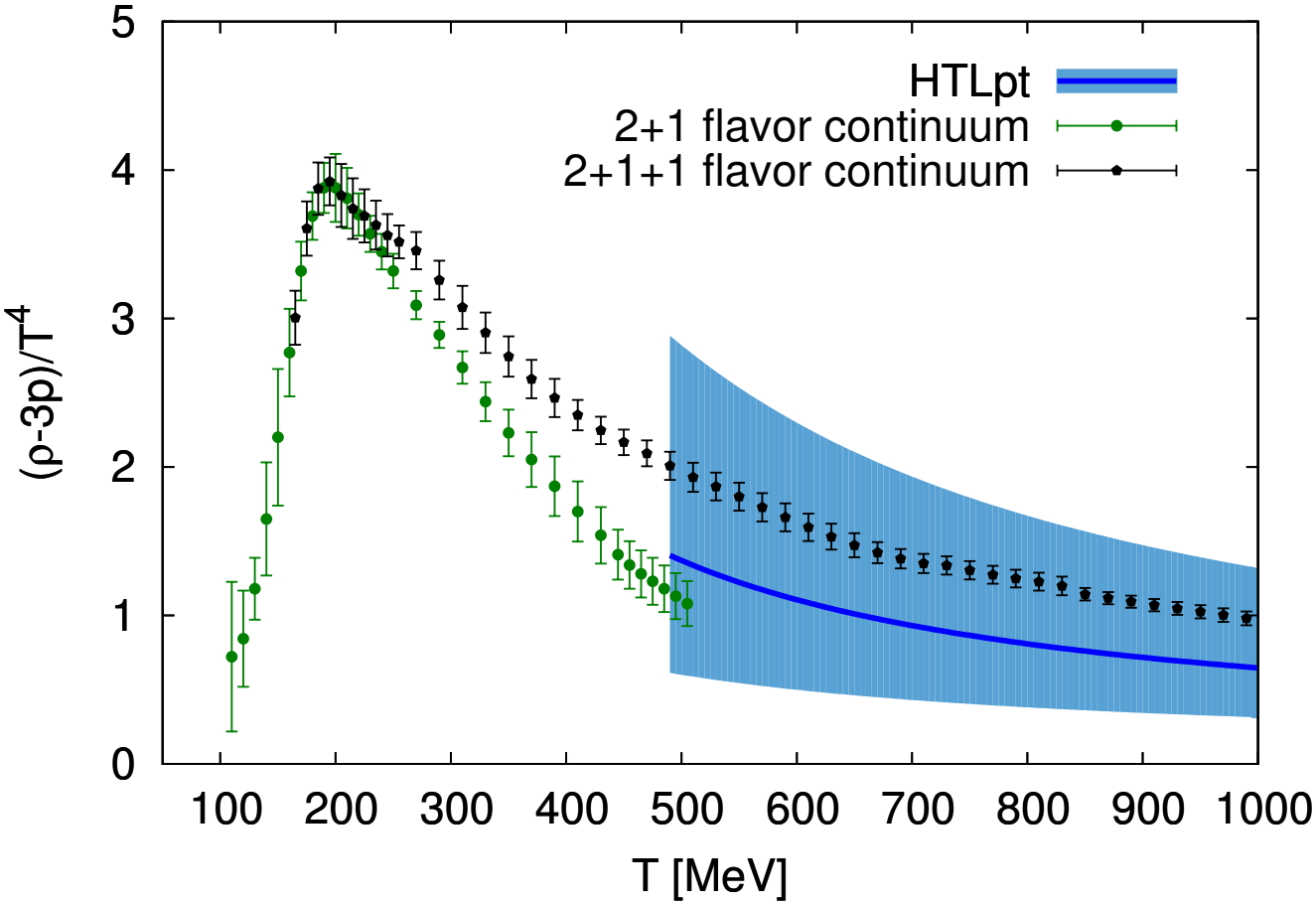
For 2+1+1 flavars see : [Wuppertal-Budapest Nature 539 (2016) 69]

HTL NLO: [Andersen et al PRD 66,085016 (2002)]

HTL NNLO: [Andersen et al PRL 104,122003 (2010)]

Equation of state at high temperatures

Effect of the charm quark: mostly relevant for **cosmology**



The ratio of the two results can be described by a tree-level threshold function.

[Wuppertal-Budapest: 1606.07494]

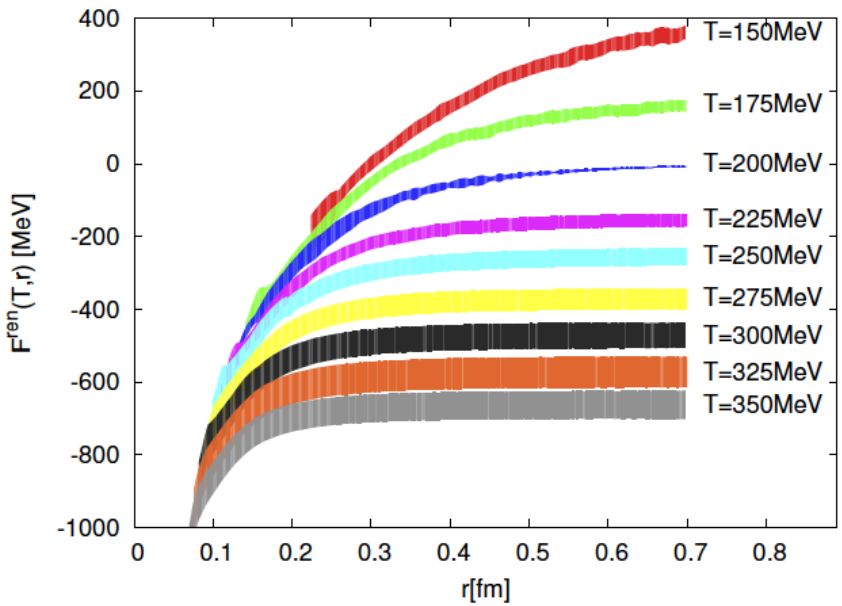
What do heavy quarks feel?

At high T the potential between heavy quark and antiquarks flattens out:

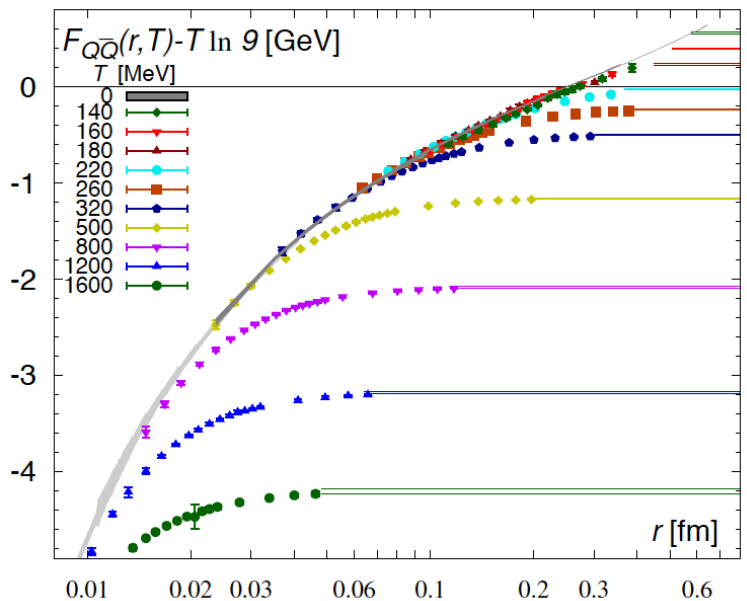
$$F_{Q\bar{Q}}(r,T) \sim f(T)\frac{1}{r}e^{-Mr} \tag{11}$$

whereas at low T the potential follows the Cornell form with string tenison σ

$$\frac{a}{r} + \sigma r + C \tag{12}$$



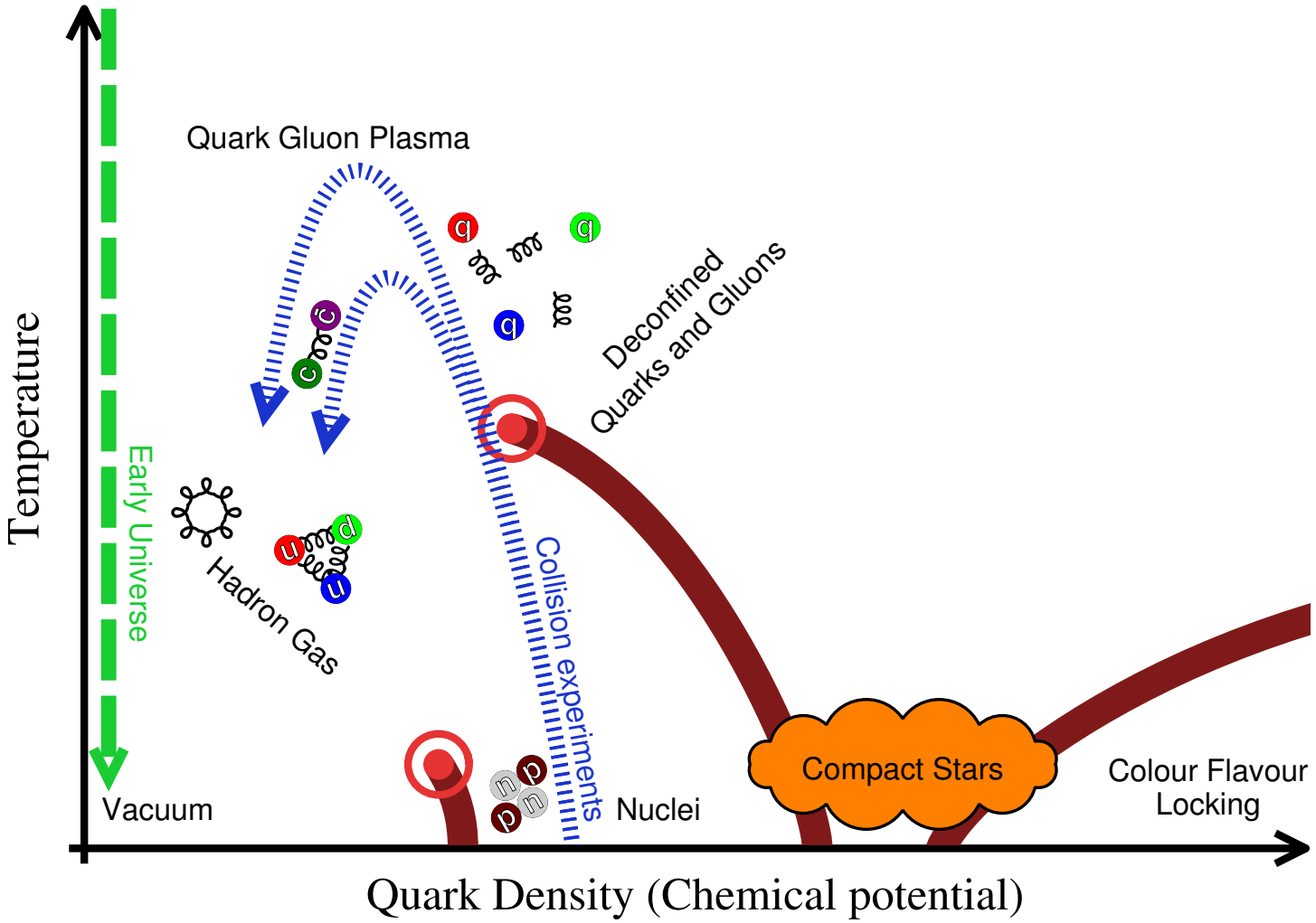
[Wuppertal-Budapest 1501.02173]



[TUM-QCD 1804.10600]

→ *running of the coupling is accessible [Peter Petreczky's talk]*

The QCD phase diagram



Fluctuations in a grand canonical ensemble

First thing you need is a conserved charge: e.g. Baryon number, not $p + \bar{p}$.
Start with a grand canonical partition function: $Z = \mathrm{Tr}\left(e^{-(H-\mu N)/T}\right)$

$$\langle N_q \rangle = \frac{1}{Z}\,\mathrm{Tr}\left[N e^{-(H-\mu_q N_q)/T}\right] = T\frac{\partial \log Z(T, V, \{\mu_q\})}{\partial \mu_q}$$

The response of the system to the thermodynamic force μ_q is proportional to the fluctuation of the conserved charge:

$$\frac{\partial \langle N_i \rangle}{\partial \mu_j} = T\frac{\partial^2 \log Z(T, V, \{\mu_q\})}{\partial \mu_j \partial \mu_i} = \frac{1}{T}(\langle N_i N_j \rangle - \langle N_i \rangle \langle N_j \rangle)$$

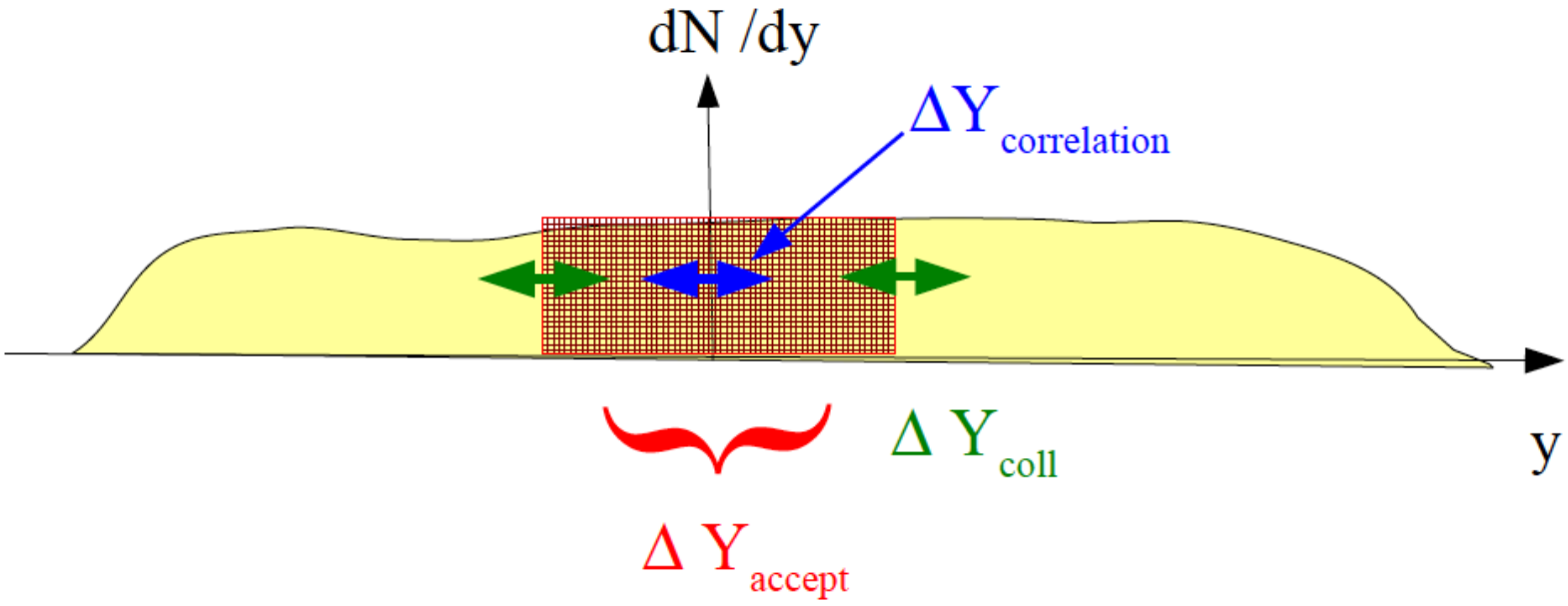
The higher derivatives are the generalized quark number susceptibilities:

$$\chi^{u,d,s,c}_{i,j,k,l} = \frac{\partial^{i+j+k+l}(p/T^4)}{(\partial \hat{\mu}_u)^i (\partial \hat{\mu}_d)^j (\partial \hat{\mu}_s)^k (\partial \hat{\mu}_c)^l}$$

with $\hat{\mu}_q = \mu_q / T$.

Do conserved charges fluctuate?

Count the net number of a charge: **electric**, **baryon**, **strangeness**.

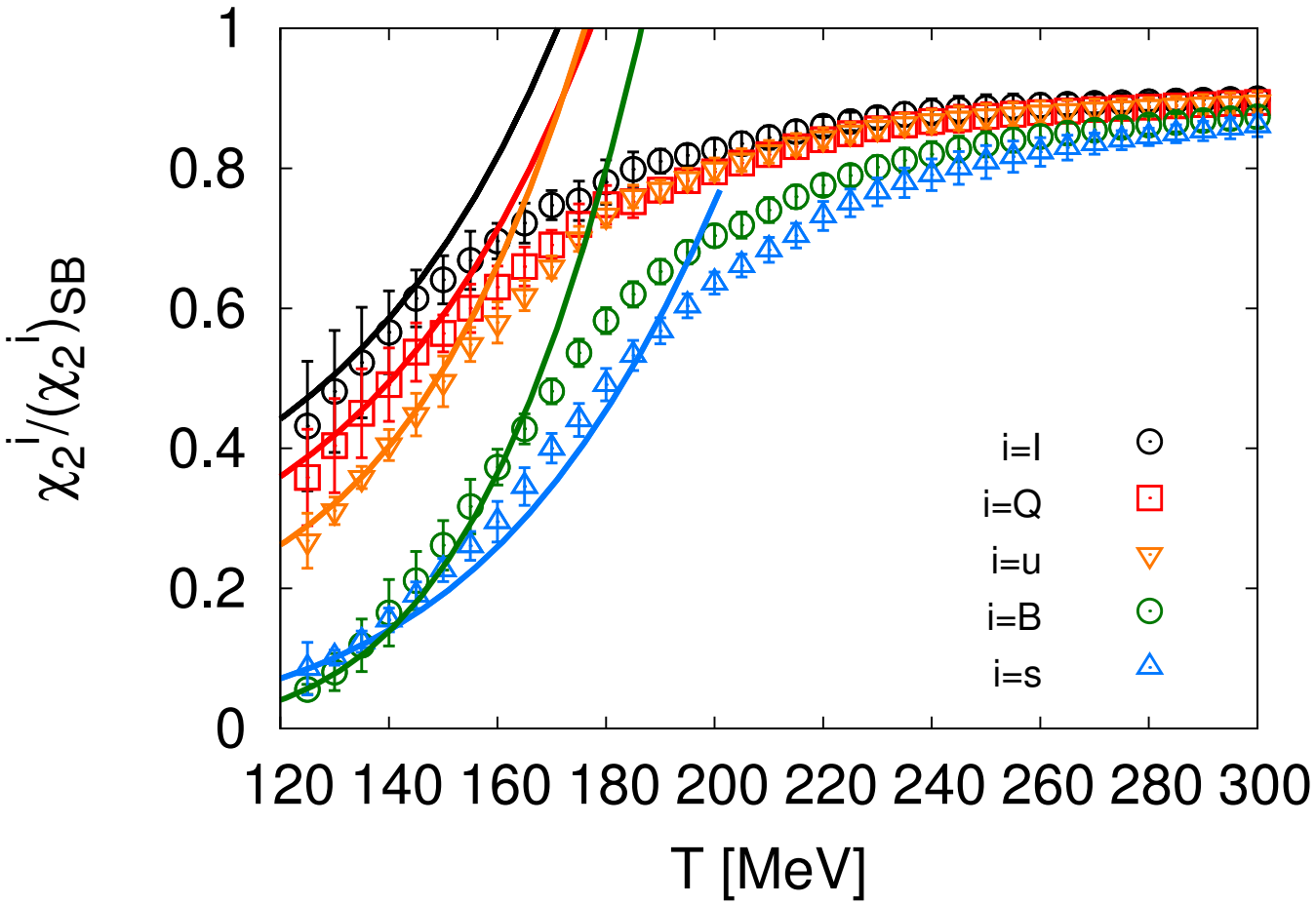


[Cartoon by V. Koch]

There is an acceptance cut in rapidity (as well as tranverse momentum), so that only particles from the fireball should be counted.
The cuts also implement a sub-volume counting: a sufficiently small sub-volume can behave as a grand-canonical ensemble.

All diagonal fluctuations

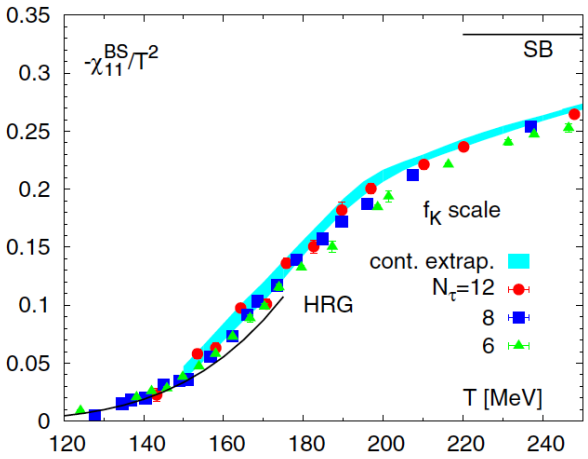
$$\chi_2 \sim \sum e^{-M_{\text{particle with quantum number}}/T} \tag{13}$$



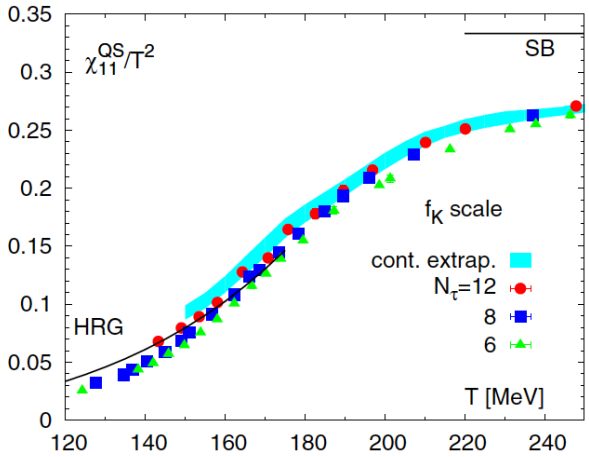
This result: [Wuppertal-Budapest 1112.4416] see also [HotQCD 1203.0784]

Off-diagonal susceptibilities

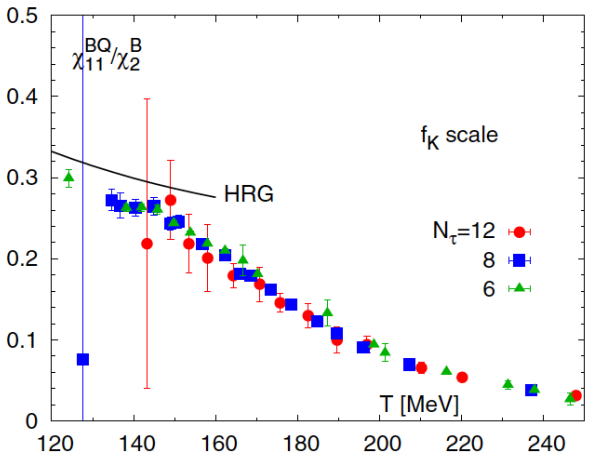
$-\chi_{11}^{BS}$ [HotQCD 1203.0784]



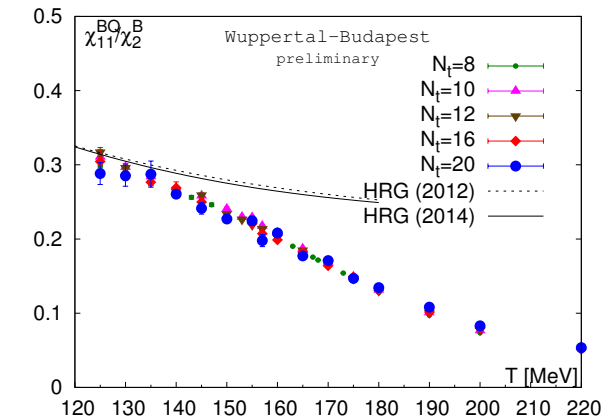
χ_{11}^{QS} [HotQCD 1203.0784]



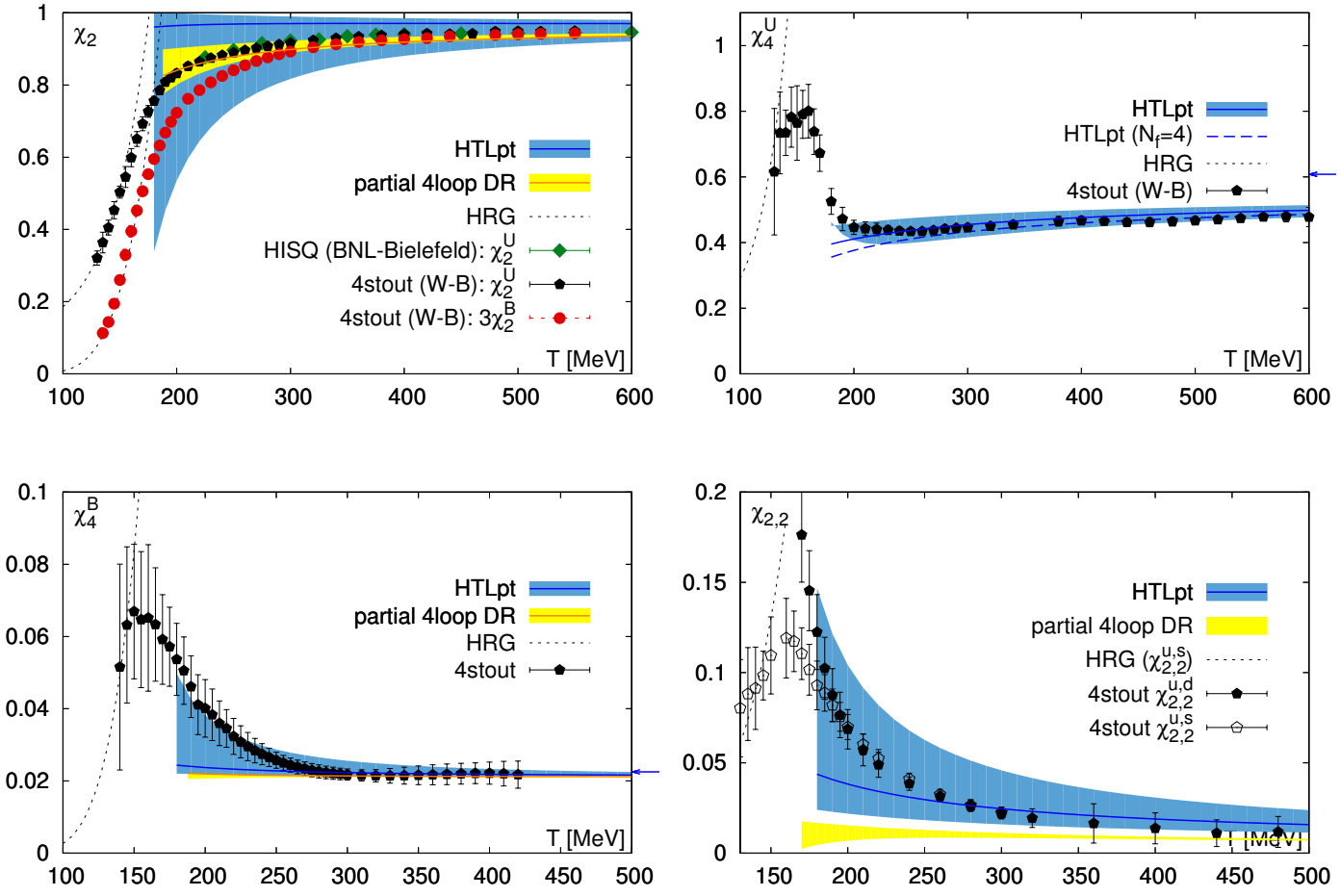
χ_{11}^{BQ}/χ_2^B [HotQCD 1203.0784]



χ_{11}^{BQ}/χ_2^B [WB preliminary]



At high temperature: lattice vs Hard Thermal Loops



HTL results: [Haque et al 1309.3968,1402.6907] Dimensional reduction: [1307.8098]

Lattice results: [Wuppertal-Budapest: 1507.04627] [BNL-Bielefeld: 1507.06637]

See also: [Swansea-Bielefeld: hep-lat/0501030] [BNL-Bielefeld 1309.2317] [WB: 1210.6901]

What is wrong with chemical potentials?

Start with a grand canonical partition function: $Z = \mathrm{Tr}\left(e^{-(H-\mu N)/T}\right)$

$$Z = \int D\psi D\bar{\psi} DA e^{-\int \mathcal{L}_{QCD}} = \int DA e^{-\int \mathcal{L}_{\mathrm{eff}}} = \int DA \det M[A,\mu] e^{-S_{\mathrm{Yang-Mils}}[A]}$$

- Maps the quantum system to a classical system, with configurations
- $w(U) =$ weight of a configuration U
- $w(U) \geq 0 \implies$ can use Monte Carlo
- $w(U)$ can be negative or complex $\implies$ a complex action problem

One can show:

$$(\det M[A,\mu])^* = \det M[A,-\mu] \tag{14}$$

The action is real (simulations are possible) if $\mu_B = 0$ or imaginary.

Euclidean path integral for QCD

Example: two color QCD

$$\begin{aligned}\mathcal{Z} &= \mathrm{Tr}\left(e^{-\beta(\hat{H}-\mu_u\hat{N}_u-\mu_d\hat{N}_d}\right) \\ &= \int \mathcal{D}U\mathcal{D}\bar{\Psi}\mathcal{D}\Psi e^{-S_{YM}-(\bar{\Psi}M\Psi)} \\ &= \int \mathcal{D}U e^{-S_{YM}[U]} \det M[U;m_u,\mu_u] \det M[U;m_d,\mu_d]\end{aligned}$$

- The gauge action S_{YM} is always real and positive in Euclidean space time. *Real time physics introduces a complex action problem*
- We do not have a complex action problem as long as the product $\det M_u \det M_d$ is real and positive.

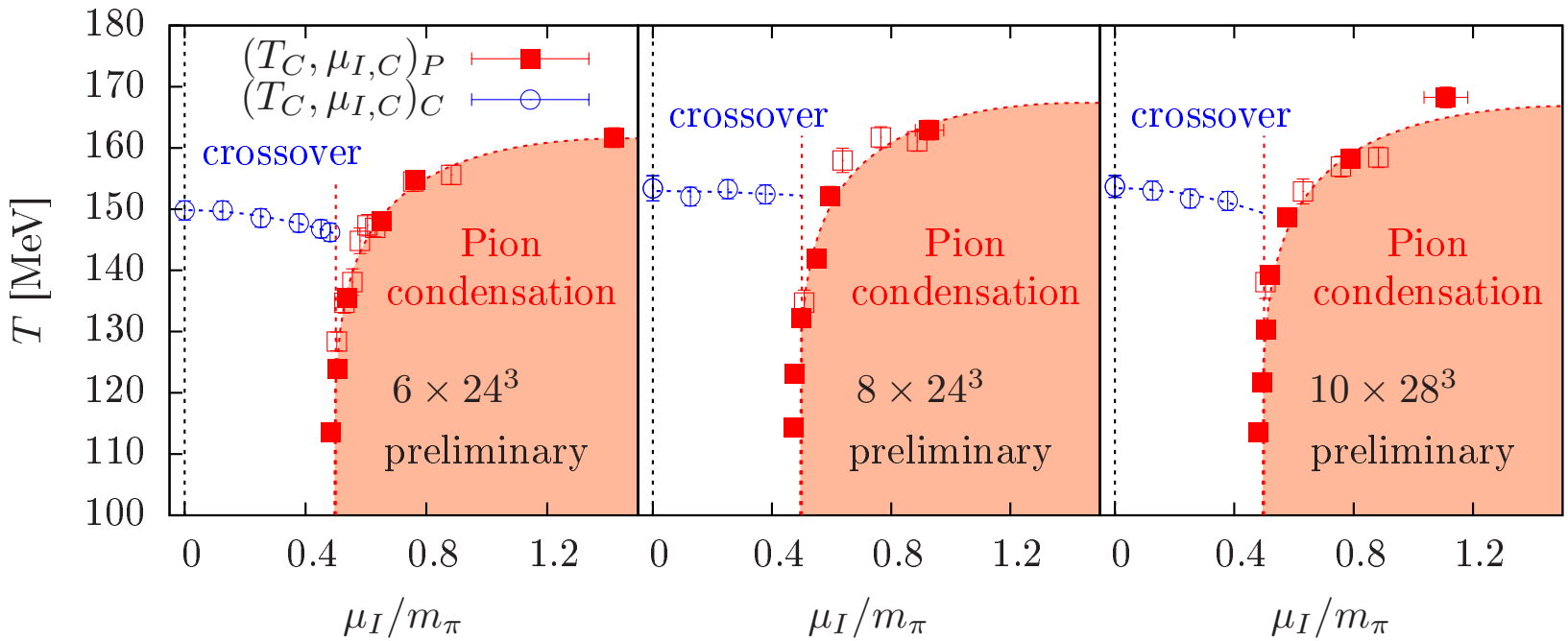
$$[\det M(\mu)]^* = \det M(-\mu^*)$$

– Product is real if $\mu_u = -\mu_d \rightarrow$ isospin chemical potential
– Each determinant is real if μ_u ad μ_d are imaginary

Phase diagram with isospin chemical potentials

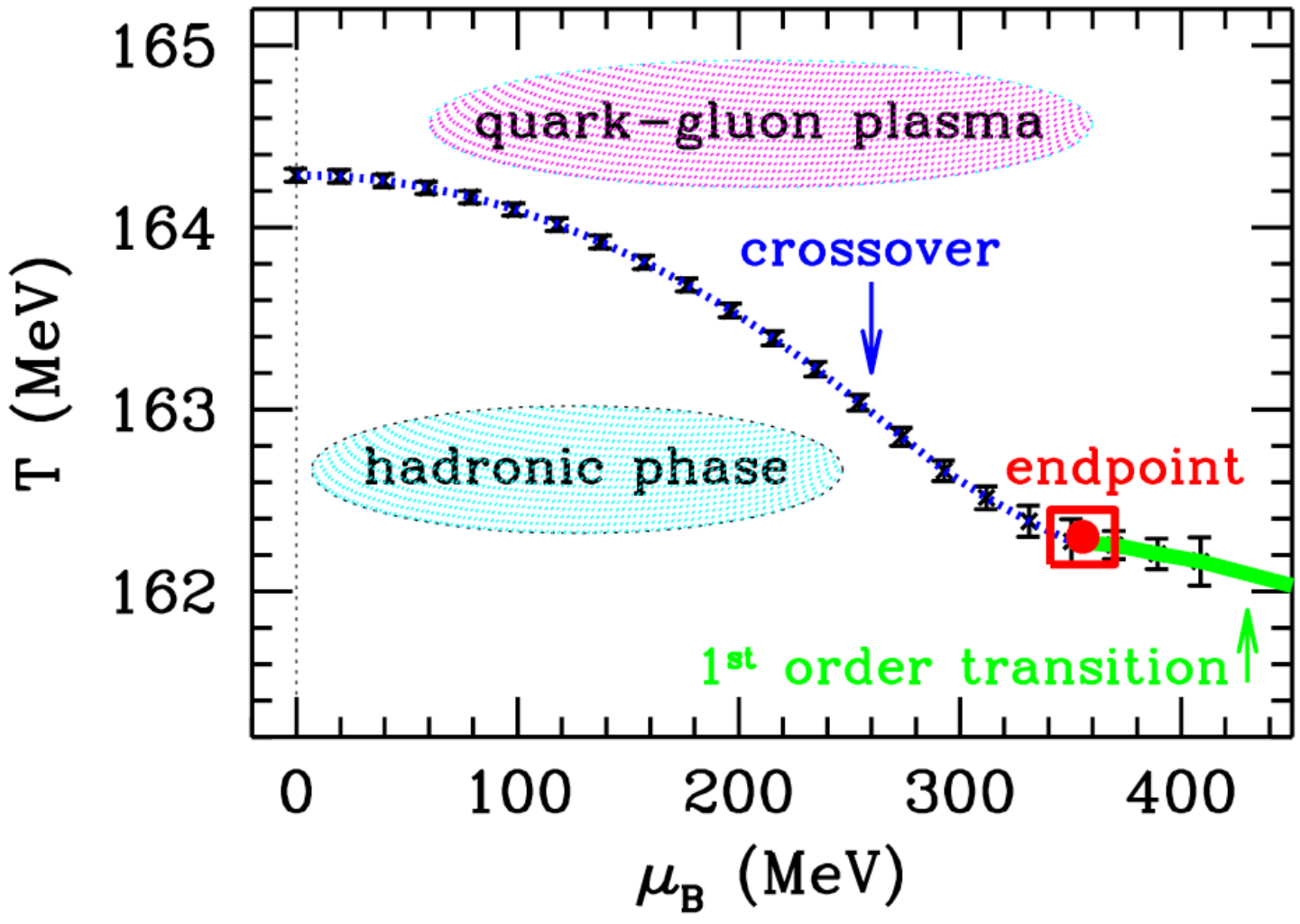
Although the action is real in the presence of an isospin chemical potential ($\mu_u = -\mu_d$), there are subtle technical difficulties.
An IR regulator λ is introduced, and $\lambda \to 0$ limit is taken. The key observables:

$$\langle \pi \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial \lambda}, \qquad \langle \bar{\psi}\psi \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial m_{ud}}, \qquad \langle n_I \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial \mu_I}.$$



[Brandt, Endrődi and Schmalzbauer, 1709.10487]

Reweighting to real μ_B



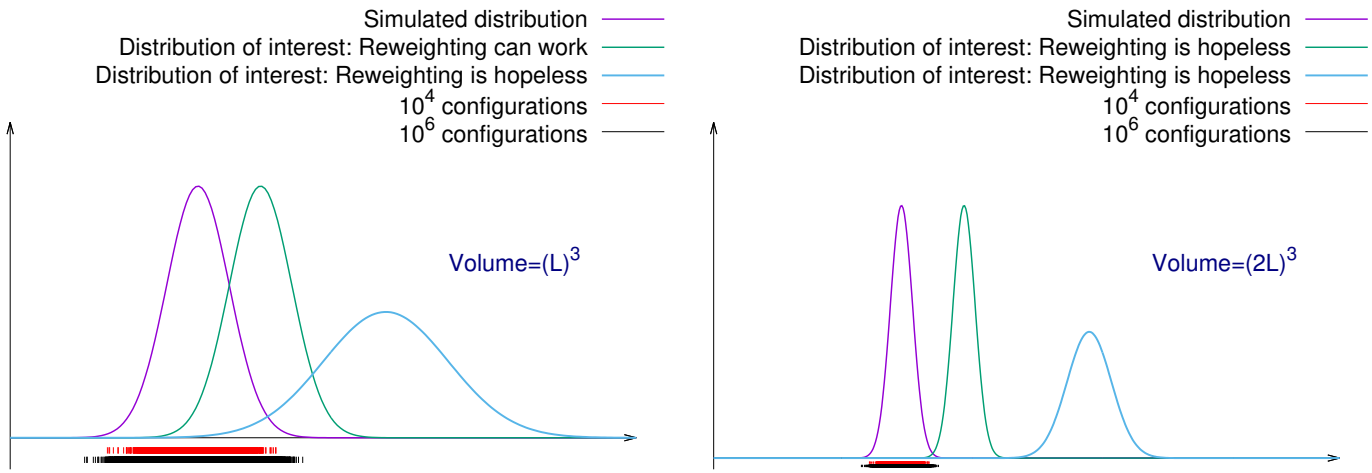
Using physical quark masses, $2+1$ *flavors,* $N_t = 4$ [Fodor&Katz hep-lat/0402006]

The overlap problem

The intregral can be transformed such that the weights are turned real:

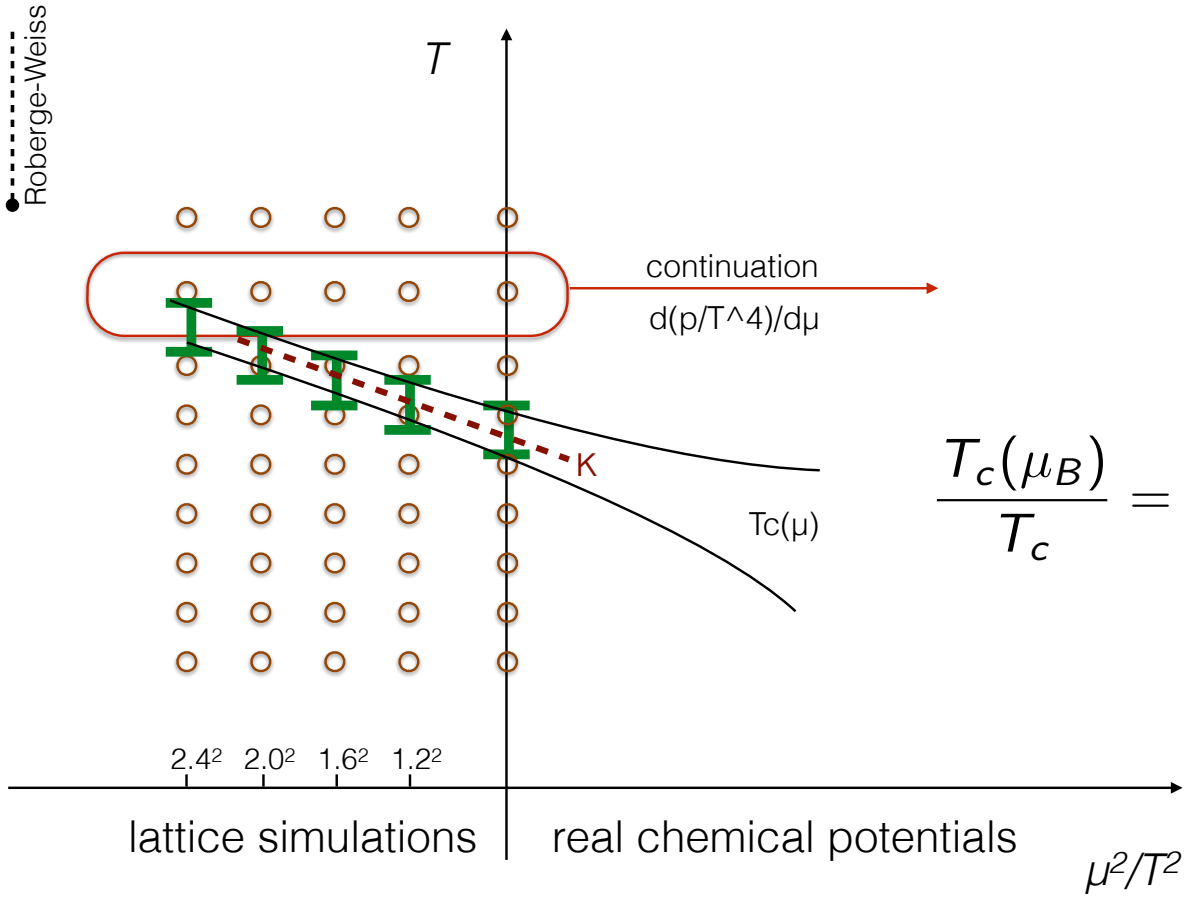
$$\langle O \rangle_w = \frac{\int \mathcal{D}U O[U] w[U]}{\int \mathcal{D}U w[U]} = \frac{\int \mathcal{D}U O[U] \frac{w[U]}{r[U]} r[U]}{\int \mathcal{D}U \frac{w[U]}{r[U]} r[U]} = \frac{\left\langle O \frac{w}{r} \right\rangle_r}{\left\langle \frac{w}{r} \right\rangle_r}$$

Using a non-physical weight (r) in the simulation will not benefit from importance sampling. In the unlucky case it will result in a 0/0 ratio.



At large volume the overlap problem makes any brute-force attempt impossible.

Analytic continuation



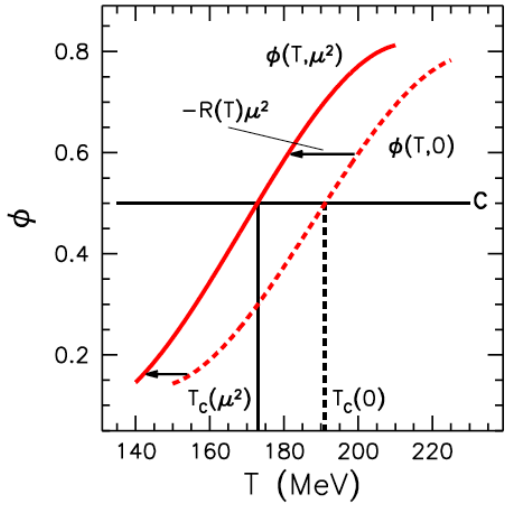
$$\frac{T_c(\mu_B)}{T_c} = 1 - \kappa \left(\frac{T_c}{m u_B} \right)^2 + \mathcal{O}(\mu_B^4)$$

Many exploratory studies: [de Forcrand & Philipsen hep-lat/0205016]

[Philipsen 0708.1293] [Philipsen 1402.0838] [Cea et al hep-lat/0612018,0905.1292,1202.5700]

Transition line form Taylor expanison

Take for example the chiral condensate $\langle\bar{\psi}\psi\rangle^r$ (sigmoid funciton).



$$\langle\bar{\psi}\psi\rangle^r(T,\mu_B^2)\big|_{T=T_c(\mu_B^2)} \equiv \langle\bar{\psi}\psi\rangle^r(T_c,0)$$

Derivative of an implicit function:

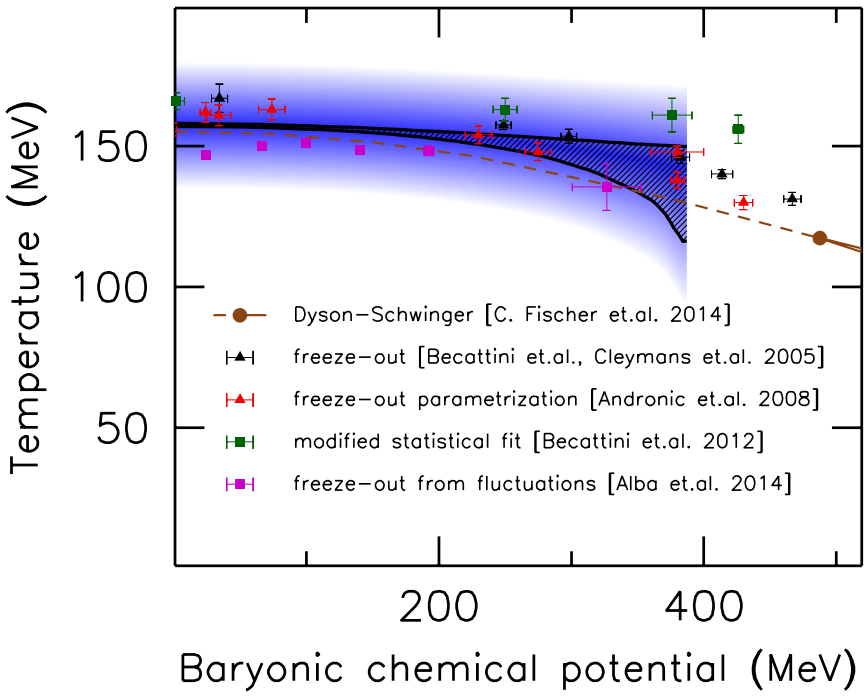
$$\kappa = -T_c\frac{dT_c}{d(\mu_B^2)} = T_c\frac{\left.\frac{\partial\langle\bar{\psi}\rangle^r}{\partial(\mu_B)^2}\right|_{\mu_B,0,T=T_c}}{\left.\frac{\partial\langle\bar{\psi}\rangle^r}{\partial T}\right|_{\mu_B,0,T=T_c}} \tag{15}$$

The agreement between Taylor and analytical continuation results was shown for the first time:

[Bonati et al 1805.02960]

Transition line from lattice

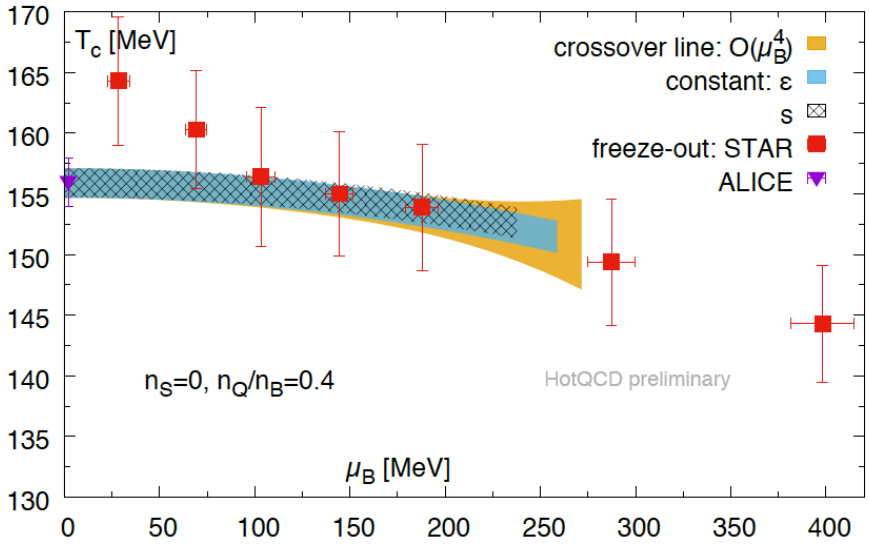
Analytical continuation:



$\kappa = 0.149 \pm 0.002$

[Jana Günther (Wuppertal) 2015, [1507.07510]]

Using Taylor coefficients:



$\kappa = 0.123 \pm 0.003$

[P. Steinbrecher's (HotQCD) talk at QM 208]

The equation of state in a grand canonical ensemble

At $\mu = 0$ lattice gives the pressure as an integral of the trace anomaly:

$$\frac{p}{T^4} = \int_0^T \frac{\epsilon(T^*) - 3p(T^*)}{{T^*}^5} dT^*$$

At finite μ_B/T one writes the pressure in a Taylor series:

$$\frac{p}{T^4}(\mu_B) = \frac{p}{T^4}(0) + \frac{1}{2}\frac{\mu_B^2}{T^2}\chi_2^B(T) + \frac{1}{24}\frac{\mu_B^4}{T^4}\chi_4^B(T) + \frac{1}{720}\frac{\mu_B^6}{T^6}\chi_6^B(T) + \dots$$

or

$$\frac{p}{T^4} = \frac{p}{T^4}(0) + \int_0^{\mu_B/T} \frac{n_B(\hat{\mu})}{T^3} d\hat{\mu}$$

$$\frac{n_B}{T^3}(\mu_B) = +\frac{\mu_B}{T}\chi_2^B + \frac{\mu_B^3}{T^3}\frac{1}{6}\chi_4^B + \frac{\mu_B^5}{T^5}\frac{1}{120}\chi_6^B + \frac{\mu_B^7}{T^7}\frac{1}{5040}\chi_8^B + \dots$$

The trace anomaly, energy, entropy are obtained as

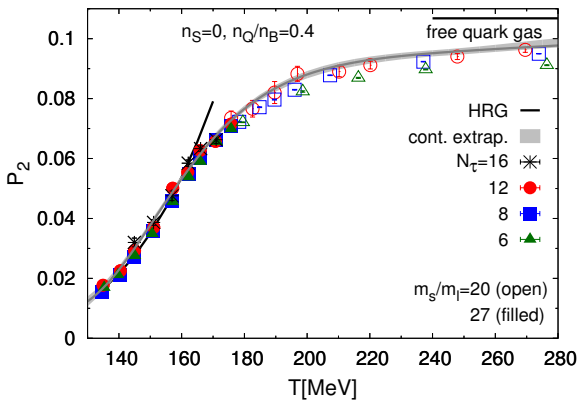
$$\frac{\epsilon - 3p}{T^4} = T\,\frac{\partial}{\partial T}\frac{p}{T^4}\bigg|_{\mu/T=\text{const}} \qquad sT = \epsilon + p - \mu_B n_B$$

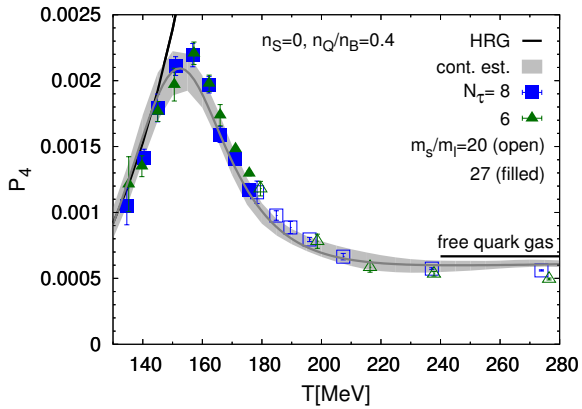
Pressure coefficients as of 2017

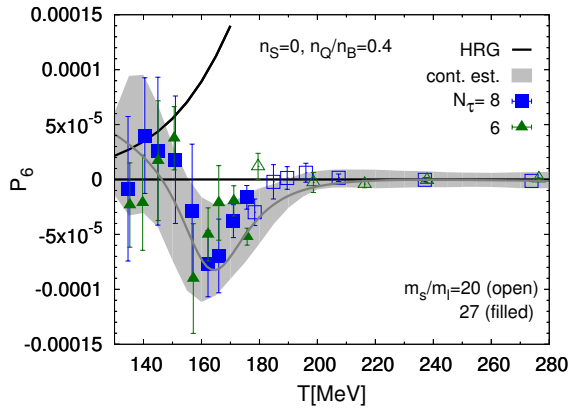
expansion coefficiens assuming strangeness neturality

Taylor method:

mostly $N_t = 8$, $\mathcal{O}(10^5)$ configurations point, [BNL-Bielefeld-CCNU: 1701.04325]



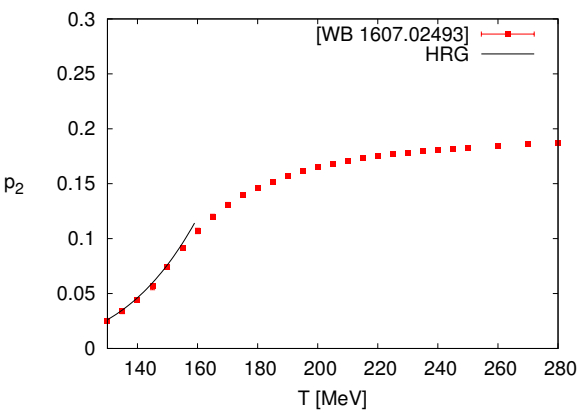


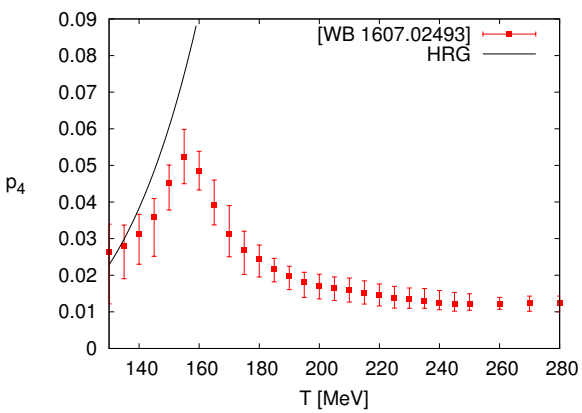


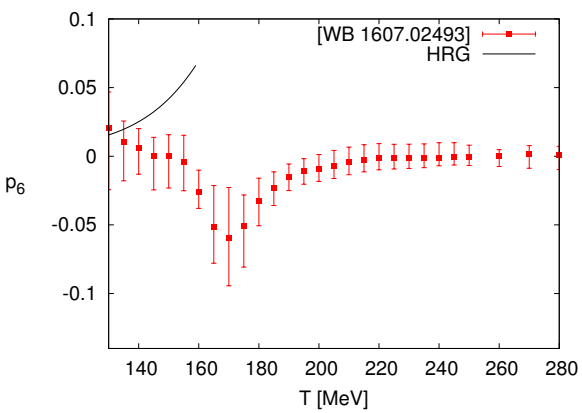
Analytical method:

continuum, $\mathcal{O}(10^4)$ configurations/point, errors include systematics

[Wuppertal-Budapest 1607.02493]







On the convergence radius

Does lattice data constrain the possible location of the critical end point? The baryon fluctuations are expanded in terms of higher order fluctuations:

$$\chi_2^B(T,\mu_B) = \sum_{n=0}^{\infty} \frac{1}{(2n)!} \chi_{2n+2}^B (\chi_B/T)^{2n}$$

An estimator for the radius of convergence:

$$r_{2n}^{\chi} = \left| \frac{2n(2n-1)\chi_{2n}^B}{\chi_{2n+2}^B} \right|^{1/2}$$

Signatrue for a critical end point:

$$r_{2n}^{\chi} \propto \ \text{Const} \tag{16}$$

In the Hadron Resonance Gas approach we have

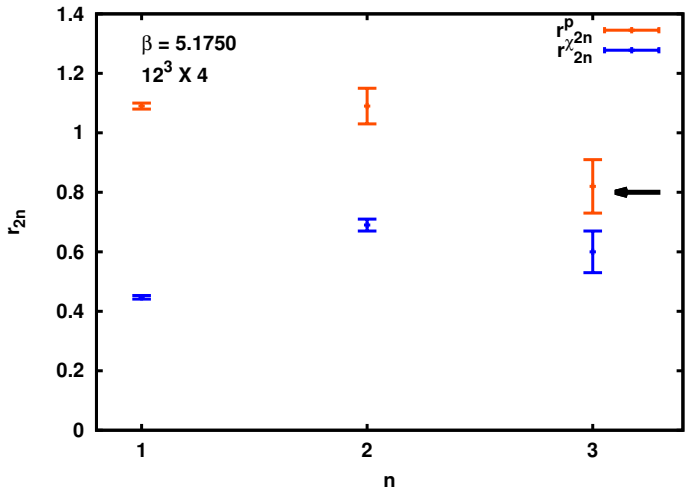
$$r_{2n}^{\chi} \propto \ n^2 \tag{17}$$

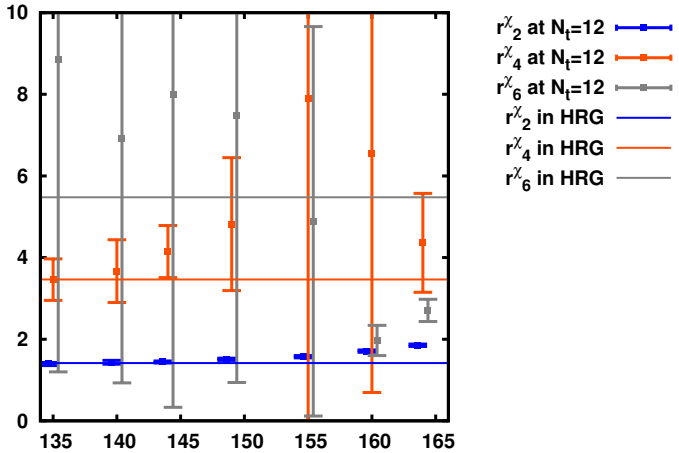
Do convergene radii converge?

The convergene radius is defined a limit.

Toy lattice:
for two observables
Here we know the CEP

Realistic lattice:
for one of the observables
Here we know nothing.





The principle might work if the end-point is not far.
Observe the difference in the scale of the two plots.
Results are not conclusive for realistic lattices.

[Attila Pasztor et al 1807.09862]

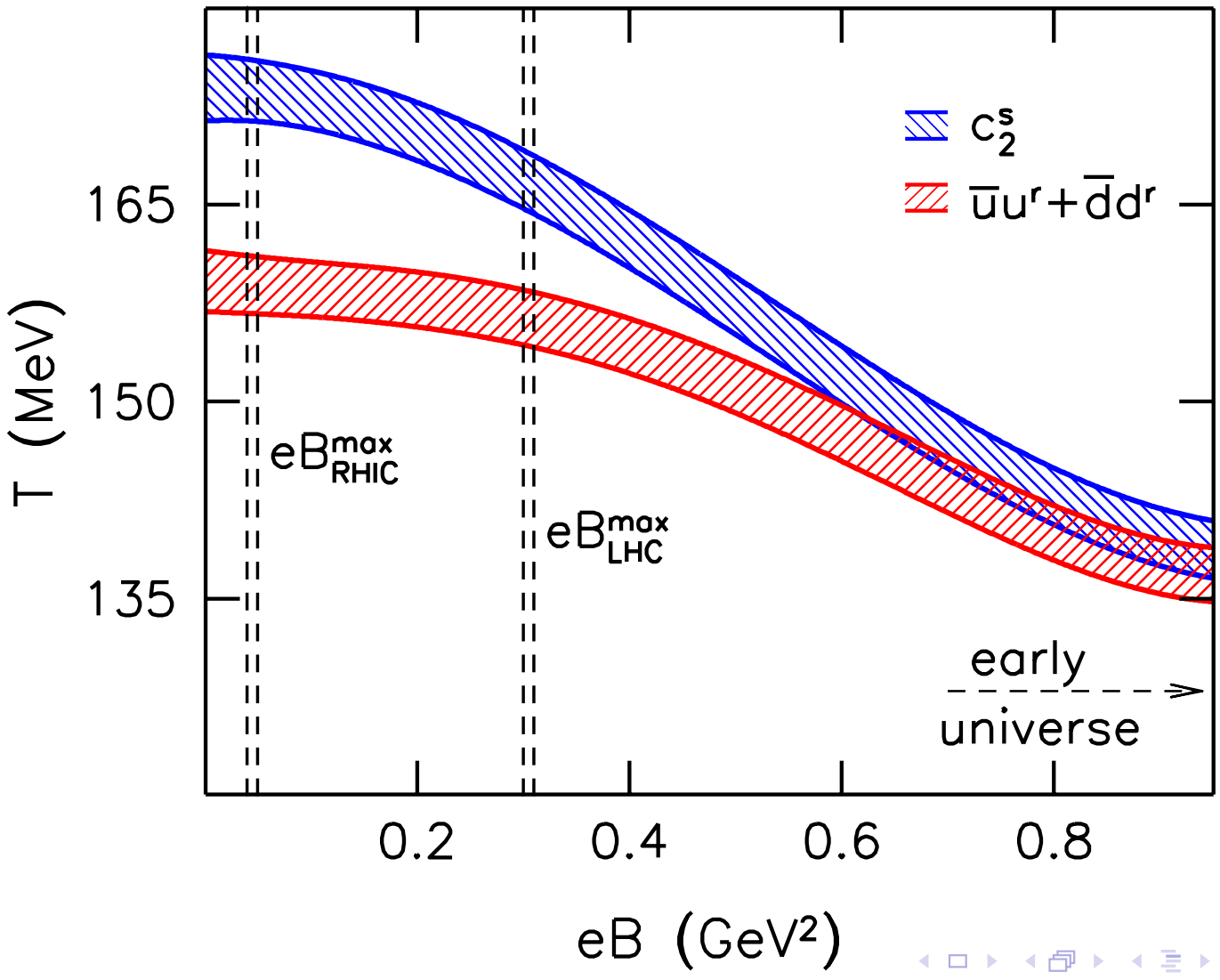
Outlook to the lattice session on Wednesday

- **Peter Petreczky:** Color screening in QCD
  The force between quark and antiquark as a function of temperature.
  $\rightarrow$ describes deconfinement, running coupling
- **Alexander Rothkopf:** Quarkonium Production in the QGP
  Two-point functions at finite temperature
  Euclidean time $\rightarrow$ real time "rotation"'
- **Christian Schmidt:** Fluctuations of conserved charges and the QCD phase diagram
  Extract physics at small μ_B from $\mu_B = 0$ simualtions.
- **Jana Guenther:** LQCD thermodynamics at finite chemical potential from analytical continuation
  Exploits that the μ_B dependence can be studied if we allow μ_B to be imagirany.

backup

T_c vs. magnetic field

The transition temperature was studied also in the presence of a magnetic field: [Bali et al: 1111.4956, 1206.4205]



Equation of state with magnetic fields

The pressure $p_i = -\frac{1}{V} L_i \frac{\partial F}{\partial L_i}$ can be anisotropic, depending on, whether the flux or the magnetic field is kept constant.

$$p_x^{(B)} = p_y^{(B)} = p_z, \qquad p_x^{(\Phi)} = p_y^{(\Phi)} = p_z eB \cdot \mathcal{M}$$

Trace anomaly:

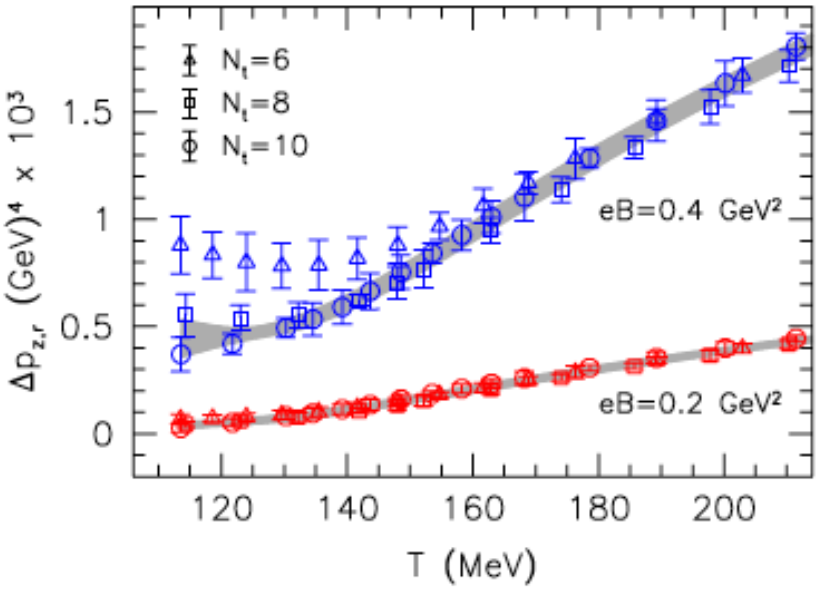
$$I^{(B)} = \epsilon - 3p_z \qquad I^{(\Phi)} = \epsilon - 3p_z + 2eB \cdot \mathcal{M}$$

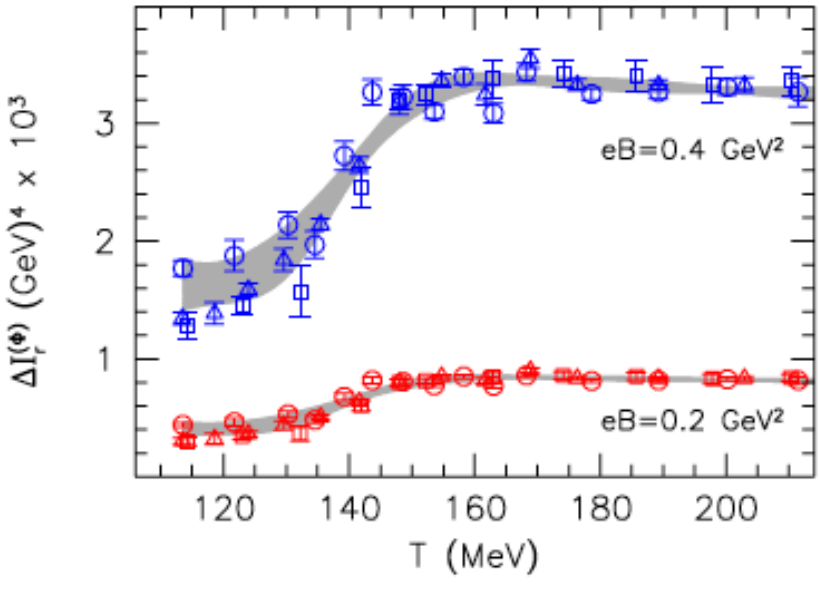
And the magnetic susceptibility:

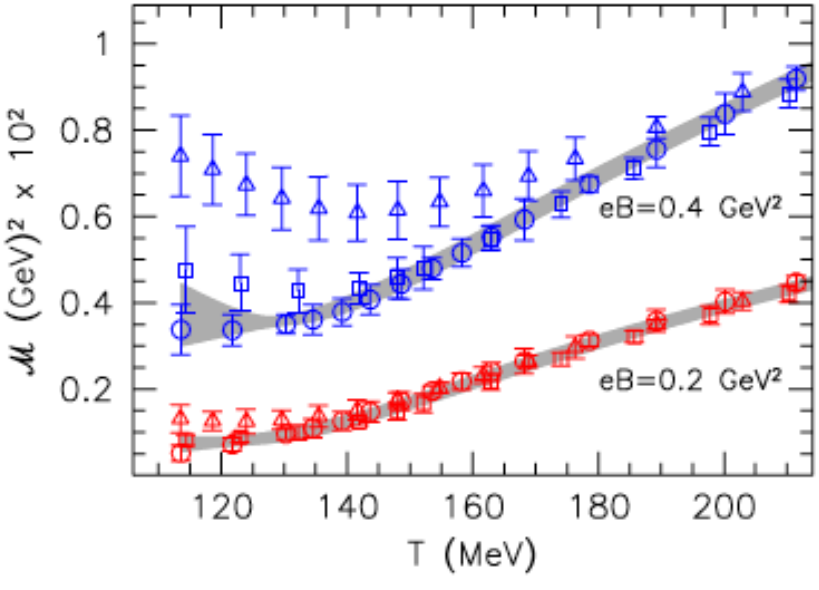
$$\chi_B = \left. \frac{\partial \mathcal{M}}{\partial (eB)} \right|_{B=0} = - \left. \frac{1}{V} \frac{\partial^2 F}{\partial (eB)^2)} \right|_{B=0}$$

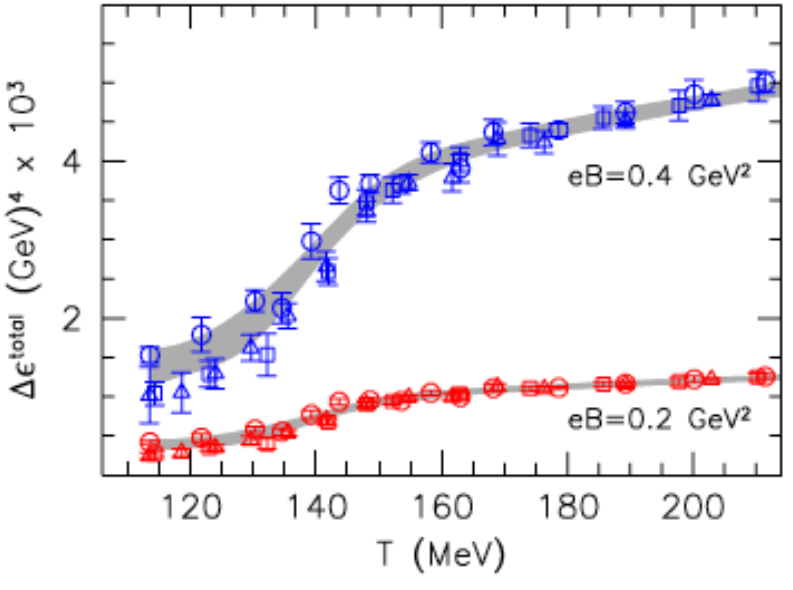
The pressure can be calculated with a variant of the integral method e.g. using integrals in the mass space [Bali et al, 1406.0269]

Equation of state with magnetic fields



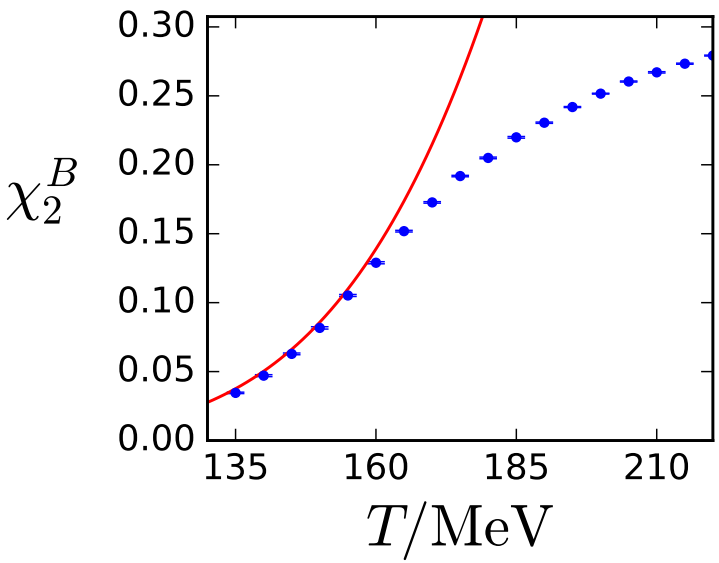


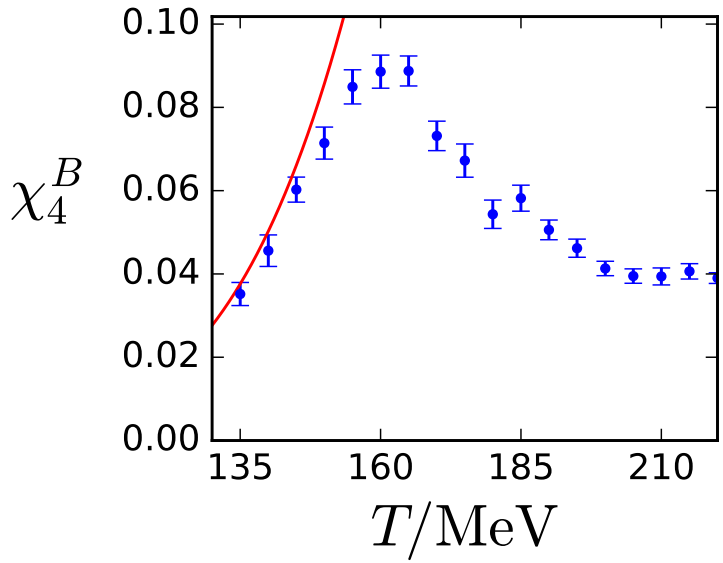


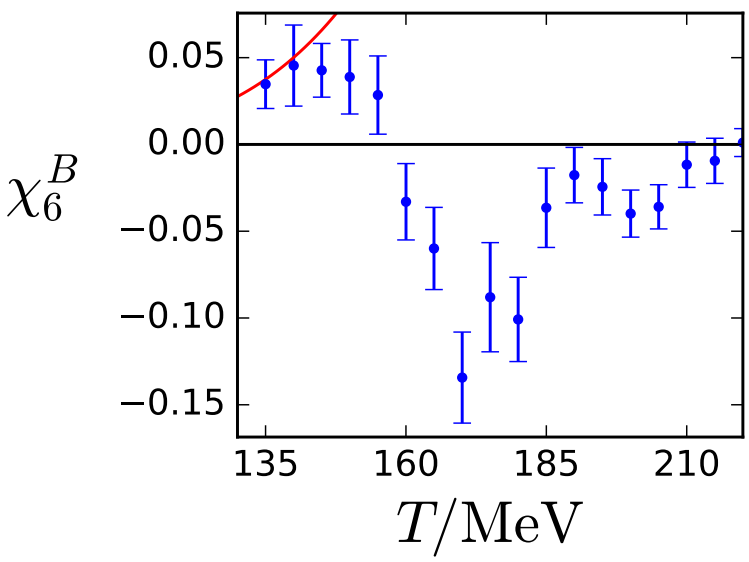


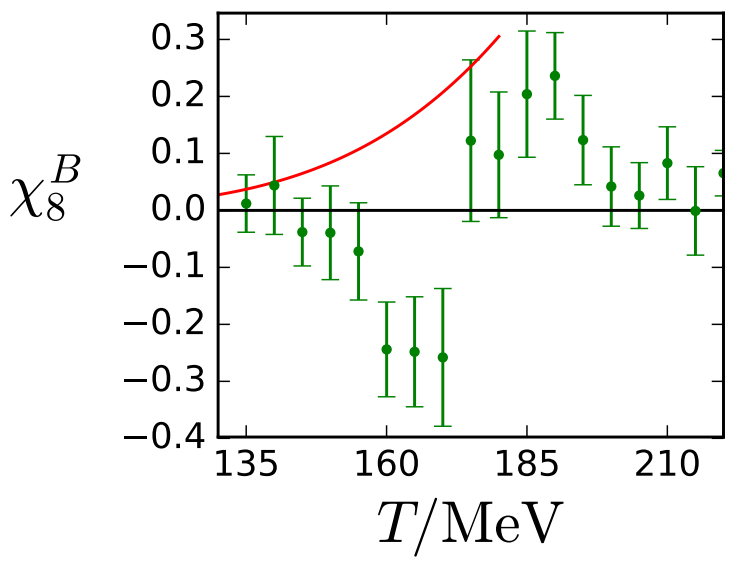
[Bali et al, 1406.0269]

Results for χ_n^B





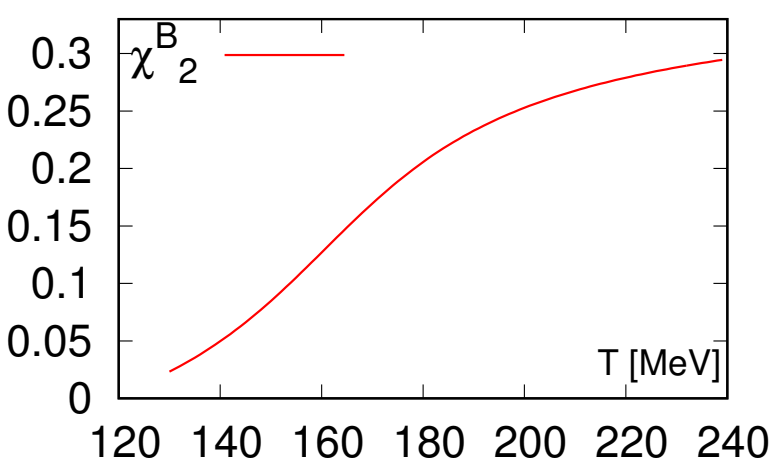


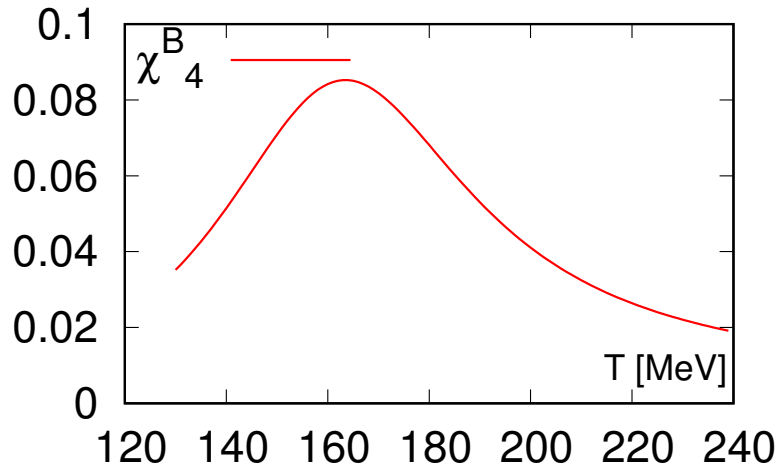


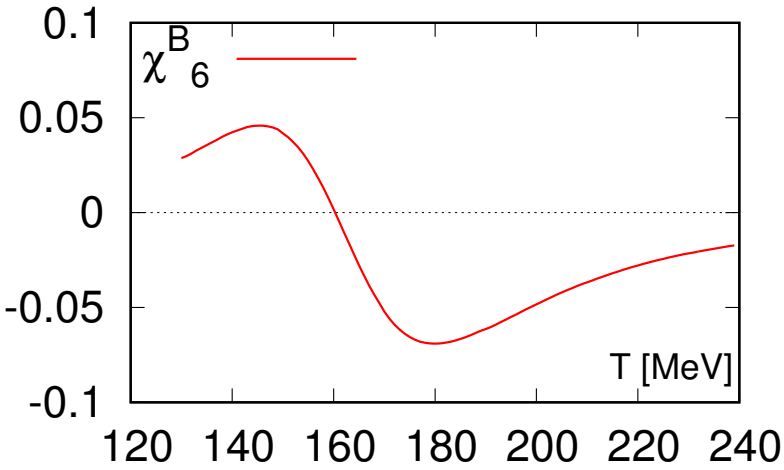
Simulation results published: **1805.04445** (Wuppertal-Budapest)

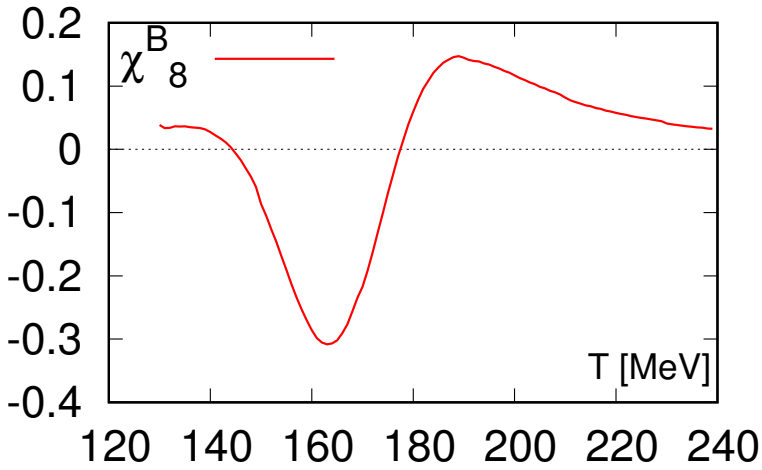
Higher order χ_B in the simple model

Input: $\chi_2^B(T, \mu = 0)$ from Wuppertal-Budapest, and $\kappa = 0.02$ [see 1508.07599]:



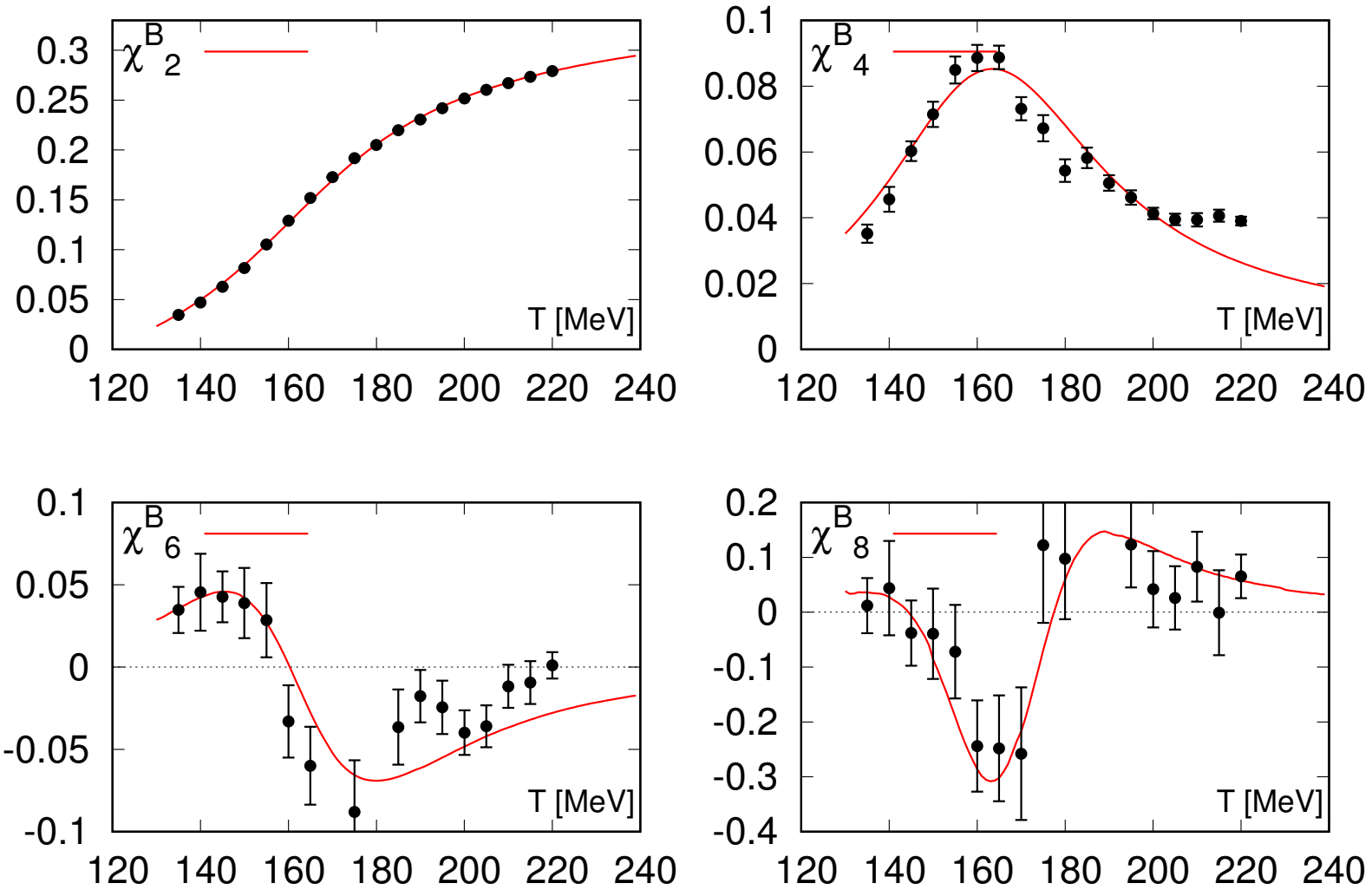






Higher order χ_B in the simple model

Comparing the simple model with our lattice result:



Simple model describes lattice result surprisingly well.

Result is consistent with the no-critical-end-point scenario.

The complex action problem at finite μ

$$[\det M(\mu)]^* = \det M(-\mu^*) \ \textit{in} \ \mathbb{C}$$

$w := e^{-S_{YM}} \det M_u \det M_d$ complex $\implies$ cannot use importance sampling

Appearance of a sign problem has to do with the absence of particle-antiparticle symmetry.

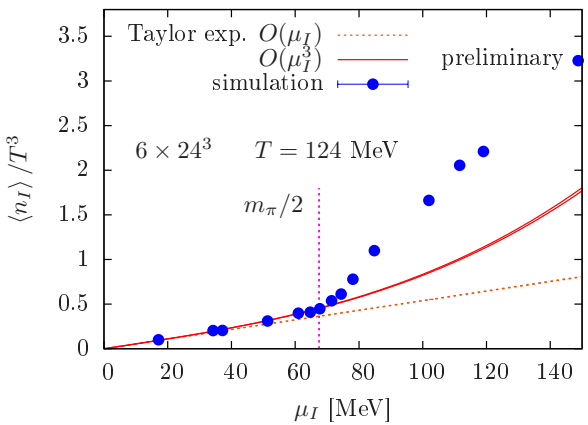
Cases without a complex action/sign problem:

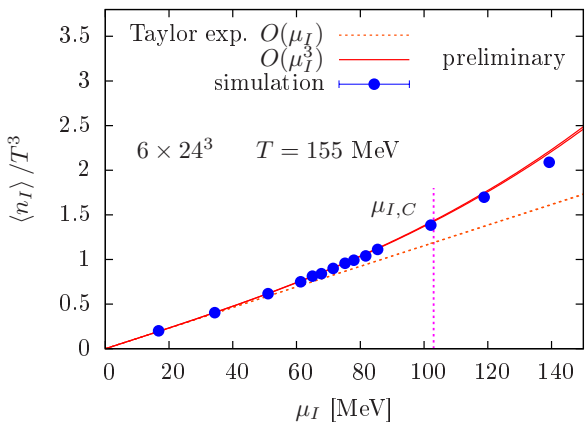
- $\mu = 0$ Calculate derivatives of $\log \mathcal{Z}$ at $\mu = 0$
- Purely imaginary μ
- The complex phase of the two determinants may cancel: Isospin chemical potential $\mu_u = -\mu_d$ $\implies$ Study pion condensation.
- The Dirac operator can have an additional symmetry, e.g. SU(2) gauge theory with N_f =even
- No complex action problem for magnetic fields.

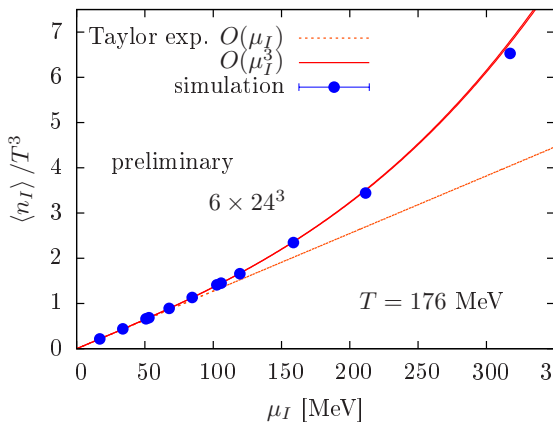
Towards the equation of state with isospin chemical potentials

Let us first look at the μ_I derivative, n_I. It is interesting to compare to the Taylor expansion:

$$\frac{\langle n_I \rangle}{T^3} = c_2 \left(\frac{\mu_I}{T}\right) + \frac{c_4}{6}\left(\frac{\mu_I}{T}\right)^3,$$







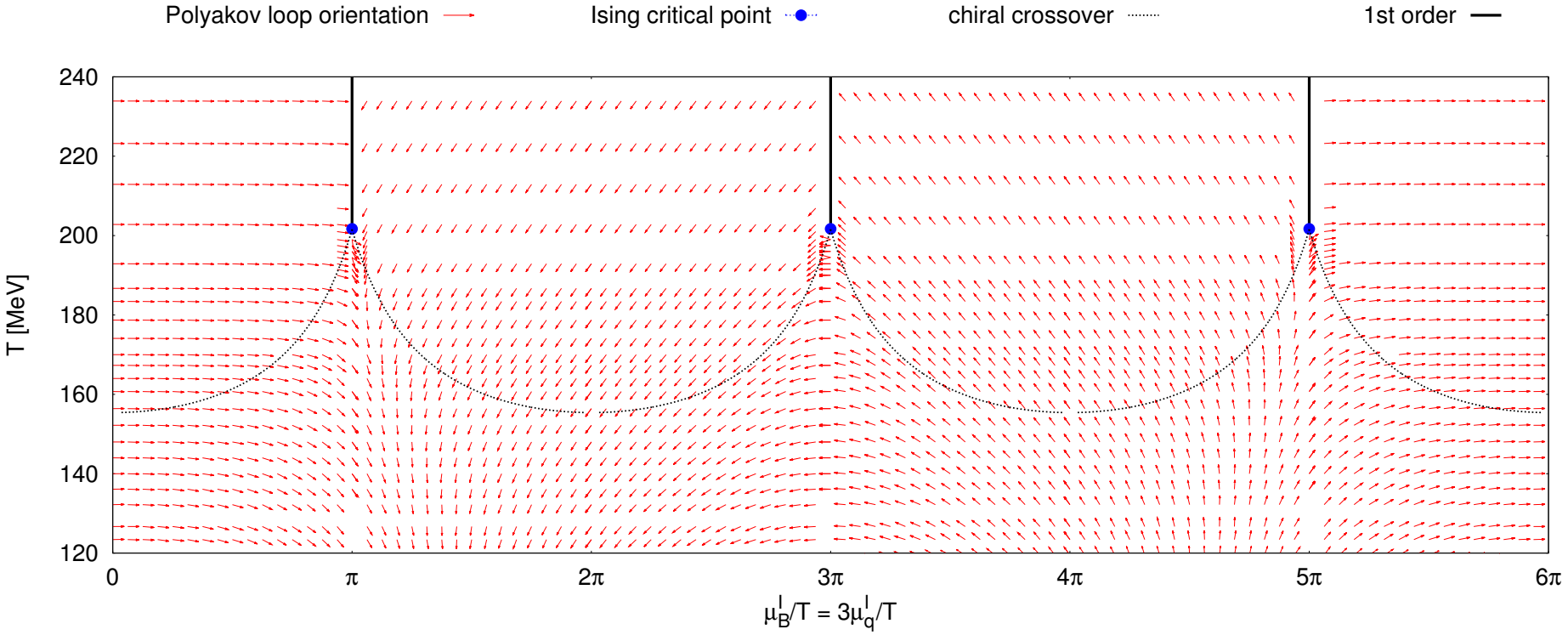
[Brandt, Endrődi and Schmalzbauer, 1709.10487]

Physics at imaginary μ_B

Many exploratory studies: [de Forcrand & Philipsen hep-lat/0205016]

[Philipsen 0708.1293] [Philipsen 1402.0838] [Cea et al hep-lat/0612018,0905.1292,1202.5700]

At imaginary μ_B there is no sign problem. The observables, including the crossover line, are analytical functions of μ_B^2.



The phase diagram is perodic $\mu_B \to \mu_B + i2\pi T$, with simultaneous rotation between the Z(3) sectors.

Periodicity in imaginary μ

$$Z = \int \mathcal{D}U \; e^{-S_g} (\det M_u)^{1/4} (\det M_d)^{1/4} (\det M_s)^{1/4}$$

where there is a separate μ^I in each determinant: $U_0(\mu) = e^{i\mu_q^I} U_0$
Gauge invariance allows to put all μ^I on one time slice:

$$U_0(\mu_q; x, t) = \delta_{t,0} e^{i\mu_q^I / T} U_0(x, t)$$

$\mu_q^I \to \mu_q^I + 2\pi T$ is a trivial symmetry of the determinant. Shifting $\mu_q^I \to \mu_q^I + \frac{2\pi}{3} T$ for all flavors at the same time is an additional symmetry of the integral. It follows from the Z(3) center symmetry of the gauge action ($U_0(t = 0) \to U_0(t = 0) e^{i\pi/3}$).

$$\begin{aligned} \mu_u &= \frac{1}{3}\mu_B + \frac{2}{3}\mu_Q \,, \\ \mu_d &= \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q \,, \\ \mu_s &= \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q - \mu_S \,. \end{aligned}$$

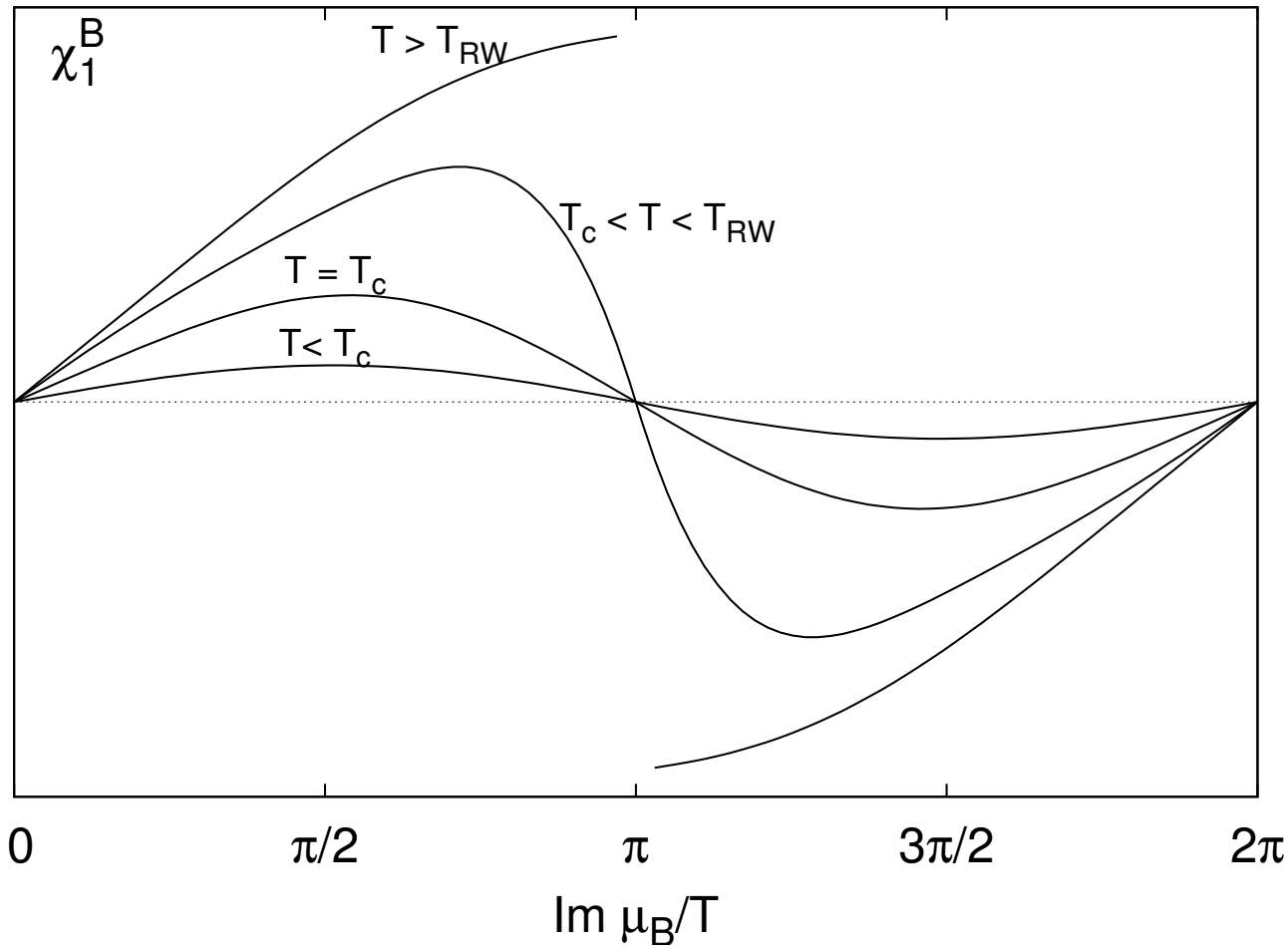
$\mu^I \to \mu^I + 2\pi T$ symmetry holds for B, Q and S.

Imaginary baryon number

Free particle of baryon number B: $\frac{p}{T^4} \sim \cosh(B\frac{\mu}{T})$ and $\chi^B(T) = \frac{dp/T^4}{d(\mu/T)}$

Hadrons Gas (baryons): $\chi_1^B(T) \sim \sin(\mu^I/T)$

At high T we see: $\chi_1^B(T) \sim \sin(\mu^I/T/3)$



Every sign problem is different

Incomplete list of **solved sign problems**:

- Charged scalar field theories
  G. Aarts, PRL 102, 2009 (Complex Lagevin)
  C. Gattringer, T. Kloiber, NPB 869, 2013 (dual variables)
  M. Cristoforetti et al, PRD88 (2013) (Lefschetz thimbles)
  Pellegrini et al, PoS LATTICE2015 (2016) 192 (Density of States)
- Abelian Higgs models
  Y. D. Mercado, C. Gattringer, A., PRL111 (2013) (dual variables)
- Yukawa models
  S. Chandrasekharan, PRD86 (2012) 021701 (dual variables/fermion bags)
- Heavy-Dense QCD
  Aarts, Attansio, Jager, Sexty JHEP 1609 (2016) 087 (Complex Langevin)
  Garron, Langfeld, Eur.Phys.J. C76 (2016) no.10, 569 (Density of States)

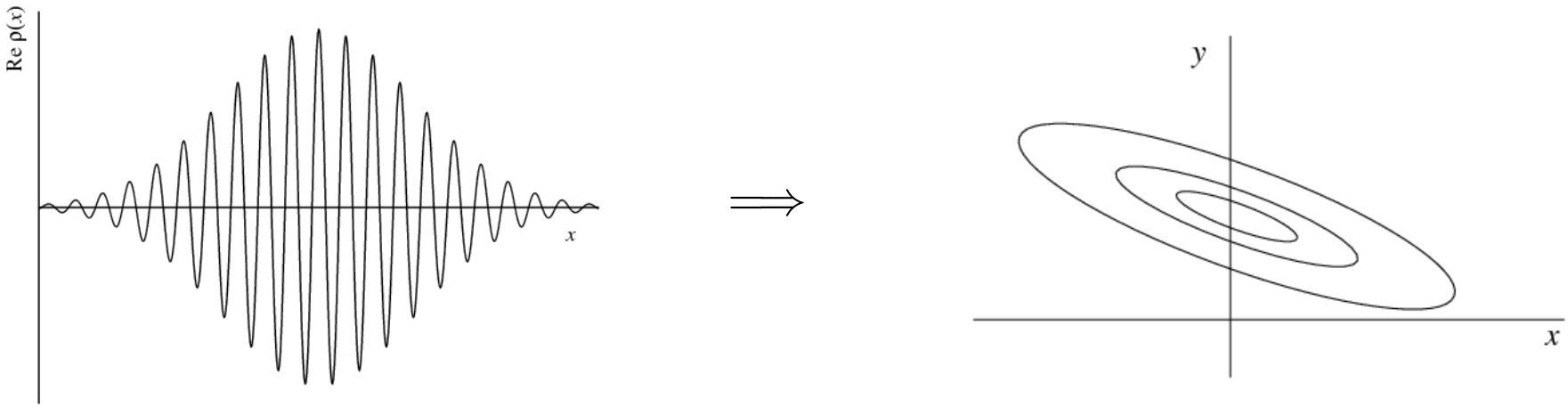
Complex Langevin - Complexification

What are the dominant configurations for an oscillating integral?

$$\int dx e^{-S} \text{ where } \mathrm{S(x)} = \frac{1}{2}\mathrm{ax}^2 - \mathrm{ibx}$$

To calculate it, you complete the square $\Longrightarrow$ go to the complex plane

- Idea: go to the complex plane, i.e. complexify your field $z = x + iy$
- Enlarged complex field space means new directions to explore, maybe can define a positive definite probability distribution there



Complex Langevin - Stochastic Quantization

Stochastic quantization Parisi, Wu 1981

- Given a real action $S(x)$, write down a Langevin equation for x:

$$\frac{\partial x}{\partial \tau} = -\frac{\partial S}{\partial x} + \eta(\tau)$$

with Gaussian noise with $< \eta(\tau) >= 0$ and $< \eta(\tau)\eta(\tau') >= \delta(\tau - \tau')$.

- Calculate the averages along the trajectories:

$$< O >= \lim_{T\to\infty} \frac{1}{T} \int_0^T O(x(\tau))d\tau = \frac{\int dx e^{-S(x)} O(x)}{\int dx e^{-S(x)}}$$

- $\Longrightarrow$ This is the basis of the real Langevin algorithm.

Complex Langevin

- The field is complexified: $SU(N) \to SL(N, \mathbb{C})$
- Can explore new directions in complexified field space
- Langevin $\to$ Fokker-Planck: allows def. of a real prob. density

Proof of convergence

- If there is fast decay $P(x, y) \to 0$ as $y \to \infty$
- and a holomorphic action $S(x)$

then CLE converges to the correct result (Aarts, James, Seiler, Stamatescu (2011))

Non-holomorphic action for non-zero density QCD

$$S = S_{\mathrm{YM}} - \sum_{q=1}^{N_f} \ln \det M(m_q, \mu_q)$$

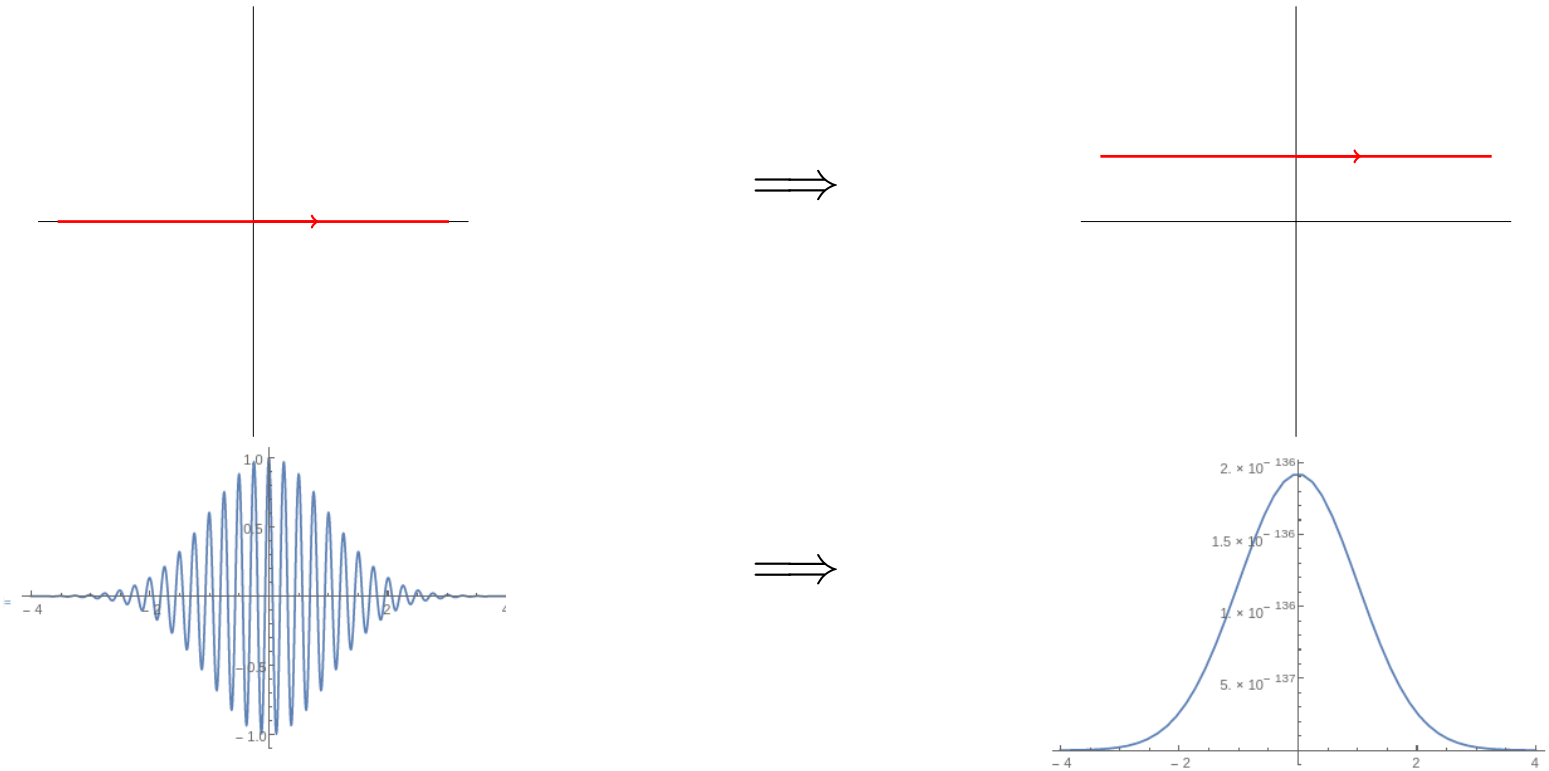
$$\det M(m_q, \mu_q) \in \mathbb{C} \text{ if } \mu_{\mathrm{q}} > 0$$

Determinant has zeros ($\det M = 0$) $\implies$ complex logarithm has a branch cut $\implies$ meromorphic drift

Complexification - Lefshetz Thimbles

What are the dominant configurations for $\int dx e^{-\frac{1}{2}x^2+ibx}$?

Deform the contour to the path of steepest descent



Multi-dimensional generalization (very non-trivial): Lefshetz thimbles.

Complexification - Comparison

Complex Langevin

- Stochastic qu.: Langevin equ. $\Longleftrightarrow$ Path Integral
- Allow for complex drift in Langevin equation
- A positive weight can be defined via Fokker-Planck equation
- Dynamics allows to explore the 2D complex space

$$\frac{1}{Z}\int P_{\mathrm{comp}}(x)O(x)dx = \frac{1}{Z}\int dxdyP_{\mathrm{real}}(x,y)O(x+iy)dxdy$$

Lefschetz thimbles

- Start from Path Int, deform the contour into the complex plane
- Look for critical points. Find the contributing thimbles.
- Phase on the Thimble changes smoothly, Reweight the residual sign problem
- Dynamics should stay on the Thimble

$$\frac{1}{Z}\int P_{\mathrm{comp}}(x)O(x)dx = \frac{1}{Z}\int_{\mathrm{Thimble}} dzP(z)O(z)dz$$

Nice ideas. They don't work for full QCD (yet?)

Density of states

$$\mathcal{Z}(\mu) = \int \mathcal{D}U\Phi e^{S_R[U]+iS_I[U]}$$

$$P(s) \equiv N \int \mathcal{D}U\delta\left(s - S_I[U]\right) e^{S_R[U]}$$

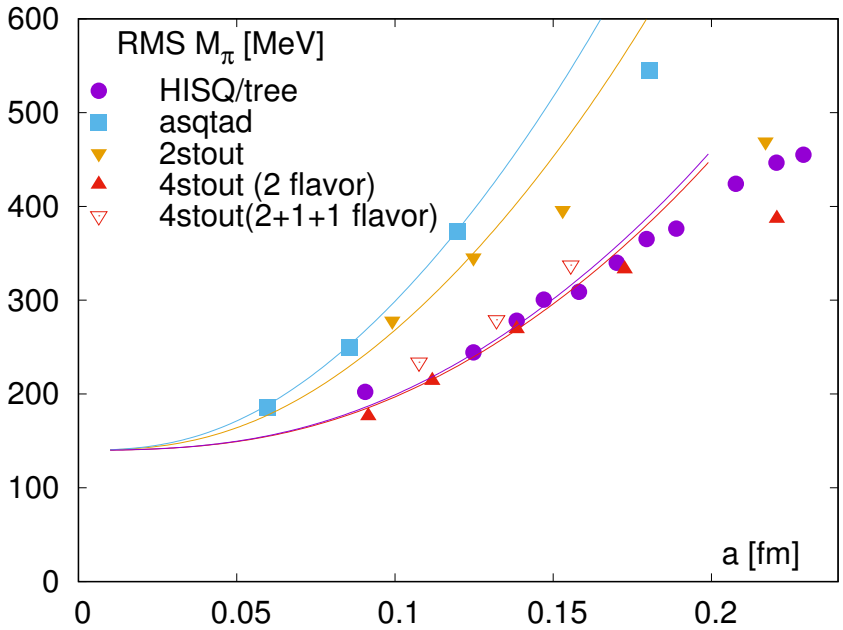
$$\mathcal{Z}(\mu) = \int dsP(s)e^{i\mu s}$$

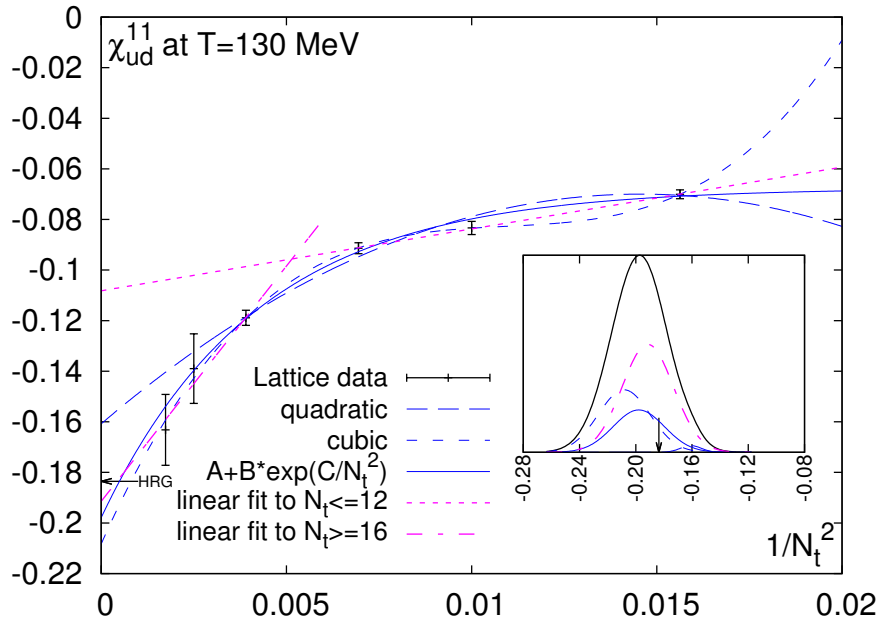
- The oscillating integral is now 1 dimensional. $\Longrightarrow$ If I know $P(s)$ exactly, I can do thermodynamics at finite μ.
- On the other hand, $P(s)$ has to be known at a high precision over a large range, and determination of $P(s)$ with usual MC methods suffers from overlap problem.
- For interesting recent progress on that front, see: Langfeld, 1610.09856v2

Challenges of lattice QCD – discretization errors

Action: the discretizaton scheme
improved actions have better than usual (e.g. $\mathcal{O}(a^2)$ scaling) at the price of more computations for a given lattice spacing.
Some actions only reduce the coefficient of the leading discretization effects, targeting a specific problem.

For staggered fermions the taste breaking distorts the pion spectrum. In the continuum limit the correct spectrum is reproduced.





The Hadron Resonance Gas model

Hadrons are free particles in a heat bath, their interactions are introduced by adding all their resonances to the heat bath, as free particles. [Dashen, Ma, Bernstein 1969]

$$\frac{p^{\mathrm{HRG}}}{T^4} = \frac{1}{VT^3} + \sum_{i\in\mathrm{mesons}} \log \mathcal{Z}^M(T, V, m_i, \{\mu\}) + \sum_{i\in\mathrm{baryons}} \log \mathcal{Z}^B(T, V, m_i, \{\mu\})$$

$$\begin{aligned} \log \mathcal{Z}^{M/B}_{m_i} &= \mp \frac{V d_i}{2\pi^2} \int_0^\infty dk k^2 \log\left(1 \mp z_i e^{-\sqrt{m_i^2+k^2}/T}\right) \\ &= \frac{VT^3}{2\pi^2} d_i \frac{m_i^2}{T^2} \sum_{k=1}^{\infty} (\pm)^{k+1} \frac{z_i^k}{k^2} K_2(k m_i/T) \end{aligned}$$

with the fugaciy factor $z_i = \exp(B_i\hat{\mu}_B + Q_i\hat{\mu}_Q + S_i\hat{\mu}_S)$ and $\hat{\mu} = \mu/T$. For $m_i \gg T$ (e.g. baryons) only the $k = 1$ term is relevant (Boltzmann approximation). The contribution of a particle and antiparticle combined:

$$\log \mathcal{Z}^{M/B}_{m_i} \approx 2\frac{VT^3}{2\pi^2} d_i \frac{m_i^2}{T^2} K_2(m_i/T) \cosh(B_i\hat{\mu}_B + Q_i\hat{\mu}_Q + S_i\hat{\mu}_S)$$

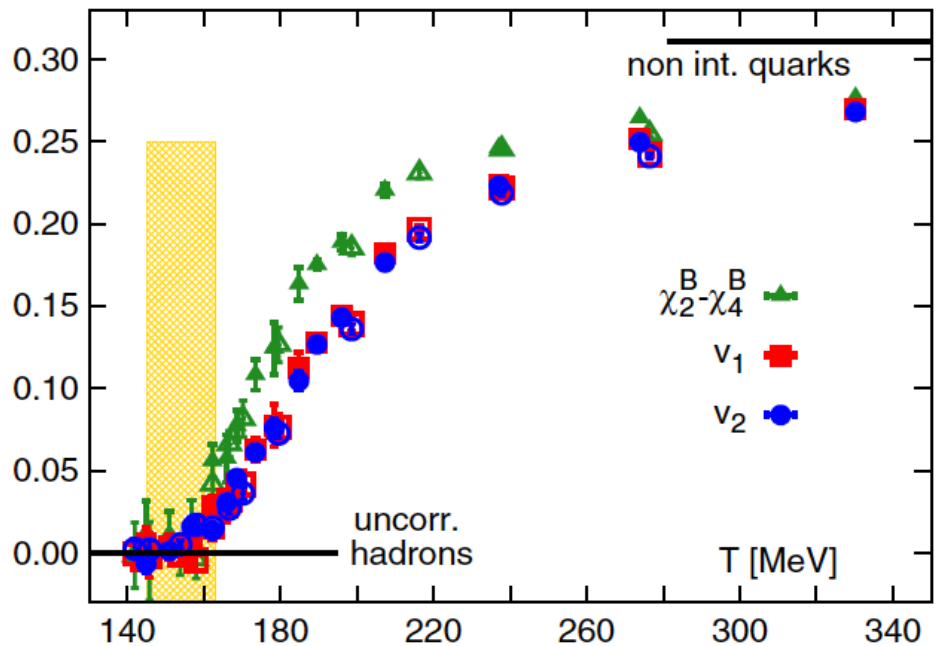
In this approximation and $\mu_Q = 0$ the pressure can be simply written as as sum:

$$\begin{aligned} p^{\mathrm{HRG}}(\hat{\mu}_B, \hat{\mu}_S) &= p^{\mathrm{mesons}}_{S=0} + p^{\mathrm{baryons}}_{S=0} \cosh(\hat{\mu}_B) \\ &+ p^{\mathrm{mesons}}_{|S|=1} \cosh(\hat{\mu}_S) + p^{\mathrm{baryons}}_{|S|=1} \cosh(\hat{\mu}_B - \hat{\mu}_S) \\ &+ p^{\mathrm{baryons}}_{|S|=2} \cosh(\hat{\mu}_B - 2\hat{\mu}_S) + p^{\mathrm{baryons}}_{|S|=3} \cosh(\hat{\mu}_B - 3\hat{\mu}_S) \end{aligned}$$

And so one can form identities independently of the resonance list:

$$\begin{aligned} \chi_4^B - \chi_2^B &= 0 \\ v_1 = \chi_{31}^{BS} - \chi_{11}^{BS} &= 0 \\ v_2 = \frac{1}{3}(\chi_2^S - \chi_4^S) & \\ -2\chi_{13}^{BS} - 4\chi_{22}^{BS} & \\ -2\chi_{31}^{BS} &= 0 \end{aligned}$$

[BNL-Bielefleld 1304.7220]



For the light flavors, see: [WB 1305.6297] For the charm sector, see: [BNL-Bielefeld 1404.4043]