### Lattice QCD at non-zero temperature and density

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- QCD in a nutshell, non-perturbative physics, lattice-regularized QCD, Monte Carlo simulations
- the phase diagram on strongly interacting matter, chiral symmetry restoration, the equation of state
- finite density QCD, cumulants of conserved charge fluctuations, thermal masses & transport properties

#### Phases of strong-interaction matter



#### **Symmetries of QCD**

$$
\mathcal{L}_{E}=\frac{1}{4}F_{\mu\nu}^{a}F_{\mu\nu}^{a}+\bar{\psi}_{j,a}\left(\sum_{\nu=0}^{3}\gamma_{\nu}\left(\partial_{\nu}-i\frac{g}{2}\mathcal{A}_{\nu}^{a}\lambda^{a}\right)+m_{j}\right)^{a,b}\psi_{j,b}
$$

– symmetries of QCD:  $U_V(1) \times U_A(1) \times SU_L(n_f) \times SU_R(n_f)$ 

– chiral decomposition:  $\psi \equiv (\psi_1, ...\psi_{n_f}) = \psi_L + \psi_R$ 

 $P_{\epsilon} = \frac{1}{2} \left( 1 + \epsilon \gamma_5 \right) \; , \; \epsilon = \pm 1 \;\;\;\;\;\;\;\;\;\; P_{\epsilon}^2 = P_{\epsilon} \; , \; P_{+} P_{-} = 0$  $\psi_L = P_+ \psi \;\; , \;\; \psi_R = P_- \psi \qquad \quad \bar \psi_L = \bar \psi P_- \;\; , \;\; \bar \psi_R = \bar \psi P_+$  $\mathcal{L}_F \sim \bar{\psi}_L \mathcal{P}_{\mu} \psi_L + \bar{\psi}_R \mathcal{P}_{\mu} \psi_R - m_q (\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L)$  $U_V(1)$ : baryon number  $\psi^\Theta = e^{i\Theta}\psi$ ,  $\bar{\psi}^\Theta = \bar{\psi}e^{-i\Theta}$  $U_A(1):$  axial symmetry  $\psi^\Theta = e^{i\Theta\gamma_5}\psi$ ,  $\bar\psi^\Theta = \bar\psi e^{i\Theta\gamma_5}$  $SU_{L/R}(n_f)$  : flavor symmetry  $G_{\epsilon} \equiv P_{-\epsilon} \cdot 1 + P_{\epsilon} U_{\epsilon}$  ,  $U_{\epsilon} \in U(n_f)$  $G \equiv G_{+}(U_{+})G_{-}(U_{-})$ 

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#### **Chiral phase transition**

#### **Which symmetry is restored?**

$$
U_L(n_f) \times U_R(n_f) \Leftrightarrow U_V(1) \times U_A(1) \times \underbrace{SU_L(n_f) \times SU_R(n_f)}_{\text{exact: baryon}}
$$
\n
$$
U_L(n_f) \times \underbrace{SU_R(n_f)}_{\text{exact: baryon}}
$$
\n
$$
n_f = 2 (u, d) : O(4)
$$

 $n_f=2:$ 

standard scenario:  $U_A(1)$  remains broken, chiral limit controlled by  $O(4)$ 



alternative scenario:  $U_A(1)$  "effectively" restored, first order transition possible



R. Pisarski, F. Wilczek, PRD29 (1984) 338

#### **Chiral symmetry breaking and restoration**

staggered (or Kogut-Susskind) fermions do have a global  $U(1)xU(1)$  symmetry (remnant of the chiral SU(nf)xSU(nf))

 $U(1) \times U(1)$ : independent phase transformations on even and odd sites of the lattice

$$
\psi'_e = \mathrm{e}^{i\theta_1}\psi_e \;\; , \;\; \bar\psi'_e = \mathrm{e}^{-i\theta_2}\bar\psi_e
$$
  

$$
\psi'_o = \mathrm{e}^{i\theta_2}\psi_o \;\; , \;\; \bar\psi'_o = \mathrm{e}^{-i\theta_1}\bar\psi_o
$$

one parameter, continuous global symmetry

 $\longrightarrow$  its spontaneous breaking generates one Goldstone pion  $m_\pi \sim m_l^2$ 



#### **Universality and the Chiral Phase Transition**



$$
\frac{p}{T^4} = \frac{1}{VT^3} \ln Z(V,T) = -f_s(t/h^{1/\beta\delta}) - f_r(V,T)
$$
\n
$$
\frac{t}{t} = 0 \text{ , } h \equiv 0 \qquad t \sim \frac{T - T_c}{T_c} \text{ , } h \sim \frac{m_l}{T}
$$
\n
$$
M_b \equiv \frac{m_s \langle \bar{\psi}\psi \rangle_l}{T^4} = \frac{1}{VT^3} \frac{m_s}{T} \frac{1}{2} \frac{\partial \ln Z}{\partial m_l/T} = h^{1/\delta} f_G(z)
$$
\n
$$
\frac{\chi_l}{T^2} = \frac{\partial \langle \bar{\psi}\psi \rangle_l/T^3}{\partial m_l/T} \sim h^{1/\delta - 1} f_\chi(t/h^{1/\beta\delta}) \text{ , } z = t/h^{1/\beta\delta}
$$
\n
$$
v = t/h^{1/\beta\delta}
$$

$$
\frac{\mathrm{d}f_{\chi}(z)}{\mathrm{d}z} = 0 \Leftrightarrow z_{max} \begin{cases} - \text{ defines pseudo-critical } T_c(m_l) \\ - \text{scaling: } \chi_l(m_l) / T^2 \sim m_l^{1/\delta - 1} \end{cases}
$$

#### **Chiral phase transition**



#### 3-flavor QCD:



1) A. Bazavov et al., arXiv:1701.03548 2) X.-J. Jin et al., arXiv:1706.01178

#### 2 and (2+1)-flavor QCD: **O(4) scaling?**



magnetic equation of state:  $M = h^{1/\delta} f_G(z)$ 

– scaling analysis in (2+1)-flavor QCD with HISQ fermions

 $\implies m_{\pi}^{crit} < 80 \rm{MeV}$ 

not yet sensitive to  $O(4)$  scaling in the chiral limit vs.  $Z(2)$  critical behavior at  $m_c > 0$ 

staggered fermions: O(2) instead of O(4) for non-zero cut-off

#### **The QCD crossover transition – extracting the pseudo-critical temperature –**

#### **Crossover transition temperature**



#### $T_c = (154 \pm 9) \;{\rm MeV}$

- well defined pseudo-critical temperature
- quark mass dependence of susceptibilities consistent with O(4) scaling
- A. Bazavov et al. (hotQCD), Phys. Rev. D85, 054503 (2012), arXiv:1111.1710

lattice: 
$$
N_{\sigma}^{3} \cdot N_{\tau}
$$
  
temperature:  $T = 1/N_{\tau}a$ 

Critical temperature from location of peak in the fluctuation of the chiral condensate (order parameter):



### **Symmetries and in-medium properties of hadrons**

Which symmetries are restored at Tc?

 $\bullet$  thermal hadron correlation functions

Greens functions G of quark-antiquark pair in different quantum number channels H, controlled by operators J

$$
\boldsymbol{J_H(x)} = \bar{q}(x)\Gamma_H q(x)
$$



scalar, pseudo-scalar, vector, axial-vector

$$
q(\bar{q}) = u(\bar{u}), \ d(\bar{d}), \dots \Rightarrow \qquad \qquad \bar{q}q = \bar{u}u \text{ flavor singlet}
$$

 $qq = ua$  flavor non-singlet

$$
G_H(\tau, \vec{x}) = \langle J_H(\tau, \vec{x}) \, J_H^{\dagger}(0, \vec{0}) \rangle \sim e^{-m_H \tau}
$$
  
at T=0

### **Thermal modification of the hadron spectrum**

quark propagator: 
$$
\bar{q}(x)q(0) = M_q^{-1}(x,0)
$$
connected  
\n
$$
G_{\pi}(x) = \langle \text{Tr } \gamma_5 M_l^{-1}(x,0) \gamma_5 M_l^{-1}(0,x) \rangle
$$
  
\n
$$
G_{\eta}(x) = G_{\pi}(x) - \langle \text{Tr } [\gamma_5 M_l^{-1}(x,x)] \text{Tr } [\gamma_5 M_l^{-1}(0,0)] \rangle
$$
  
\n
$$
G_{\delta}(x) = -\langle \text{Tr } M_l^{-1}(x,0) M_l^{-1}(0,x) \rangle
$$
  
\n
$$
G_{\sigma}(x) = G_{\delta}(x) + \langle \text{Tr } M_l^{-1}(x,x) \text{Tr } M_l^{-1}(0,0) \rangle
$$
  
\n
$$
-\langle \text{Tr } M_l^{-1}(x,x) \rangle \langle \text{tr } M_l^{-1}(0,0) \rangle
$$

hadronic susceptibilities

$$
\chi_{\pi} = \sum_{x} G_{\pi}(x) \equiv \chi_{5,con} , \quad \chi_{\delta} = \sum_{x} G_{\delta}(x) = \chi_{con}
$$
  

$$
\chi_{\eta} = \sum_{x} G_{\eta}(x) \equiv \chi_{5,con} - \chi_{5,disc}
$$
  

$$
\chi_{\sigma} = \sum_{x} G_{\sigma}(x) = \chi_{con} + \chi_{disc}
$$

disconnected

 $\cup$   $\cup$ 

### **Thermal modification of the hadron spectrum**

 $\mathbf{T}$   $\leq$   $\mathbf{T}_c$ : broken chiral symmetry is reflected in the hadron spectrum



 $T \geq T_c$ : restoration of symmetries is reflected in the (thermal) hadron spectrum

 $SU(2)_L \times SU(2)_R: (\pi, \sigma), (a_1, \rho)$  degenerate

 $U(1)_A: (\pi, \delta)$  degenerate

### **Symmetry restoration and correlation functions**



### **Restoration of the axial symmetry**

 $T \nvert T_c$ : broken chiral symmetry is reflected in the hadron spectrum



 $U(1)_A$  restored  $\implies$   $\chi_{5,con} = \chi_{con}$ 

 $\Leftrightarrow \chi_{disc} = 0 \Leftrightarrow \chi_{\pi}(x) - \chi_{\delta}(x) = 0?$ 

# **U(1)** remains broken

the difference of the scalar  $(\delta)$ and pseudo-scalar $(\pi)$  drops by an order of magnitude but stays non-zero



above Tc (but still for m>0):

$$
\frac{\chi_{\pi}-\chi_{\delta}}{T^2}=\frac{\chi_{disc}}{T^2}=\frac{\chi_{5,disc}}{T^2}>0
$$

thermodynamics with domain wall fermions hotQCD, arXiv:1205.3535 nonetheless, chiral limit remains controversial

S. Aoki et al., PR D86 (2012) 114512



## Lattice QCD at non-zero baryon number density  $\mu > 0$

THE PROBLEM in QCD Thermodynamics

partition function again:

$$
Z(V, T, \mu) = \int \mathcal{D}A \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{\bar{\psi} \mathcal{M}(\mathcal{A}, m_q, \mu)\psi} e^{-S_G}
$$

$$
= \int \mathcal{D}A \det M(\mathcal{A}, m_q, \mu) e^{-S_G}
$$

The fermion determinant **– is no longer positive definite standard simulation techniques fail**

$$
\mathrm{det M}(\mathcal{A},\mathrm{m}_\mathrm{q},\mu)=\mathrm{e}^{i\theta(\mu)}|\mathrm{det} M(\mathcal{A},m_q,\mu)|
$$

#### Lattice QCD at non-zero baryon number density – the infamous sign problem –

 $Z(\boldsymbol{V},\boldsymbol{T},\mu)=\int \mathcal{D}\mathcal{A} \ \mathrm{det} M(\mathcal{A},m_q,\mu) \ \mathrm{e}^{-S_G}$ partition function:  $M(\mu)=m_q\delta_{i,j} \hspace{3mm} + \hspace{3mm} \frac{1}{2}\eta_i\biggl(\sum_{i=1}^3(U_{i,k}\delta_{i,j-\hat k}-U^\dagger_{i-\hat k,k}\delta_{i,j+\hat k})\biggr)$ staggered fermion matrix:  $+ \qquad \ \ \mathrm{e}^{\mu} \; U_{i,0} \delta_{i,j-\hat{0}} - \mathrm{e}^{-\mu} \; U_{i-\hat{0},0}^{\dagger} \delta_{i,j+\hat{0}} \bigg)$  $\lambda=m_q\cdot 1+\sum D_i+D_0(\mu)$ e o e o

#### Lattice QCD at non-zero baryon number density – the infamous sign problem –



#### **Probing the properties of matter through the analysis of conserved charge fluctuations**

Taylor expansion of the **QCD** pressure: 
$$
\frac{P}{T^4} = \frac{1}{VT^3} \ln Z(T, V, \mu_B, \mu_Q, \mu_S)
$$

$$
\frac{P}{T^4}=\sum_{i,j,k=0}^\infty \frac{1}{i!j!k!}\chi^{BQS}_{ijk}(T)\left(\frac{\mu_B}{T}\right)^i\left(\frac{\mu_Q}{T}\right)^j\left(\frac{\mu_S}{T}\right)^k
$$

cumulants of net-charge fluctuations and correlations:

$$
\chi_{ijk}^{BQS}=\left.\frac{\partial^{i+j+k}P/T^4}{\partial\hat{\mu}_B^i\partial\hat{\mu}_Q^j\partial\hat{\mu}_S^k}\right|_{\mu_{B,Q,S}=0}\quad,\quad\hat{\mu}_X\equiv\frac{\mu_X}{T}
$$

the pressure in hadron resonance gas (**HRG**) models:

$$
\frac{p}{T^4} = \sum_{m \in meson} \ln Z_m^b(T, V, \mu) + \sum_{m \in baryon} \ln Z_m^f(T, V, \mu)
$$

$$
\sim e^{-m_H/T} e^{(B\mu_B + S\mu_S + Q\mu_Q)/T}
$$

#### Equation of state of (2+1)-flavor QCD:  $\,\mu_B/T > 0$

$$
\frac{P}{T^4}=\sum_{i,j,k=0}^\infty \frac{1}{i!j!k!}\chi_{i,j,k}^{BQS}(T)\left(\frac{\mu_B}{T}\right)^i\left(\frac{\mu_Q}{T}\right)^j\left(\frac{\mu_S}{T}\right)^k
$$

the simplest case:  $\mu_S = \mu_Q = 0$ 

$$
\frac{P(T, \mu_B)}{T^4} = \frac{P(T, 0)}{T^4} + \frac{\chi_2^B(T)}{2} \left(\frac{\mu_B}{T}\right)^2 + \frac{\chi_4^B(T)}{24} \left(\frac{\mu_B}{T}\right)^4 + \mathcal{O}((\mu_B/T)^6)
$$
\nAn  $\mathcal{O}((\mu_B/T)^4)$  expansion is  
\nexact in a QGP up to  $\mathcal{O}(g^2)$   
\nHRG vs. QCD:  
\n $\mathcal{O}((\mu_B/T)^4)$ :difference is less  
\nthan 3% at  $\mu_B/T = 2$   
\n
$$
\mathcal{O}((\mu_B/T)^6)
$$
:difference is less  
\nthan 2% at  $\mu_B/T = 3$ 

### Equation of state of (2+1)-flavor QCD:  $\mu_B/T > 0$



– leading and next-to-leading order corrections agree well with HRG for T<150 MeV – already in the crossover region deviations from HRG can reach ~40% for T~165 MeV

#### Equation of state of (2+1)-flavor QCD:  $\,\mu_B/T > 0$

$$
\frac{\Delta(T,\mu_B)}{T^4} = \frac{P(T,\mu_B) - P(T,0)}{T^4} = \frac{\chi_2^B}{2} \left(\frac{\mu_B}{T}\right)^2 \left(1 + \frac{1}{12} \frac{\chi_4^B}{\chi_2^B} \left(\frac{\mu_B}{T}\right)^2\right)
$$

$$
+ \frac{1}{720} \frac{\chi_6^B}{\chi_2^B} \left(\frac{\mu_B}{T}\right)^6
$$

$$
\frac{\chi_6}{T^2} \left(\frac{\mu_B}{T}\right)^6
$$

$$
\frac{\chi_6}{T^2} \left(\frac{\mu_B}{T}\right)^6
$$

$$
\frac{\chi_6}{T^2} \left(\frac{\mu_B}{T}\right)^{6.5}
$$
<

or equivalently

#### **Searching for a critical point at**  $\mu_B > 0$

**Does it exist?**



– signatures for a critical point: large fluctuations in e.g. the net baryon-number

 break-down of Taylor series expansion → **radius of convergence**

#### **Chiral transition, hadronization and freeze-out**

- pseudo-critical temperature  $T_c = 154(9) \text{MeV}$
- hadronization temperatures  $T_h = 164(3) \text{ MeV}$
- freeze-out temperatures:



$$
T_{fo} = [164(5)-168(4)]~{\rm MeV}
$$



#### **Where does hadronization set in?**

**physics is quite different at lower and upper end of the current error bar on Tc**

**probed with net-charge correlations&fluctuations**

#### **HRG vs. QCD net baryon-number fluctuations**

$$
\mathcal{L}_2^B(T,\mu_B) = \chi_2^B + \frac{1}{2}\chi_4^B \left(\frac{\mu_B}{T}\right)^2 + \frac{1}{24}\chi_6^B \left(\frac{\mu_B}{T}\right)^4 + \mathcal{O}(\mu_B^6)
$$

- **agreement between HRG and QCD will start to deteriorate for T>150 MeV**
- **net baryon-number fluctuations in QCD always smaller than in HRG for T>150 MeV**



### **HRG vs. QCD net baryon-number fluctuations**

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$$

- **agreement between HRG and QCD will start to deteriorate for T>150 MeV**
- **net baryon-number fluctuations in QCD always smaller than in HRG for T>150 MeV**

no evidence for enhanced net baryon-number fluctuations for  $T\geq~135{\rm MeV} \; , \; \mu_B\leq 2T$ no evidence for getting closer to a ''critical region''



### **Taylor expansion of the pressure and critical point**

$$
\boxed{\frac{P}{T^4} = \sum_{n=0}^\infty \frac{1}{n!} \chi_n^B(T) \left(\frac{\mu_B}{T}\right)^n}
$$

for simplicity :  $\mu_Q = \mu_S = 0$ 

estimator for the radius of convergence:

$$
\left(\frac{\mu_B}{T}\right)_{crit,n}^{\chi} \equiv r_n^{\chi} = \sqrt{\left|\frac{n(n-1)\chi_n^B}{\chi_{n+2}^B}\right|}
$$

– radius of convergence corresponds to a critical point only, iff

 $\chi_n > 0$  for all  $n \geq n_0$ 

forces  $P/T^4$  and  $\chi_n^B(T,\mu_B)$ to be monotonically growing with  $\mu_B/T$ 

at  $T_{CP}: \kappa_B \sigma_B^2 = \frac{\chi_4^B(T,\mu_B)}{\gamma_2^B(T,\mu_B)} > 1$ 

#### if not:

- radius of convergence does not determine the critical point
- Taylor expansion can not be used close to the critical point

#### **estimates/constraints on critical point location**



#### 01/01/17: based on ongoing calculations of  $6<sup>th</sup>$  order Taylor expansion coefficients performed by the Bielefeld-BNL-CCNU collaboration A. Bazavov et al., arXiv:1701.04325

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 $\chi^B_6< 0$ 

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 $\chi^B_6 < 0$ 

Explore the **structure of matter** close to the QCD transition temperature using **fluctuations of conserved charges**

baryon number, strangeness, electric charge



**ideal quark (fermi) gas, m=0**



#### **fractional charges integer charges**

baryon number:  $B = +/- 1/3$ 

electric charge:  $Q = +/- 1/3, +/- 2/3$ 

Low T: HRG

#### **hadron resonance gas**





#### **Correlations and Fluctuations of conserved charges**

- construct QCD observables that would project onto specific quantum numbers,  $if QCD = HRG$
- obtain fluctuations of quantum numbers and correlations between them from the grand canonical potential (~pressure)

$$
\frac{P}{T^4} = \ln Z(T, V, \mu_B, \mu_Q, \mu_S, ...)
$$

#### charge fluctuations charge correlations:

$$
\chi_n^X = \frac{\partial^n \ln Z(T, V, .. \mu_X ..)}{\partial \mu_X^n} \bigg|_{\mu=0}
$$
  

$$
n = 2: \ \chi_2^X = \langle X^2 \rangle - \langle X \rangle^2
$$

$$
\chi_{XY}^{nm} = \frac{\partial^{n+m} \ln Z(T, V, .. \mu_X, \mu_Y..)}{\partial \mu_X^n \partial \mu_Y^m}
$$
  

$$
n = m = 1: \ \chi_{11}^{XY} = \langle XY \rangle - \langle X \rangle \langle Y \rangle
$$

#### **Net baryon-number fluctuations**

ratio of  $4<sup>th</sup>$  and  $2<sup>nd</sup>$  order cumulants:



BNL-Bielefeld-CCNU: Phys. Rev. Lett. 111, 082301 (2013) Phys. Lett. B737, 210 (2014)

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#### **Net baryon-number fluctuations**

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#### Ratio of baryon number – strangeness correlation and net strangeness fluctuations



PDG-HRG: uses experimentally known hadron spectrum listed by the Particle Data Group QM-HRG: uses additional hadrons predicted to exist in Quark Model calculations

#### **Probing the hadron spectrum using QCD thermodynamics**



#### **Probing the hadron spectrum using QCD thermodynamics**



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### **Correlations and Fluctuations: HRG vs. LQCD**

- construct QCD observables that would project onto specific quantum numbers, if QCD = HRG
- E.g.: HRG pressure:



#### **Evidence for many charmed baryons in thermodynamics**



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#### **Evidence for many charmed baryons in thermodynamics**



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### **Thank you for your attention and the**

many interested/interesting questions

### you asked during the lectures and the breaks

Brookhaven National Laboratory



Bielefeld University

