









#### LGT:

- equilibrium thermodynamics of QCD;
- formulated in terms of basic degrees of freedom: quarks and gluons;
- observables expressed in terms of temperature and chemical potential







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- evolution of a dense interacting medium described by QCD;
- observable properties in terms of hadrons, leptons and photons;
- observables parametrized in terms of energy and particle multiplicities







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## MODELS

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Where lattice calculations do/will contribute to the development of theoretical concepts and the analysis of experimental observables



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 $T_c, \ \epsilon_c$ phase diagram in the  $(T, \ \mu_B)$ -plane;  $\mu \simeq 0$  : RHIC (LHC)  $\mu > 0$  : SPS (GSI future) chiral critical point



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#### EoS

energy density, pressure, velocity of sound,...; susceptibilities (baryon number fluctuations);

strangeness contribution



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experimental observables

In - medium

charmonium spectroscopy;

light quark bound states;

thermal dilepton rates

hadron properties

heavy quark potential, screening;

F. Karsch, HP2004 – p.2/26



Where lattice calculations do/will contribute to the development of theoretical concepts and the analysis of

experimental observables

*short vs. long distance physics* 

running coupling constant; transport coefficients (??)



#### Progress in lattice calculations... depends on...

- development of (special purpose) computer hardware
- ٩





# Setting a standard: Computational requirements in EoS calculations

only integrated luminosity counts (!), i.e. peak spead of a computer itself is of little significance



#### a PETAFLOP calculation



### Progress in lattice calculations... depends on...

- development of (special purpose) computer hardware
- progress in algorithm development

1987	invention of Hybrid Monte Carlo Algorithm
early '90s	development of various preconditioning schemes
late '90s	new algorithms: polynomial / shifted HMC; multi-boson algorithm

1987 - 2004: gain of factor 15 - 20 from algorithm development



#### Progress in lattice calculations... depends on...

- development of (special purpose) computer hardware
- progress in algorithm development
- new ideas, new conceptual developments!!!
- 1988/89 multi-parameter Ferrenberg-Swendsen reweighting
   ⇒ accurate location of transition points, scaling analysis
  - 1996 Non-perturbative definition of bulk thermodynamics  $\Rightarrow$  integral method for reliable pressure calculations
  - 1999 Maximum Entropy Method (MEM) for QCD
     ⇒ spectral functions, in-medium properties of hadrons
  - 2002 reweighting and Taylor expansion techniques for  $\mu > 0$  $\Rightarrow$  QCD phase diagram at finite baryon density



# Outlook: Next generation computers for lattice gauge theory



today: APEmille

so far the only dedicated large-scale computer installation used predominantly for QCD thermodynamics exists in Bielefeld: 120 GFlops

RHIC vs. SPS: Running a dedicated machine makes a difference!



# Outlook: Next generation computers for lattice gauge theory

### **QCDOC** and apeNEXT



QCD thermodynamics on the next generation of special purpose dedicated QCD computers

installations with (10-20) TFlops peak speed are planned in the USA and Europe



## apeNEXT: Next generation of APE computers



BackPlane



## apeNEXT: Next generation of APE computers



#### BackPlane



## apeNEXT: Next generation of APE computers



BackPlane



## QCDOC: Next generation of Columbia-RIKEN computer

#### Columbia-RIKEN/BNL-UKQCD Collaboration



2 - node daughter card



64 - node mother board

prototypes exist since 07/2003



## QCDOC: Next generation of Columbia-RIKEN computer

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10/2004: 12288-node machine:  $\sim$  10 TFlops

• first QCDOC machine; built for UKQCD



## QCDOC: Next generation of Columbia-RIKEN computer

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#### $QCDOC\ computing\ center\ at\ BNL:$

- 10 TFlops machine for RBRC:  $\sim$  12/2004
- 10 TFlops machine for american LGT community:  $\sim$  early in 2005
- •... larger installations possible and needed!



### Bulk Thermodynamics: What do we (want to) know?

#### $\mu = 0:$

Properties of transition in  $2, \ (2+1)$ -flavor QCD:

crossover or phase transition, deconfinement vs. chiral symmetry restoration, universality, ...



confront resonance gas, quasi-particle gas, high-T pert. theory, HTL-resummation, ... with lattice calculations

#### $\mu > 0:$

 ${} {\scriptstyle 
m extsf{le}} \ T_c(\mu) \ \Leftrightarrow \ T_{
m freeze}(\mu):$ 

location of the chiral critical point, direct evidence for  $1^{
m st}$  order regime; density fluctuations;  $T_c(\mu)\equiv T_{
m freeze}$  ?



# Critical behavior in hot and dense matter: phase diagram

### crossover vs. phase transition





# Critical behavior in hot and dense matter: phase diagram





#### Critical temperature, equation of state





#### Critical temperature, equation of state





#### Critical temperature, equation of state



- $a\simeq 0.2\,fm$  (continuum limit??)
- improved staggered fermions,
   ⇒ flavor symmetry breaking (need even better fermion actions)

 $\epsilon_c$ 

- $m_{PS}\simeq 770~MeV$  (!!!)
- ullet  $V\simeq (4\,{
  m fm})^3$  (thermodynamic limit)





non-zero baryon number density:  $\mu > 0$ 

$$Z(\mathbf{V}, \mathbf{T}, \boldsymbol{\mu}) = \int \mathcal{D}\mathcal{A}\mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S_E(\mathbf{V}, \mathbf{T}, \boldsymbol{\mu})}$$
$$= \int \mathcal{D}\mathcal{A}\mathcal{D} \det M(\boldsymbol{\mu}) e^{-S_E(\mathbf{V}, \mathbf{T})}$$
$$\uparrow \text{complex fermion determinant;}$$

long standing problem

 $\Rightarrow$  three (partial) solutions for large T, small  $\mu$ 



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- $\Rightarrow$  three (partial) solutions for large T, small  $\mu$
- exact evaluation of *det M*: works well on small lattices; requires reweighting
   Z. Fodor, S.D. Katz, JHEP 0203 (2002) 014
- Taylor expansion around  $\mu = 0$ : works well for small  $\mu$ ; requires reweighting C. R. Allton et al. (Bielefeld-Swansea), Phys. Rev. D66 (2002) 074507
- imaginary chemical potential: works well for small  $\mu$ ; requires analytic continuation Ph. deForcrand, O. Philipsen, Nucl. Phys. B642 (2002) 290



analysis of volume dependence of Lee-Yang zeroes for  $\mu > 0$ 





first (exploratory) results on the quark mass dependence of the transition line:



### $m_q$ -dependence

(3-flavor QCD, pert.  $\beta$ -function, Taylor expansion)

$$\begin{array}{l} \frac{T_c(\mu)}{T_c(0)} : & 1-0.025(6)(\mu_q/T)^2 \ , \ ma=0.1 \\ & 1-0.114(46)(\mu_q/T)^2 \ , \ ma=0.005 \\ & \text{Bielefeld-Swansea} \\ & (\text{hep-lat/0309116, Lattice 2003}) \end{array}$$



first (exploratory) results on the quark mass dependence of the transition line:



## $\begin{array}{l} m_q \mbox{-dependence not confirmed in} \\ \mbox{simulations with imaginary } \mu \\ \mbox{Ph. de Forcrand, O. Philipsen, NP B673 (2003) 170} \end{array}$

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Bielefeld-Swansea  
(hep-lat/0309116, Lattice 2003)

a systematic analysis of cut-off effects, scaling violations AND volume + truncation effects still needs to be done



non-zero baryon number density:  $\mu > 0$ 

$$egin{aligned} Z(oldsymbol{V},oldsymbol{T},oldsymbol{\mu}) &= \int \mathcal{D}\mathcal{A}\mathcal{D}\psi\mathcal{D}ar{\psi} \ \mathrm{e}^{-S_E(oldsymbol{V},oldsymbol{T},oldsymbol{\mu})} \ &= \int \mathcal{D}\mathcal{A}\mathcal{D} \ det \ M(oldsymbol{\mu}) \ \mathrm{e}^{-S_E(oldsymbol{V},oldsymbol{T})} \end{aligned}$$



 ${T_c(\mu)\over T_c(0)}$  :

- $: 1 0.0056(4)(\mu_B/T)^2$ 
  - deForcrand, Philipsen (imag.  $\mu$ , pert)  $1 - 0.0078(38)(\mu_B/T)^2$

**Bielefeld-Swansea** 

 $(\mathcal{O}(\mu^2)$  reweighting, non-pert)

 $1-0.0032(1)(\mu_B/T)^2$ 

Fodor,Katz(Lee-Yang zeroes, pert)



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current studies of  $T_c(\mu)$  are exploratory! uncertainties in scale-determination and systematics of quark mass dependencee



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 $T_c(\mu) \equiv T_{
m freeze}$ ?

P. Braun-Munzinger, J. Stachel,C. Wetterich, hep-nucl/0311005

Will be answered by LGT calculations



# Analyzing the (quasi-particle) structure of HG and QGP phases

### Response and correlation functions:

#### $T \leq T_c$ : chiral symmetry restoration

- hadronic resonance gas;
  MEM analysis of thermal masses and widths,  $\pi, \rho, \dots$ 
  - (baryon) density fluctuations, strangeness fluctuations, ...

#### $T > T_c$ : deconfinement

- free energies, potentials and screening masses, running coupling at short and large distances,...
- MEM analysis of heavy and light quark bound states, quark and gluon propagators, dilepton and photon rates, ...



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requires light dynamical quarks ⇒ PETAFLOPs era

> meaningful already in quenched QCD → TERAFLOPs era



# Thermal meson correlation functions and spectral functions

Thermal correlation functions: 2-point functions which describe propagation of a  $\bar{q}q$ -pair

spectral representation of correlator  $\Rightarrow$  dilepton and photon rates



spectral representation of

Euclidean correlation functions

spectral representation of thermal photon rate:  $\omega = |\vec{p}|$  $\omega \frac{\mathrm{d}^3 R^{\gamma}}{\mathrm{d}^3 p} = \frac{5\alpha}{6\pi^2} \frac{\sigma_V(\omega, \vec{p}, T)}{\omega^2(\mathrm{e}^{\omega/T} - 1)}$ 

spectral representation of thermal dilepton rate  $\frac{\mathrm{d}^4 W}{\mathrm{d}\omega \mathrm{d}^3 p} = \frac{5\alpha^2}{27\pi^2} \frac{\sigma_V(\omega, \vec{p}, T)}{\omega^2(\mathrm{e}^{\omega/T} - 1)}$ 

$$G_H^{eta}( au,ec{r}) = \int_0^\infty \mathrm{d}\omega \,\int rac{\mathrm{d}^3ec{p}}{(2\pi)^3} \, \sigma_H(\omega,ec{p},T) \, \mathrm{e}^{iec{p}ec{r}} \, rac{\mathrm{cosh}(\omega( au-1/2T))}{\mathrm{sinh}(\omega/2T)}$$

### Dilepton rate: HTL and lattice calculations



#### thermal dilepton rate

$$\frac{\mathrm{d}W}{\mathrm{d}\omega\mathrm{d}^3p} = \frac{5\alpha^2}{27\pi^2} \frac{\sigma_V(\omega,\vec{p},T)}{\omega^2(\mathrm{e}^{\omega/T}-1)}$$

HTL and lattice disagree for  $\omega/T \lesssim (3-4)$ 

● infra-red sensitivity of HTL-calculations ⇔ "massless gluon" cut in HTL-propagator

- ullet infra-red sensitivity of lattice calculations  $\Leftrightarrow$  thermodynamic limit,  $V 
  ightarrow \infty$
- $VT^3 = (N_\sigma/N_\tau)^3 < \infty \Rightarrow$  momentum cut-off:  $p/T > 2\pi N_\tau/N_\sigma$

need large lattices to analyze infra-red regime

in future also thermal photon rates

### Dilepton rate: HTL and lattice calculations



thermal dilepton rate

$$\frac{\mathrm{d}W}{\mathrm{d}\omega\mathrm{d}^3p} = \frac{5\alpha^2}{27\pi^2} \frac{\sigma_V(\omega,\vec{p},T)}{\omega^2(\mathrm{e}^{\omega/T}-1)}$$

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need large lattices to analyze infra-red regime



need  $N_ au \sim \mathcal{O}(30)$  AND $N_\sigma \sim 6 \; N_ au$ 



#### Heavy quark spectral functions and correlation functions

reconstructed correlation functions above  $T_c$  from data below  $T_c$ SC,  $\beta$ =6.64,  $\kappa$ =0.1290, G<sub>recon</sub> from  $\rho$ (0.75T<sub>c</sub>) 0.75T  $(\chi_{c0})^{1.8}$  $G(\tau)/G_{recon}(\tau)$ 1.1T 1.5 1.2 0.9 0.2 0.3 0.5 0.1 0.4 0 τ[fm] 1.1 0.75T 1.1T  $G(\tau)/G_{recon}(\tau)$  $(J/\psi)$ 1.5T<sub>c</sub><sup>6</sup> ⊢ 1 0.9 VC,  $\beta$ =6.64,  $\kappa$ =0.1290, G<sub>recon</sub> from  $\rho$ (0.75T<sub>c</sub>) 0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 τ[fm]

reconstructed spectral functions using the Maximum Entropy Method





#### Heavy quark spectral functions and correlation functions



reconstructed spectral functions using the Maximum Entropy Method



F. Karsch, HP2004 - p.21/26



#### Heavy quark spectral functions and correlation functions



reconstructed spectral functions using the Maximum Entropy Method



#### Heavy quark spectral functions comparison of different approaches

S. Datta et al., hep-lat/0312037





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S. Datta et al., hep-lat/0312037

M. Asakawa, T. Hatsuda, hep-lat/0308034 S. Dat  $J/\psi$  spectral function



#### Heavy quark spectral functions comparison of different approaches





## Fluctuations of the baryon number density ( $\mu \geq 0$ )

baryon number density fluctuations: (MILC coll., hep-lat/0405029)



$$egin{aligned} &rac{\chi_q}{T^3} = \left(rac{\mathrm{d}^2}{\mathrm{d}(\mu/T)^2}rac{p}{T^4}
ight)_{T \,\,\mathrm{fixed}} \ &= rac{9 \, T}{V} \left(\langle N_B^2 
angle - \langle N_B 
angle^2
ight) \end{aligned}$$

susceptibilities = integrated correlation functions
= integrated spectral functions

to be studied in event-by-event fluctuations



# Fluctuations of the baryon number density ( $\mu \geq 0$ )







# Fluctuations of the baryon number density ( $\mu \geq 0$ )





## Outlook: Next generation lattice calculations

- Thermodynamics of pure gauge theory has been "solved" on (1-10)GFlops computers (1996)
- Thermodynamics of QCD with "still too heavy" quarks has been studied on (10-100) GFlops computers
- Analysis of "continuum and thermodynamic limit" of bulk thermodynamics with light quarks and spectral functions in quenched QCD requires computers with ~10 TFlops peak speed.

Germany: LatFor proposal 2003

http://www.zeuthen.desy.de/latfor/paper.pdf

US: White Paper 2004

http://www-ctp.mit.edu/~negele/WhitePaper.pdf

Studies of spectral functions of light quark bound states below  $T_c$  require simulations with light, dynamical quarks on computers with  $\gtrsim 100$  TFlops peak speed.



## Outlook: projects coming soon...

Thermodynamics on a 10 TFlops computer (5 TFlops sustained)

•  $T_c$ , EoS ( $\mu = 0$  and  $\mu > 0$ ) with light dynamical quarks: (2+1)-flavor QCD, close to physical  $m_{\pi}/m_K$  ratio; exploring the continuum limit:  $a \simeq (0.1 - 0.2)$  fm analyzing the thermodynamic limit:  $V \simeq 500$  fm<sup>3</sup>

> ⇒ lattice sizes up to:  $32^3 \times 8$ ; CPU-time: ~ 5 TFlops-years ( $\mu = 0$ ) ~ 5 TFlops-years ( $\mu > 0$ )

In-medium hadron properties, charmonium, dilepton rates: quenched QCD on fine lattices (a ~ 0.02 fm); analyzing light quark mesons with improved fermion formulations; exploring infra-red sensitivity of dilepton rates; analyzing charmonium spectra;

 $\Rightarrow$  lattice sizes up to:  $128^3 \times 32$ ; CPU-time:  $\sim 3$  TFlops-years



### Outlook: projects on future machines...

Thermodynamics on Petaflops computers

(exploratory studies already on up-coming TFlops computers)

In-medium properties of light quark bound states: QCD with light, dynamical quarks on fine lattices become possible; mass shifts and modification of widths below T<sub>c</sub>

finite density QCD at low temperature: temperatures around  $T \sim 0.5 T_c$  should be accessible

transport properties:

calculation of "gluonic correlator" (energy momentum tensor) should become possible; spectral functions in the  $\omega \to 0$  limit may become accessible