Lattice simulation of QCD on supercomputers

V.V. Braguta

JINR

October 28, 2024

Outline:

- Introduction
  - Statistical mechanics
  - QED as a gauge theory
  - Building gluodynamics and QCD
- Lattice gluodynamics and QCD
- Numerical methods for lattice QCD
- Applications

Partition function

- Partition function:
  $Z = \sum_n e^{-\frac{E_n}{T}} = \sum_n \langle n| e^{-\frac{\hat{H}}{T}} |n\rangle = Tr\left[e^{-\frac{\hat{H}}{T}}\right]$,
  $\hat{H}|n\rangle = E_n|n\rangle$

- Free energy:
  $F = -T\log Z = E - TS, \quad Z = e^{-\frac{F}{T}}$

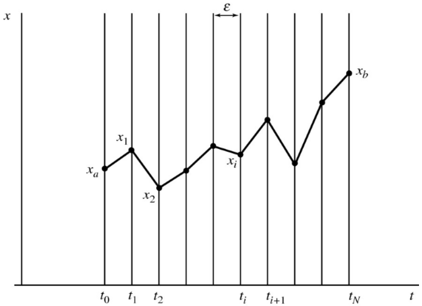
- Probability to find a system at the n-th level:
  $P_n = \frac{e^{-\frac{E_n}{T}}}{Z}$

- $\langle O\rangle = \sum_n P_n \langle n|\hat{O}|n\rangle = \frac{1}{Z}\sum_n \langle n|O|n\rangle e^{-\frac{E_n}{T}}$

- Z contains an important information about system:
  - $\langle E\rangle = T^2 \frac{\partial logZ}{\partial T} = -T^2 \frac{\partial}{\partial T}\left(\frac{F}{T}\right)$
  - $p = -\frac{\partial F}{\partial V}$
  - $S = \frac{\partial T logZ}{\partial T} = -\frac{\partial F}{\partial T}$

Path integral formulation for partition function

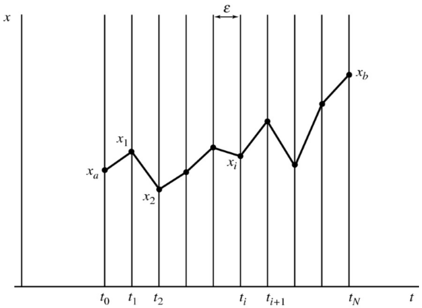
- $Z = Tr\left[e^{-\frac{\hat{H}}{T}}\right] = \sum_q \langle q| e^{-\frac{\hat{H}}{T}} |q\rangle = \int dq \langle q| e^{-\frac{\hat{H}}{T}} |q\rangle$
- Quantum evolution in time: $\langle q'| e^{-i\frac{\hat{H}}{\hbar}t} |q\rangle$, $q(0) = q$, $q(t) = q'$
- Z looks like quantum evolution in *imaginary* time
  $t = -i\tau = -i\frac{1}{T}$, $q(0) = q$, $q(\tau = \frac{1}{T}) = q$
- $Z \sim \lim_{N\to\infty} \int \prod_{\tau=1}^{N} dq(\tau) e^{-S_E}$
  $S_E = \int_0^{1/T} d\tau (\frac{m\dot{q}(\tau)^2}{2} + V(q(\tau)))$, $\quad q(0) = q(\tau = \frac{1}{T}) = q$



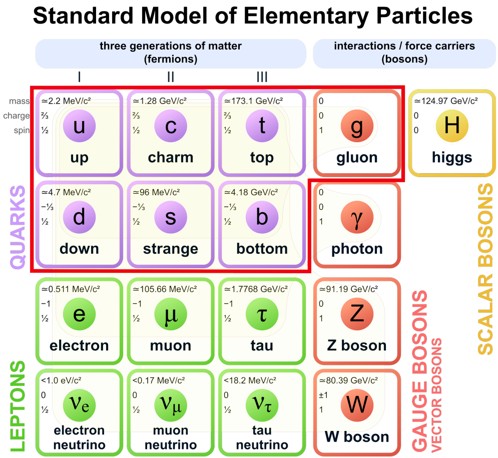
N degrees of freedom

- $q_i(\tau)$, $i = 1..N$

- $Z \sim \int \prod_\tau \prod_{i=1}^N dq_i(\tau) e^{-S_E}$
  $S_E = \int_0^{1/T} d\tau \left(\frac{m \sum_i \dot{q}_i(\tau)^2}{2} + V(q_i(\tau))\right), \quad q_i(0) = q_i(\tau = \frac{1}{T}) = q_i$



Elementary particles



Properties of QED

- Interaction of charged particles
- Vector potential
  $A_\mu = (A_0, A_x, A_y, A_z), \quad \mu = 0, 1, 2, 3$
  $\vec{E} = -\frac{\partial \vec{A}}{\partial t} - \vec{\nabla} A_0, \quad \vec{B} = rot\vec{A}$
- Gauge transformation:
  $A_\mu \to A_\mu + \partial_\mu f, \quad \psi \to e^{if}\psi$
  electric field: $\vec{E} \to \vec{E}$
  magnetic field: $\vec{B} \to \vec{B}$
- QED action: $S = \int d^4x \left[-\frac{1}{2e^2}(\vec{H}^2 - \vec{E}^2) + \bar{\psi}(i\gamma^\mu D_\mu - m)\psi \right]$
- Coupling constant: $\alpha_{em} = \frac{e^2}{4\pi\hbar c} \simeq \frac{1}{137} \ll 1$

Maxwell equations

$$
\begin{aligned}
divE &= 4\pi\rho \\
divH &= 0 \\
rotE &= -\frac{1}{c}\frac{\partial H}{\partial t} \\
rotH &= \frac{4\pi}{c}j + \frac{1}{c}\frac{\partial E}{\partial t}
\end{aligned}
$$

- Maxwell equations are linear

Building QCD

- New quantum number: $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}$
- Interactions of particles with the color
- Gauge transformation: $S(x) \in SU(3)$
  $\hat{A}_\mu \to S\hat{A}_\mu S^{-1} - i\partial_\mu S S^{-1} \quad \hat{A}_\mu = t^a A^a_\mu,\ a = 1...8$
  $\psi(x) \to S(x)\psi(x)$
  chromo-electric field: $\vec{E} \to S^{-1}\vec{E}S$
  chromo-magnetic field: $\vec{B} \to S^{-1}\vec{B}S$
- QCD action:
  $S = \int d^4x \big[-\frac{1}{g^2} Tr(\vec{H}^2 - \vec{E}^2) + \bar{\psi}(i\gamma^\mu \hat{D}_\mu - m)\psi \big]$
- Coupling constant: $\alpha_s = \frac{g^2}{4\pi\hbar c} \sim 1$

Maxwell equations in QCD

$$
\begin{aligned}
divE^a &= 4\pi\rho^a + f_1(A, E, H, ...) \\
divH^a &= 0 + f_2(A, E, H, ...) \\
rotE^a &= -\frac{1}{c}\frac{\partial H^a}{\partial t} + f_3(A, E, H, ...) \\
rotH^a &= \frac{4\pi}{c}j^a + \frac{1}{c}\frac{\partial E^a}{\partial t} + f_4(A, E, H, ...)
\end{aligned}
$$

- Maxwell equations for QCD are nonlinear

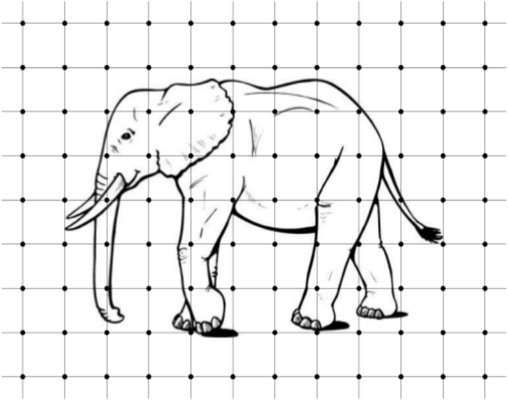
Quantum chromodynamics(QCD)

- Degrees of freedom: Quarks ψ, gluons A
- QCD Lagrangian

$$L = -\frac{1}{4}\sum_{a=1}^{8} F_a^{\mu\nu} F_{\mu\nu}^a + \sum_{f=u,d,s,\ldots} \bar{q}_f (i\gamma^\mu \partial_\mu - m) q_f + g \sum_{f=1}^{N_f} \bar{q}_f \gamma^\mu \hat{A}_\mu q_f$$

- Nonlinear equation of motion with $\alpha_s \sim 1$
- **The most complicated physical theory**
- QCD Lagrangian is well known but the calculations are not possible
  - *In particular:* Confinement from QCD lagrangian is a millenium problem
- Reliable results can be obtained on modern supercomputers

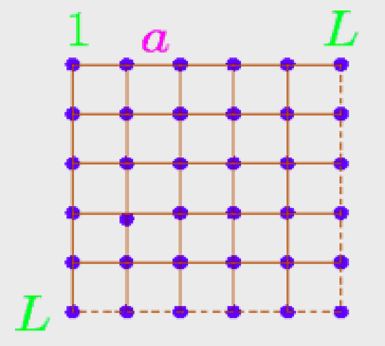
Lattice QCD

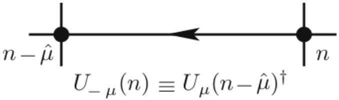


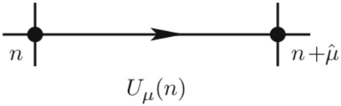
Lattice simulation

- Allows to study strongly interacting systems
- Based on the first principles of quantum field theory
- Powerful due to modern supercomputers and algorithms

Building lattice gluodynamics



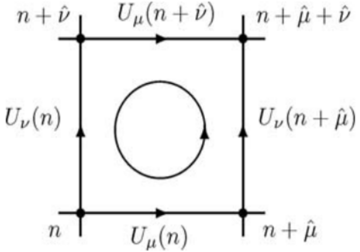




- Lattice spacing-a
- Degrees of freedom:

  $U_\mu(n) = P\exp\left(-i\int_C dx^\mu \hat{A}_\mu\right)\Big|_{a\to 0} = e^{ia\hat{A}_\mu(n)} = 1 + ia\hat{A}_\mu(n)$

Building lattice gluodynamics



- $U_{\mu\nu}(x) = U_\mu(n)U_\nu(x+\hat{\mu})U_\mu^{-1}(x+\hat{\nu})U_\nu^{-1}(n)$

- $S_l = \frac{2}{g^2}\sum_n \sum_{\mu<\nu} ReTr[1 - U_{\mu\nu}(n)]|$
  $S_l\big|_{a\to 0} \to \frac{1}{g^2}\int d^4x Tr(\vec{H}^2 - \vec{E}^2)$
- Partition function of gluodynamics
  $Z_l = \int \prod_{n,\mu} dU_\mu(n) e^{-S_l}$

Building lattice QCD

- 4-dimensional lattice: $L_s \times L_s \times L_s \times L_t = L_s^3 \times L_t$
- Lattice spacing–a
- $S = \frac{\beta}{3} \sum_n \sum_{\mu<\nu} ReTr[1 - U_{\mu\nu}(n)] + \bar{\psi}(\hat{D}(U) + m)\psi$
- $Z_l = \int \prod dU d\bar{\psi} d\psi e^{-S_l} =$
  $\int \prod dU e^{-S_G(U)} \prod_{i=u,d,s\ldots} \det(\hat{D}_i(U) + m_i) =$
  $\int \prod dU e^{-S_{eff}(U)}$

Lattice simulation of QCD

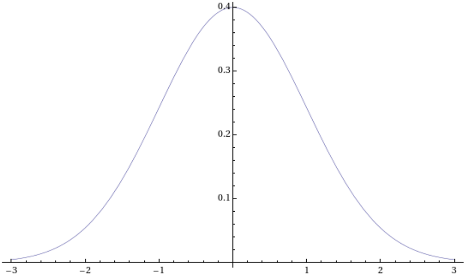
- We study QCD in thermodynamic equilibrium
- The system is in the finite volume
- Calculation of the partition function
  $Z \sim \int DU e^{-S_G(U)} \prod_{i=u,d,s...} \det\left(\hat{D}_i(U) + m_i\right) = \int DU e^{-S_{eff}(U)}$
- Monte Carlo calculation of the integral
- Carry out continuum extrapolation $a \to 0$
- Uncertainties (discretization and finite volume effects) can be systematically reduced
- The first principles based approach. No assumptions!
- Parameters: g^2 and masses of quarks

Modern lattice simulation of QCD

$$Z_l \sim \int DU e^{-S_{eff}(U)}$$

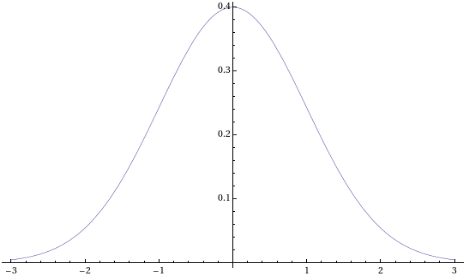
- Lattices
  - 96×48^3
  - Variables: $96 \cdot 48^3 \cdot 4 \cdot 8 \sim 300 \cdot 10^6$
  - Matrices: $100 \cdot 10^6 \times 100 \cdot 10^6$
- Dynamical u, d, s, c–quarks
- Physical masses of u, d, s, c–quarks
- Lattice spacing $a \sim 0.05\,\text{fm}$

Monte Carlo method



- We calculate the integral: $I = \int_{+\infty}^{-\infty} dx \frac{e^{-x^2/2}}{\sqrt{2\pi}} = \int_{+\infty}^{-\infty} dx f(x) = 1$
- Generate the sequence of random numbers: $(x_1, x_2, x_3, ... x_N)$ in the region $x \in [-c, c]$
- $I_N = \frac{2c}{N} \sum_{i=1}^{N} f(x_i)$
- $\lim_{N\to\infty} I_N = I$
- $I_{10} = 0.8836, \quad I_{100} = 1.0708, \quad I_{1000} = 0.9807, \quad I_{10000} = 0.9983, \quad I_{100000} = 1.0018$

Monte Carlo method



- We calculate the integral: $I = \int_{+\infty}^{-\infty} dx \frac{e^{-x^2/2}}{\sqrt{2\pi}} = \int_{+\infty}^{-\infty} dx f(x) = 1$
- Generate the sequence of random numbers: $(x_1, x_2, x_3, ...x_N)$ in the region $x \in [-c, c]$
- $I_N = \frac{2c}{N} \sum_{i=1}^{N} f(x_i)$
- $\lim_{N\to\infty} I_N = I$
- $I_{10} = 0.8836, \quad I_{100} = 1.0708, \quad I_{1000} = 0.9807, \quad I_{10000} = 0.9983, I_{100000} = 1.0018$
- Not very effective!

Metropolis algorithm

Calculation of the $\int dx e^{-S(x)}, \quad S(x) = \frac{x^2}{2}$

- The first approximation $x_0 = 0$
- Choose randomly $\Delta x \in [-c, c]$
- $x' = x_k + \Delta x$
- Metropolis algorithm(accept/reject procedure): $\Delta S = S(x') - S(x_k)$. If $\Delta S < 0, \quad S(x') < S(x_k)$, then $x_{k+1} = x'$. Else, x' is accepted with probability: $e^{-\Delta S}$.
- In practice: generate a random number $r \in [0, 1]$. If $r < e^{-\Delta S}$, then $x_{k+1} = x'$, else $x_{k+1} = x_k$.

Metropolis algorithm

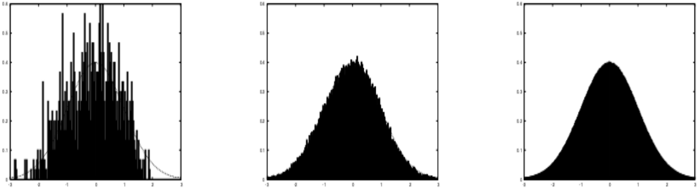
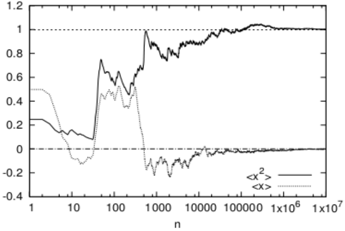
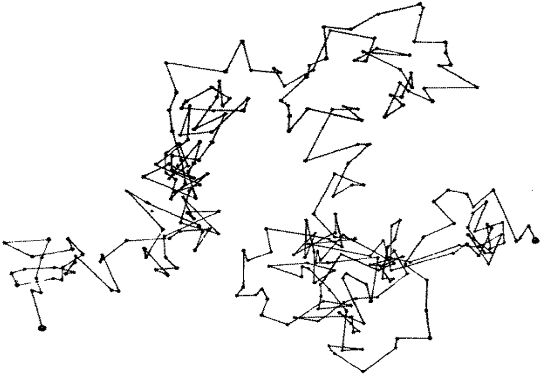


Figure 2: The distribution of $x^{(1)}, x^{(2)}, \cdots, x^{(n)}$, for $n = 10^3, 10^5$ and 10^7, and $\frac{e^{-x^2/2}}{\sqrt{2\pi}}$.



from arXiv:1808.08490

The Hybrid Monte Carlo algorithm

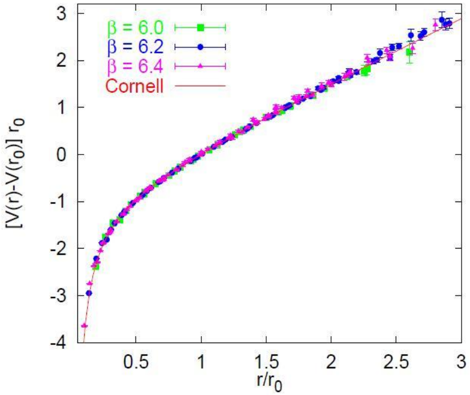


- HMC can be considered as Brownian motion of the system
- Accept/reject step at the end of the trajectory
  - if $S_{eff}(U_{n+1}) < S_{eff}(U_n)$ the U_{n+1} is accepted
  - otherwise U_{n+1} is accepted with $p \sim e^{-[S_{eff}(U_{n+1}) - S_{eff}(U_n)]}$
- Simulation of quantum system!
- For large number of the trajectories $p(U) \sim e^{-S_{eff}(U)}$

Applications

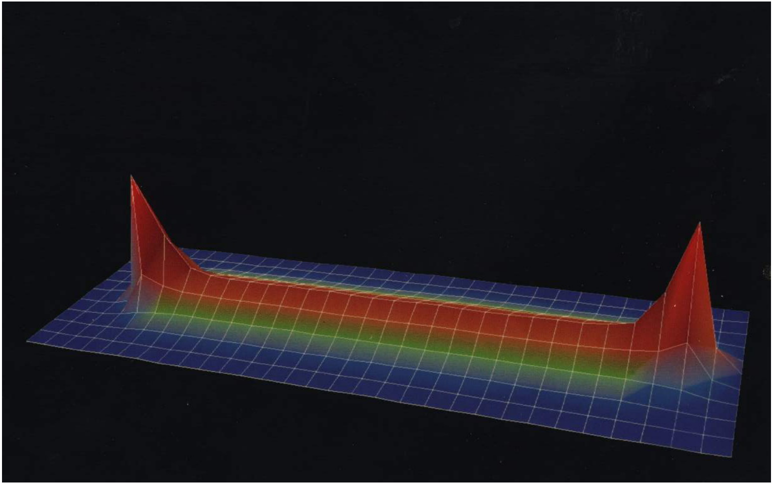
- Spectroscopy
- Matrix elements and correlations functions
- Thermodynamic properties of QCD
- Transport properties of QCD
- Phase transitions
- Nuclear physics
- Properties of QCD under extreme conditions
  - High temperature
  - Huge magnetic field
  - Large baryon density
  - Relativistic rotation
  - ...
- Vacuum structure and topological properties
- Beyond the Standard Model at strong coupling
- ...

Confinement in lattice simulation



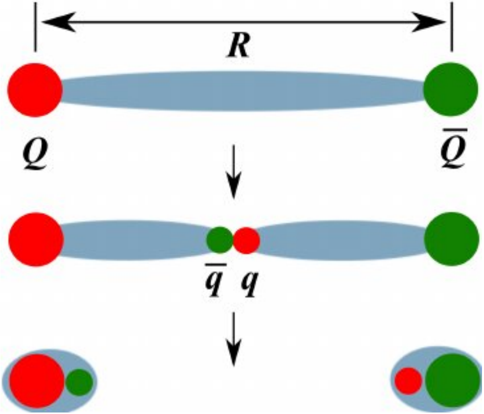
- Small distances: $V(r) = -\frac{4}{3}\frac{\alpha_s(r)}{r}$
  Asymptotic freedom $\alpha_s(r) \sim -\frac{1}{\log \Lambda r}|_{r \to 0} \to 0$
- Large distances $V(r) = \sigma_{phys} r$ - Confinement
  $F = \sigma \simeq 160000$ N
- To separate quarks one needs infinite energy

Confinement in lattice simulation



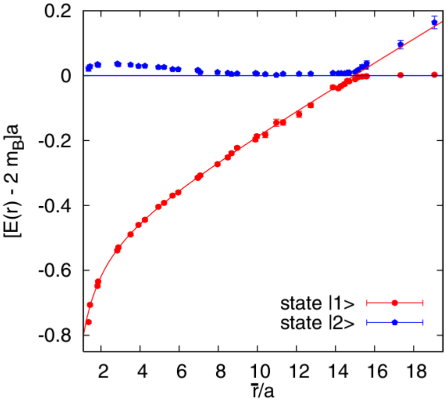
- Can be solved for one hour at modern laptop

String breaking



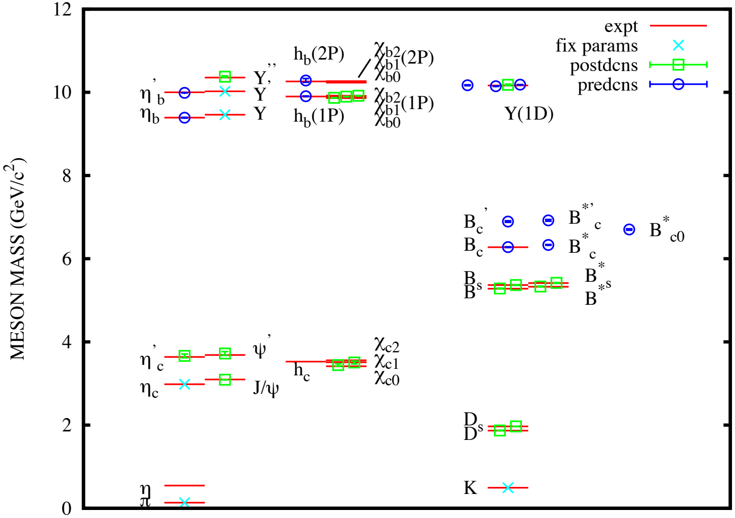
from arXiv:1001.0570

String breaking

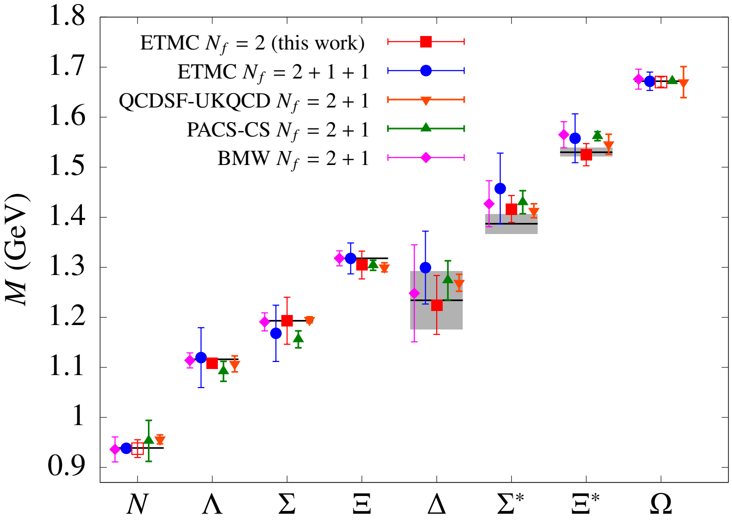


- The string is not broken
- The string is broken

Spectroscopy: Mesons



Spectroscopy: Baryons



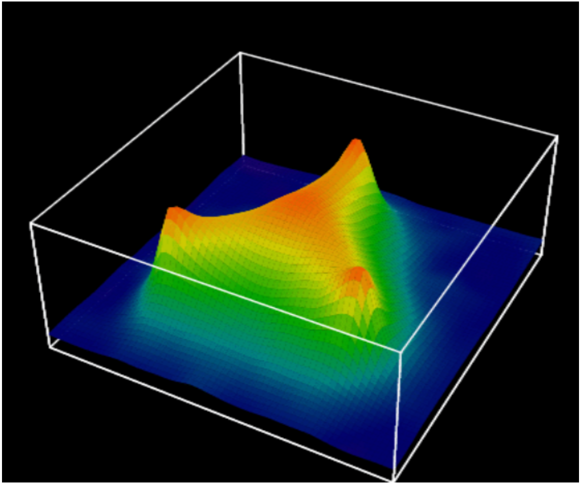
What is matter composed of?

- The following law is well satisfied in nature
  $M \simeq \sum_i M_i$
- In QCD
  $p(uud) \quad M_p c^2 = 938 \text{ MeV} \gg (m_u + m_u + m_d)c^2 = 12 \text{ MeV}$
  $n(udd) \quad M_n c^2 = 940 \text{ MeV} \gg (m_u + m_d + m_d)c^2 = 15 \text{ MeV}$

What is matter composed of?

- The following law is well satisfied in nature
  $M \simeq \sum_i M_i$
- In QCD
  $p(uud) \quad M_p c^2 = 938 \text{ MeV} \gg (m_u + m_u + m_d)c^2 = 12 \text{ MeV}$
  $n(udd) \quad M_n c^2 = 940 \text{ MeV} \gg (m_u + m_d + m_d)c^2 = 15 \text{ MeV}$
- Where is the rest of mass?

Chromoelectric fields in proton



- We are composed of gluons to 98%!

QCD vacuum

- Is vacuum an empty space ($\epsilon = 0$)?

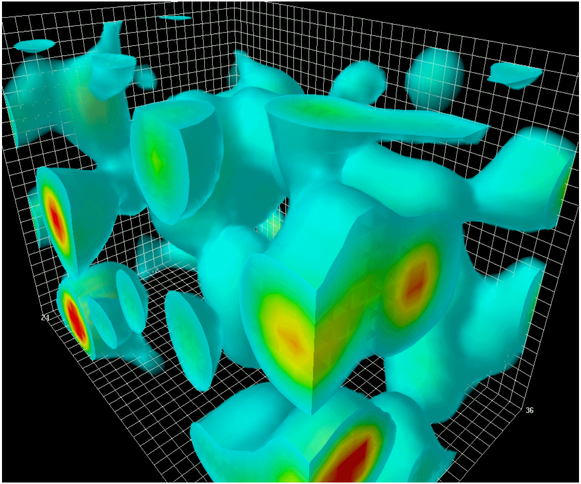
QCD vacuum

- Is vacuum an empty space ($\epsilon = 0$)?
- Vacuum is the state with the smallest energy

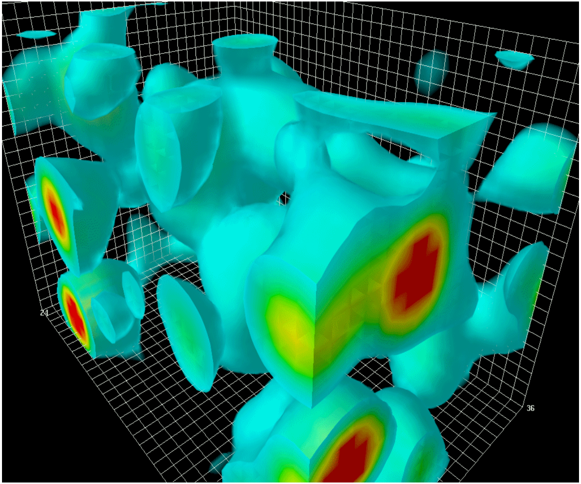
QCD vacuum

- Is vacuum an empty space ($\epsilon = 0$)?
- Vacuum is the state with the smallest energy
- QCD vacuum: $\epsilon \simeq -(265\ MeV)^4,\ \langle H^2 + E^2 \rangle \neq 0$

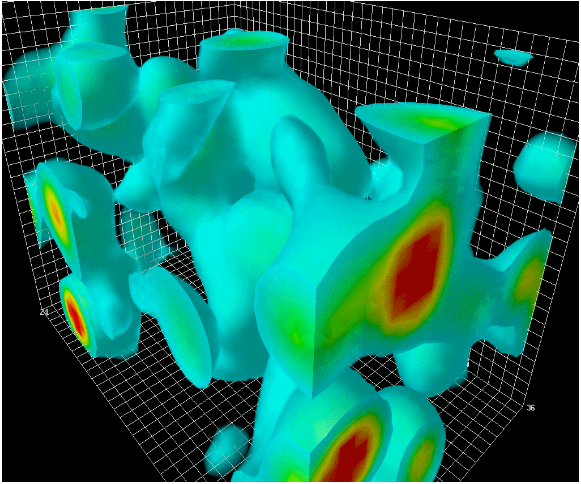
QCD vacuum



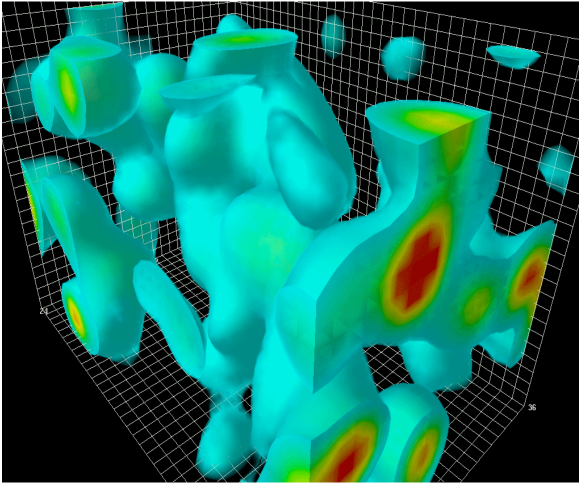
QCD vacuum



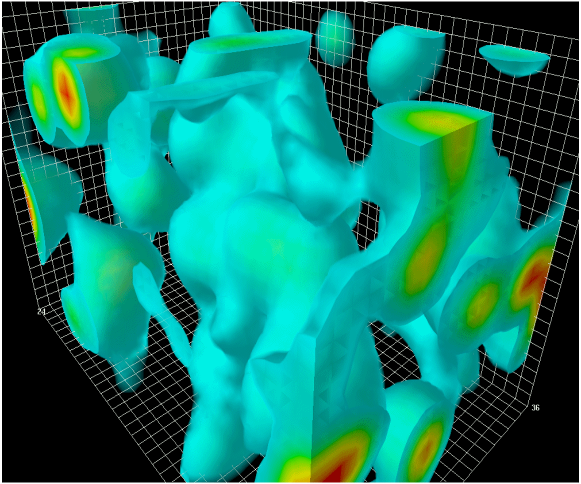
QCD vacuum



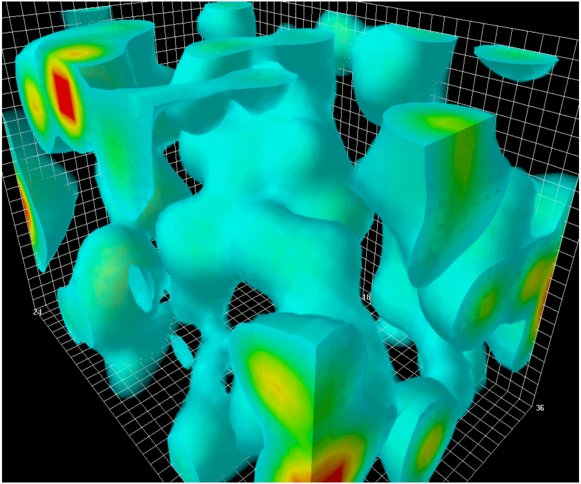
QCD vacuum



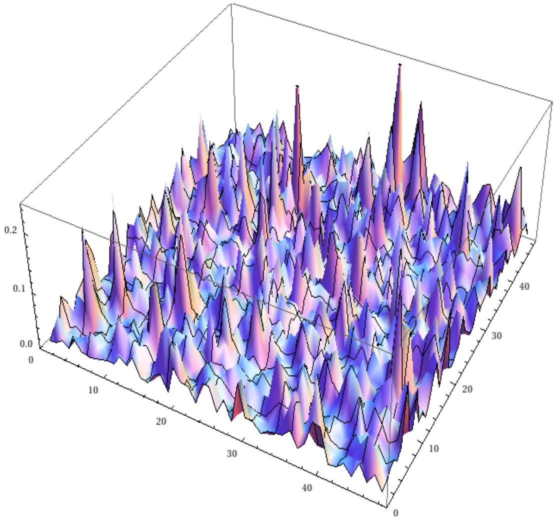
QCD vacuum



QCD vacuum

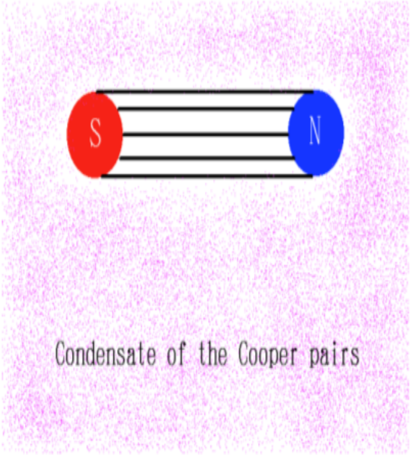


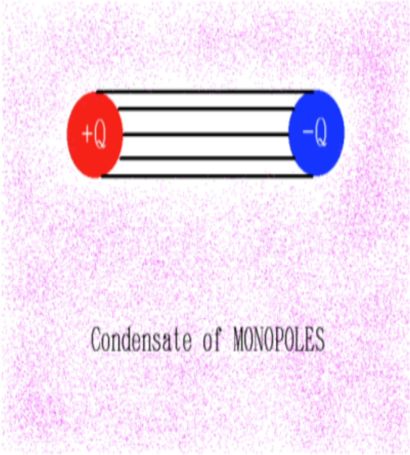
Quantum (ultraviolet) fluctuations in QCD vacuum



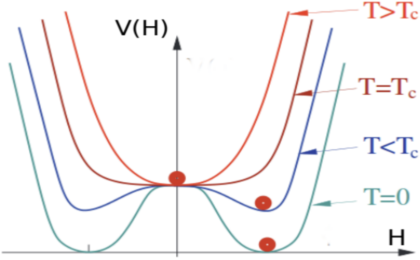
- Classical vacuum is distorted by UV fluctuations
- The fluctuations take place at distances $\sim a$

Model of dual superconductor





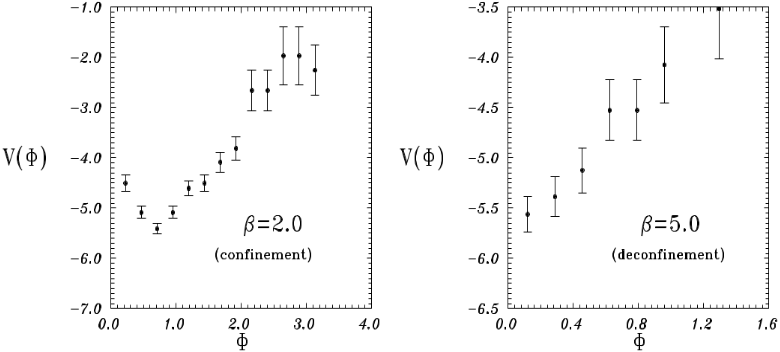
Phase transitions



Experience from φ^4-theory

- $V(\varphi) = -\frac{m^2}{2}\varphi^2 + \frac{\lambda}{4!}\varphi^4$
- Order parameter: $\langle \varphi \rangle$
- Z_2-symmetry: $\varphi \to (\pm 1)\varphi$
- $V(\varphi)$ is invariant but not the $\langle \varphi \rangle$
- Low temperature phase Z_2 is broken, $\langle \varphi \rangle \neq 0$
- High temperature phase Z_2 is restored $\langle \varphi \rangle = 0$

Condensation of monopoles

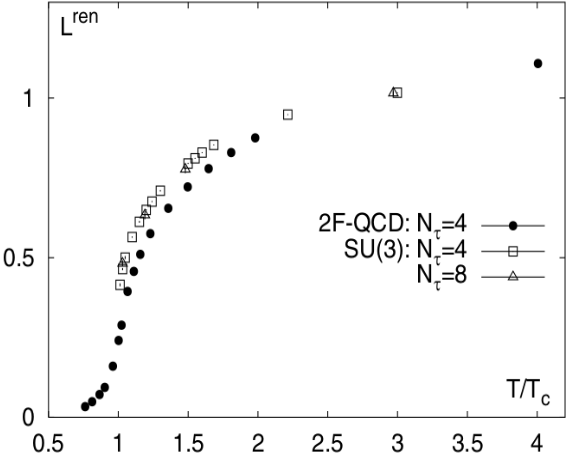


Polyakov line

Gluodynamics

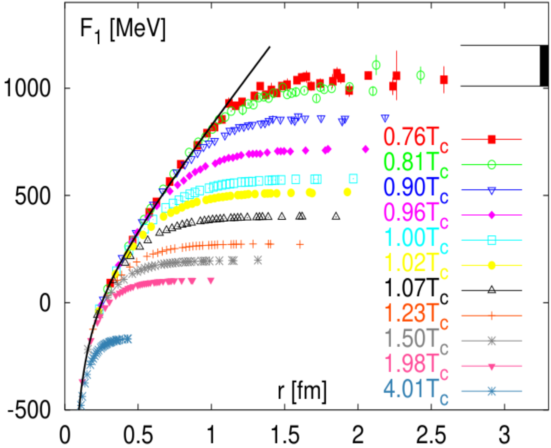
- $S_l = \frac{\beta}{3} \sum_n \sum_{\mu<\nu} ReTr[1 - U_{\mu\nu}(n)]$
- Polyakov line: $\langle P(\vec{x}) \rangle = Tr P \exp\left(i \int_0^T dx^4 \hat{A}_4(\vec{x}, x^4)\right)$
- It is gauge invariant because periodic boundary conditions
- Z_3 symmetry: $U \to e^{2\pi k/3i} U$, $k = 0, 1, 2$
- S_l is invariant but not the $\langle P(\vec{x}) \rangle$
- $P = e^{-F_Q/T}$
- Low temperature phase: $\langle P(\vec{x}) \rangle = 0$, $F_Q = \infty$, i.e. Z_3 is restored
- High temperature phase $\langle P(\vec{x}) \rangle \neq 0$, $F_Q = finite$, , i.e. Z_3 is broken

Polyakov line



*hep-lat/0506019

Static potential at finite temperature



- One needs the temperature
  $T \sim 150$ MeV $\sim 1.5 \times 10^{12}$ degrees

Chiral symmetry breaking

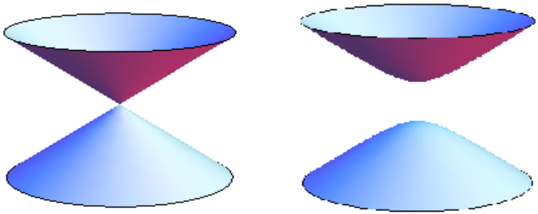
- Left and right sectors of the theory do not interact

$$\mathcal{L} = \bar{\Psi} i\hat{D}\Psi = \bar{\Psi} i\hat{D}\left(\frac{1+\gamma_5}{2} + \frac{1-\gamma_5}{2}\right)\Psi = \bar{\Psi} i\hat{D}\frac{1+\gamma_5}{2}\Psi + \bar{\Psi} i\hat{D}\frac{1-\gamma_5}{2}\Psi = \bar{\Psi}_R i\hat{D}\Psi_R + \bar{\Psi}_L i\hat{D}\Psi_L$$

- For N_f quarks chiral symmetry is $SU_L(N_f) \times SU_R(N_f)$
- Order parameter: chiral condensate $\langle\bar{\Psi}\Psi\rangle = \langle\bar{\Psi}_L\Psi_R\rangle + \langle\bar{\Psi}_R\Psi_L\rangle$
- Dynamical chiral symmetry breaking $SU_L(N_f) \times SU_R(N_f) \to SU_V(N_f)$
- The mechanism of chiral symmetry breaking is unknown
- It is connected to the confinement
- Some ideas can be gained from NJL model

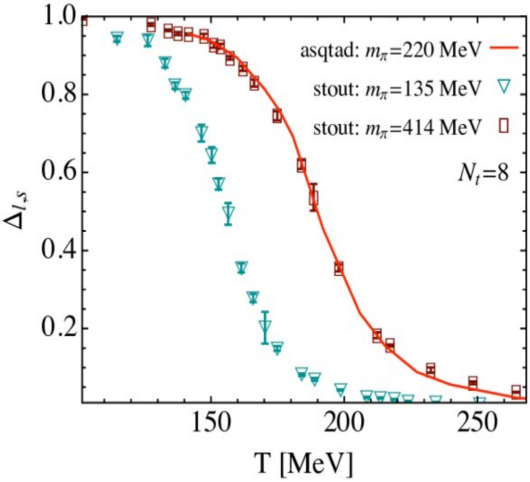
$$\mathcal{L}_S = \bar{\psi}\left[i\partial + g(\sigma + i\boldsymbol{\pi}\cdot\boldsymbol{\tau}\gamma_5)\right]\psi + \frac{1}{2}\left[(\partial\boldsymbol{\pi})^2 + (\partial\sigma)^2\right] - \frac{\mu^2}{2}(\sigma^2 + \boldsymbol{\pi}^2) - \frac{\lambda}{4}(\sigma^2 + \boldsymbol{\pi}^2)^2.$$

Chiral symmetry breaking



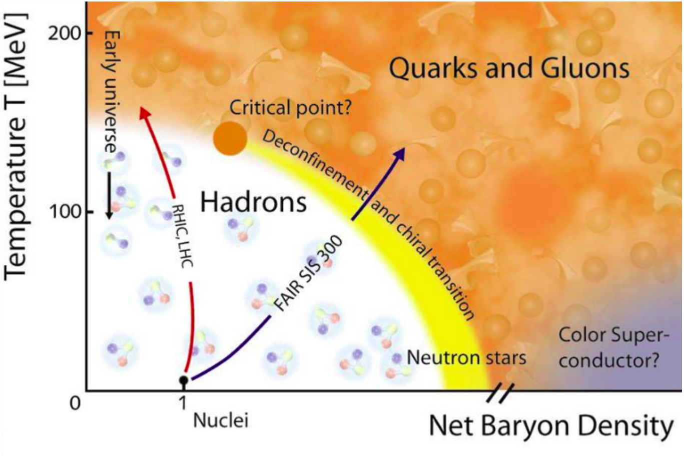
- NJL models are based on BCS theory
- The interaction term $(\bar{\psi}\psi)^4$
- $\alpha_{NJL} < 1$ no solutions, $M = 0$, $E^2 = \vec{p}^2$
- $\alpha_{NJL} > 1$ there is solution $M \neq 0$, $E^2 = \vec{p}^2 + M^2$
- Dynamical symmetry breaking
- The condensate of Cooper pairs: $\langle\bar{\psi}\psi\rangle \neq 0$
- Condensate from vacuum!
- Too simple model: no confinement

Chiral condensate $\langle\bar{\psi}\psi\rangle$



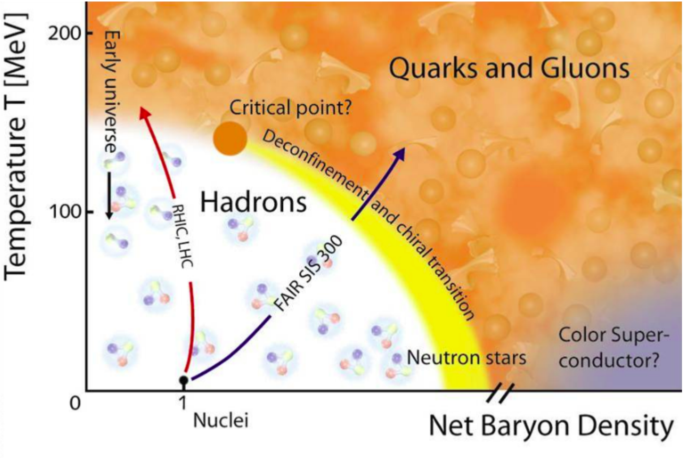
*arXiv:1005.3508

QCD under extreme conditions



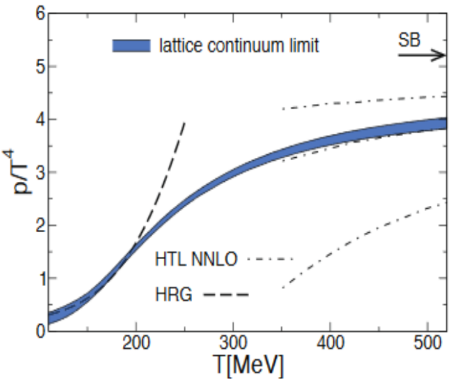
- Modern experiments: **LHC**(Switzerland), **RHIC**(USA), **FAIR**(Germany), **NICA**(Russia, Dubna, JINR)

QCD under extreme conditions



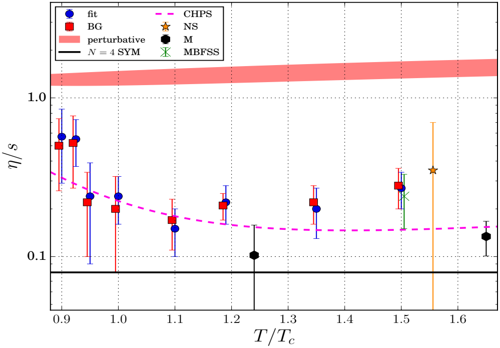
- Temperature $T \sim 150$ MeV $\sim 1.5 \times 10^{12}$ degrees
- Baryon density $n > n_0$
- Magnetic fields $eB \sim 10^{13}$ T
- Rotation with angular velocity $\omega \sim 10^{22}$ c^{-1}
- ...

QCD equation of state



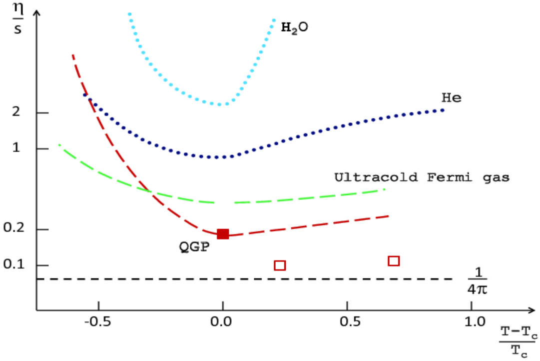
- Low temperature: HRG
- High temperature: SB - Stefan Boltzmann: $p = \sigma T^4$
- At very high temperature QGP is gas of quarks and qluons?

Shear viscosity of QGP



- QGP is close to the ideal liquid ($\frac{\eta}{s} = (1-3)\frac{1}{4\pi}$)
- Considerable deviation from gas of quarks and gluons
- The result is close to the N=4 SYM $\frac{\eta}{s} = \frac{1}{4\pi}$

Shear viscosity of QGP



- QGP is the most superfluid liquid

THANK YOU!