



Joint Institute for High Temperatures, Moscow, RAS

PATH INTEGRAL MONTE CARLO SIMULATIONS FOR THE QUARK – GLUON PLASMA – FIRST RESULTS

V. Filinov^{1,5}, Y. Ivanov^{2,3}, V. Skokov^{2,4}, M. Bonitz⁵,
P. Levashov¹, V. Fortov¹

¹Joint Institute for High Temperatures, RAS, Moscow, Russia

²GSI, Darmstadt, Germany

³Russian Research Center "Kurchatov Institute", Moscow, Russia

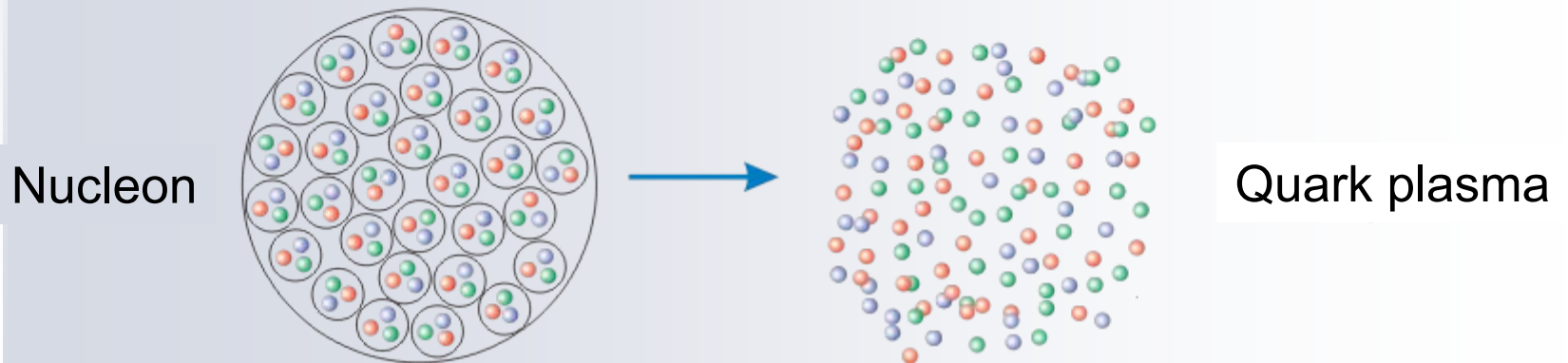
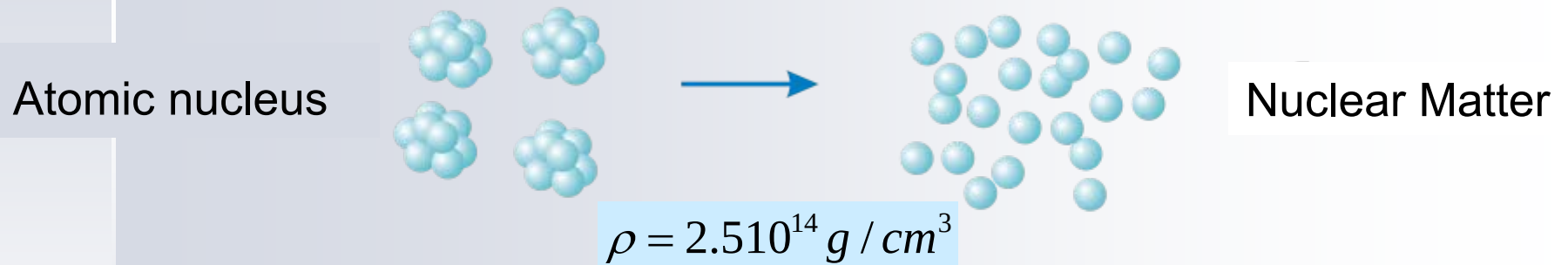
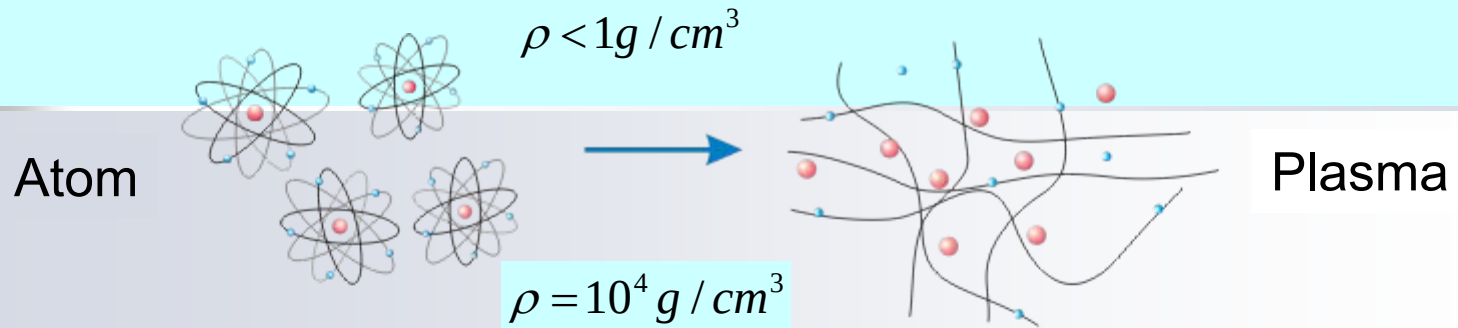
*⁴Bogoliubov Lab. of Theoretical Physics, Joint Institute for Nuclear Research,
Dubna, Moscow region Russia*

⁵Institut für Theoretische Physik und Astrophysik, Kiel, Germany

OUTLINE

- States of matter at high energy concentration
- Formation of quark-gluon plasma
- Conclusions from Lattice QCD simulations
- Simulation of quantum many-particle systems
- Path integral Monte Carlo method
- Applications to hydrogen plasmas
- Applications to the models of quark-gluon plasma

Matter transformation at high energy concentration



APPROACHES TO QUANTUM THERMODYNAMICS

- Thomas-Fermi method
- Hartree-Fock(-Slater) method
- Density Functional Theory
- Monte Carlo methods (variational, diffusion, path-integral)

Classical one-component plasma - COCP

Quantum one-component plasma - QOCP

Classical two-component plasma - CTCP

Quantum two-component plasma - QTCP

— Nonideality boundary:

$$\langle U_{Coul} \rangle = \langle E_{Kin} \rangle$$

Inside: Strong Coulomb interaction,
Many-body effects
atoms, molecules, clusters

Degeneracy boundary

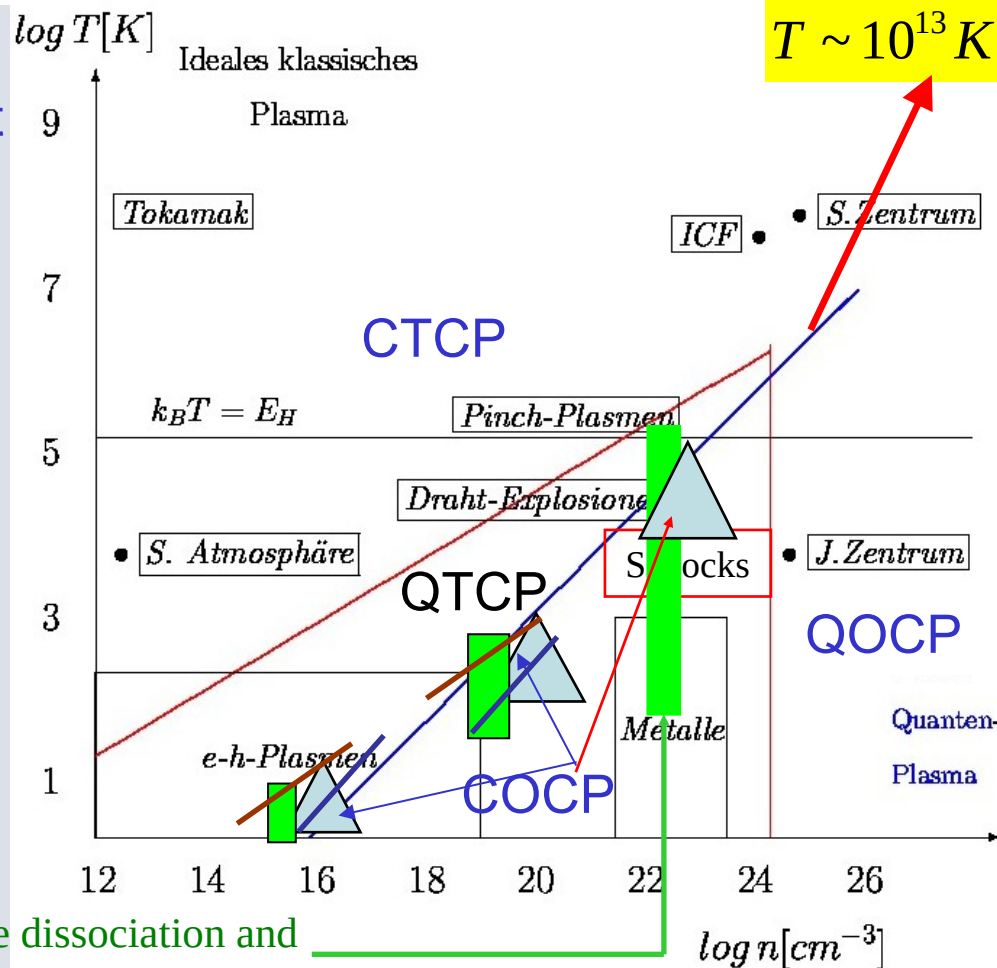
$$\lambda_e = \bar{r}$$

Below: overlapping electron
Wave functions,
Quantum and spin effects

Interaction and quantum effects in dense 3D and 2D plasma media with different mass ratio of charges.

Coulomb interaction:

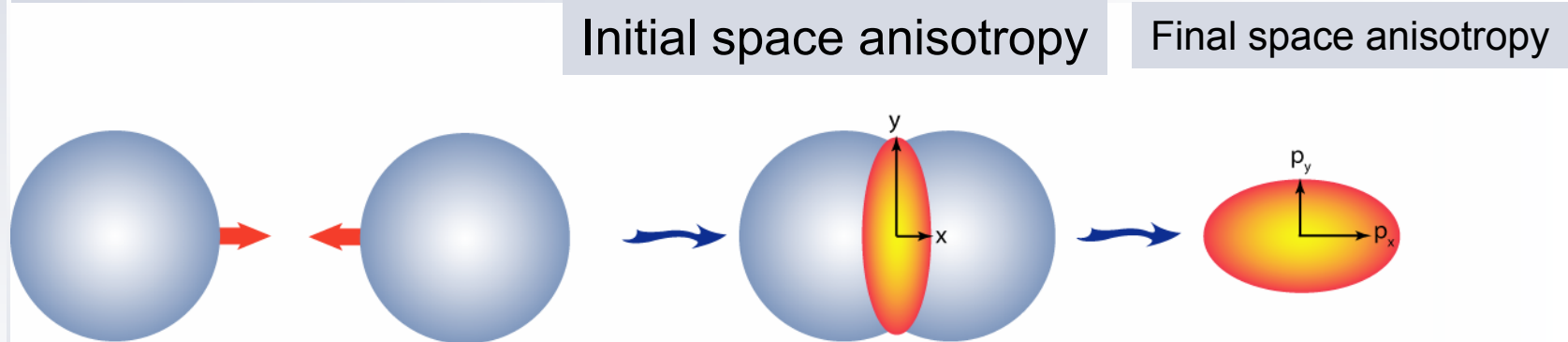
$$U_{ab}(r) = e_a e_b / r$$

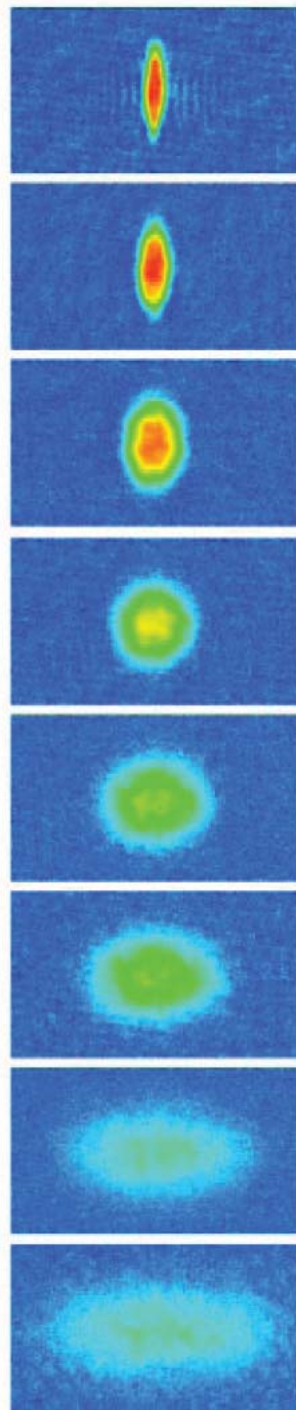


Pressure dissociation and
ionization, Mott effect

$$T \sim 10^{13} K, n \sim 10^{45} cm^{-3}$$

Relativistic collisions heavy ions, elliptic flows





100 MKC

200 MKC

400 MKC

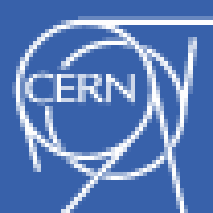
600 MKC

800 MKC

1000 MKC

1500 MKC

2000 MKC



LHCb experiment:
700 physicists
50 institutes
15 countries

Jet d' Eau
140 m

Mont Blanc,
4808 m

CERN

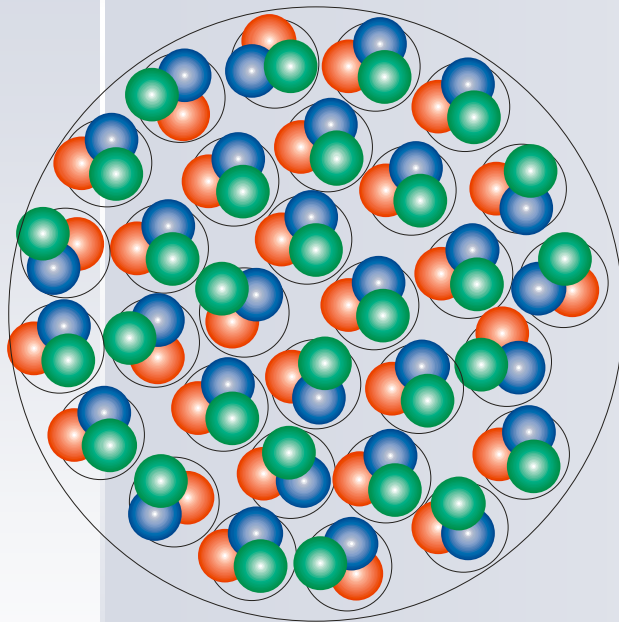
LHCb

ATLAS

CMS

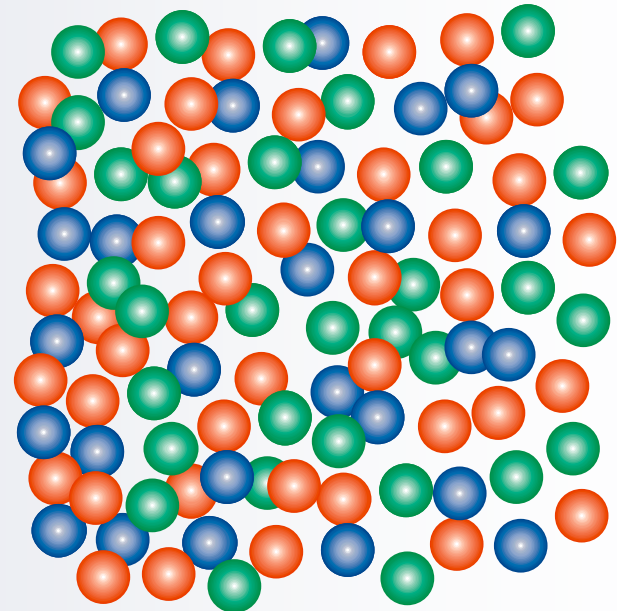
ALICE

Formation of quark-gluon plasma

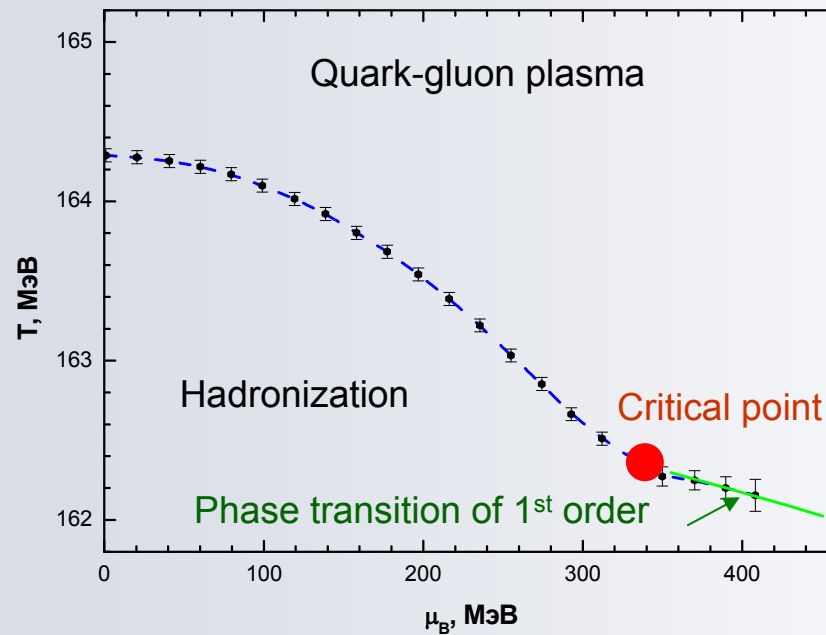


Color
deconfinement

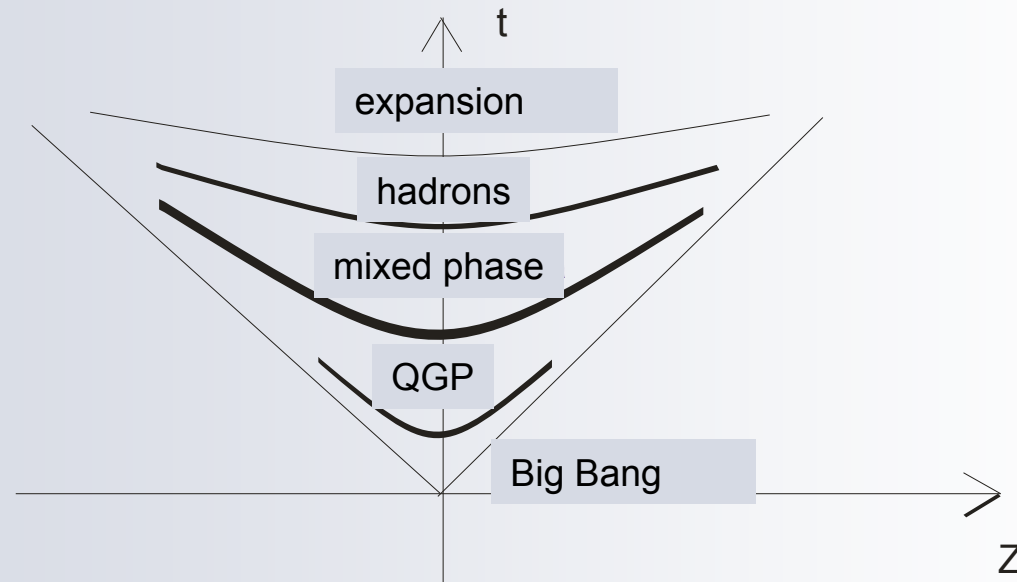
Phase transition



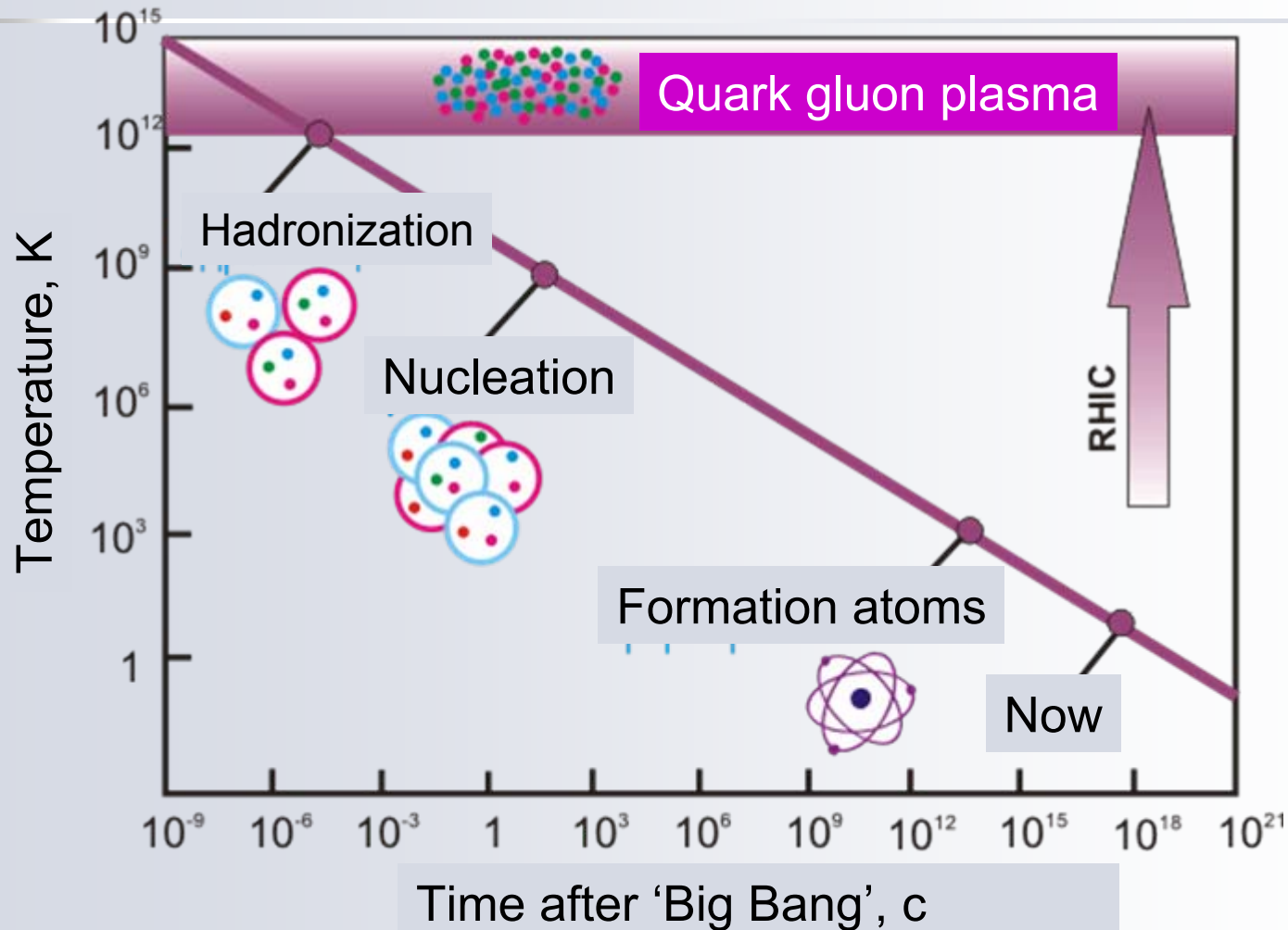
Phase diagram of quark-gluon plasma



Space-time evolution of matter after collision or 'Big Bang'



Evolution of matter after 'Big Bang'

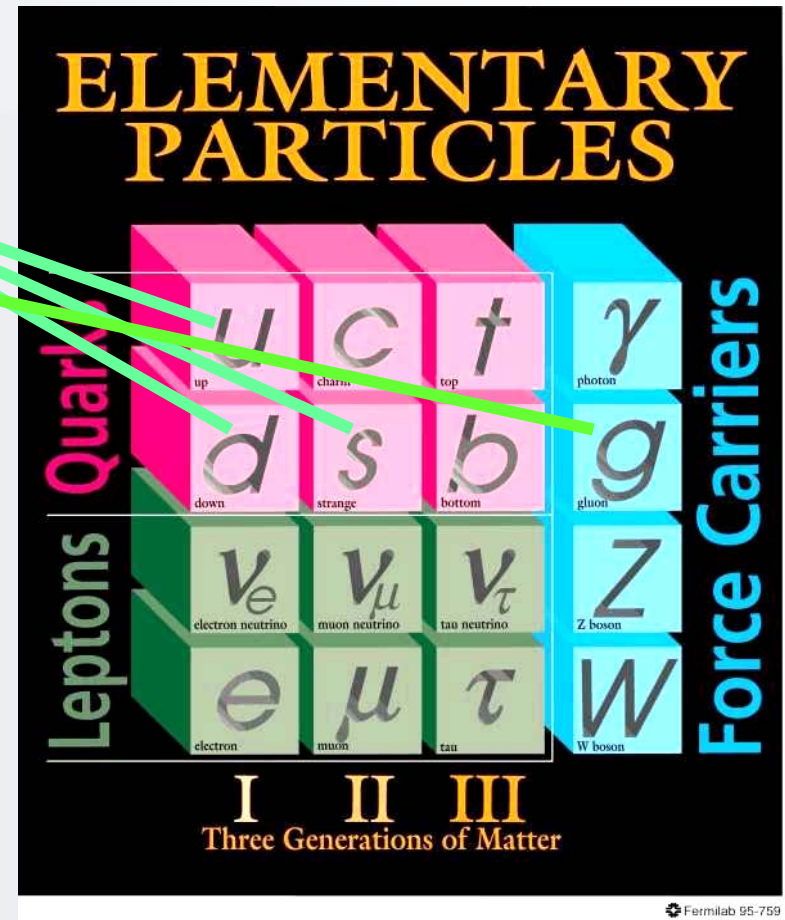


INTRODUCTION

Main Problems: starting from Lagrangian

$$L = -\frac{1}{g^2} \text{Tr } F_{\mu\nu}^2 + \sum_f \bar{\psi}_f (D + m) \psi_f$$

- (1) obtain hadron spectrum,
- (2) calculate various matrix elements,
- (3) describe phase transitions, and phase diagram
- (4) explain **confinement** of color



<http://www.claymath.org/millennium/>

INTRODUCTION

Methods

- Imaginary time $t \rightarrow it$

$$Z = \int D\varphi \exp\{i S[\varphi]\} \longrightarrow Z = \int D\varphi \exp\{-S[\varphi]\}$$

- Space-time discretization

$$D\varphi(x) \Rightarrow \prod_x d\varphi_x$$

$$Z = \int \prod_x d\varphi_x \exp\{-S[\varphi]\}$$

- Thus we get from functional integral the partition function for statistical theory in four dimensions

For lattice L^4 ($L=48, L^4=5,308,416$)

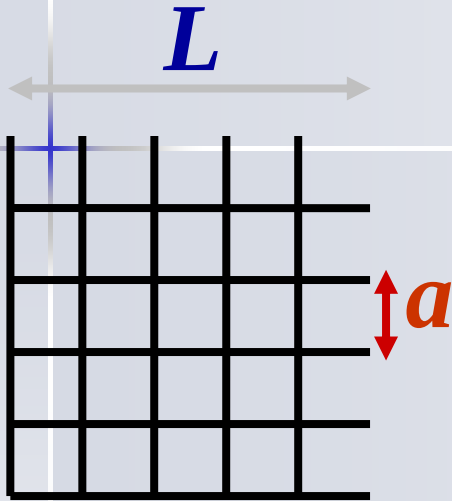
**Integrals of dimension $32L^4$ ($L=48,$
 $32L^4=169,869,312$)**

**Work with matrices $12L^4 \times 12L^4$
($L=48, 12L^4=63,700,992$)**

$$Z = \int d\varphi d\bar{\varphi} \exp\{\bar{\varphi} M \varphi\}$$

INTRODUCTION

Three limits



Lattice spacing

Lattice size

Discrete quark mass

$$a \rightarrow 0$$

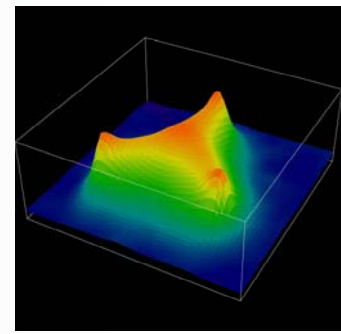
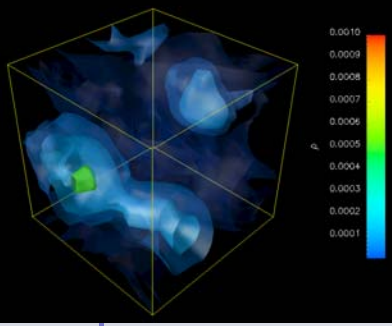
$$L \rightarrow \infty$$

$$m_q \rightarrow 0$$

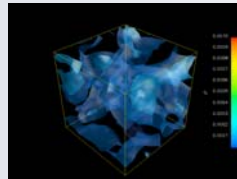
For typical lattice $L=48$, $L^4=5,308,416$

We calculate integrals of dimension $32L^4=169,869,312$

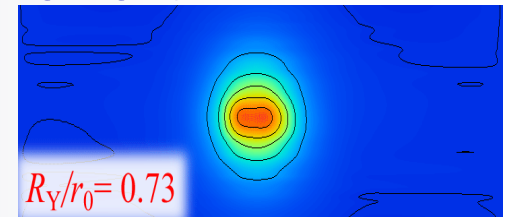
Conclusions from Lattice simulations



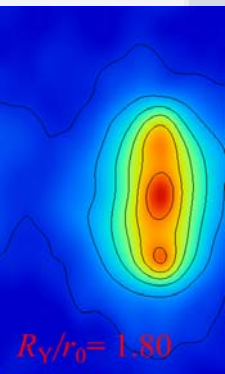
Computer simulations a) reproduce well known hadron properties b) predict new phenomena c) help to create new theoretical ideas.



Low dimensional objects (regions or **quasiparticles - dressed quarks and gluons**) are responsible for most interesting nonperturbative effects: chiral symmetry breaking, topological susceptibility and confinement.



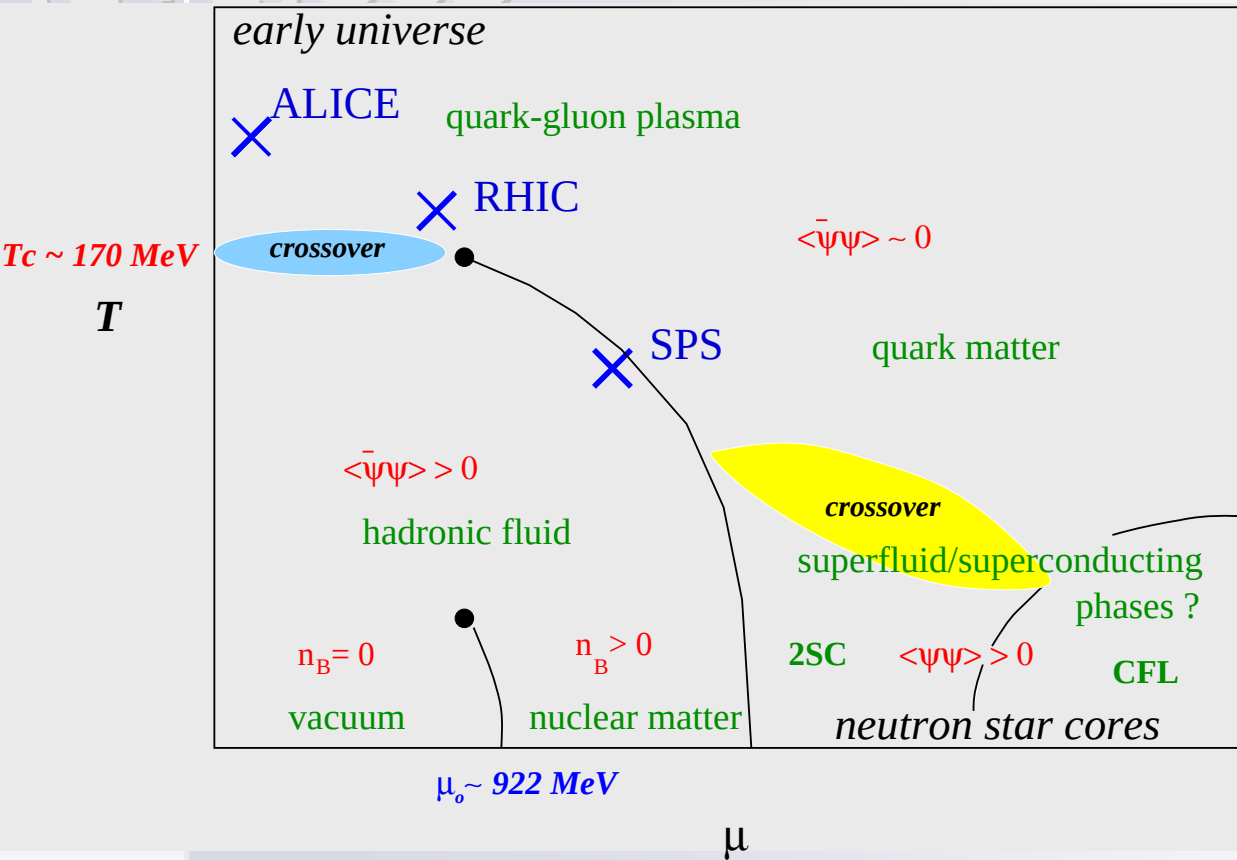
The era of traditional quantum field theory (Feynman graphs, perturbation theory) is over, nonperturbative field theory is close in spirit to solid state theory; we have to study dislocations, fractals, phase transitions etc.



<http://www.ihed.ras.ru/fortov/polikarpov.ppt>

SU(2) glue SU(3) glue 2qQCD (2+1)QCD

Phase diagram
(F. Karsch)



Talks at Lattice 2006!

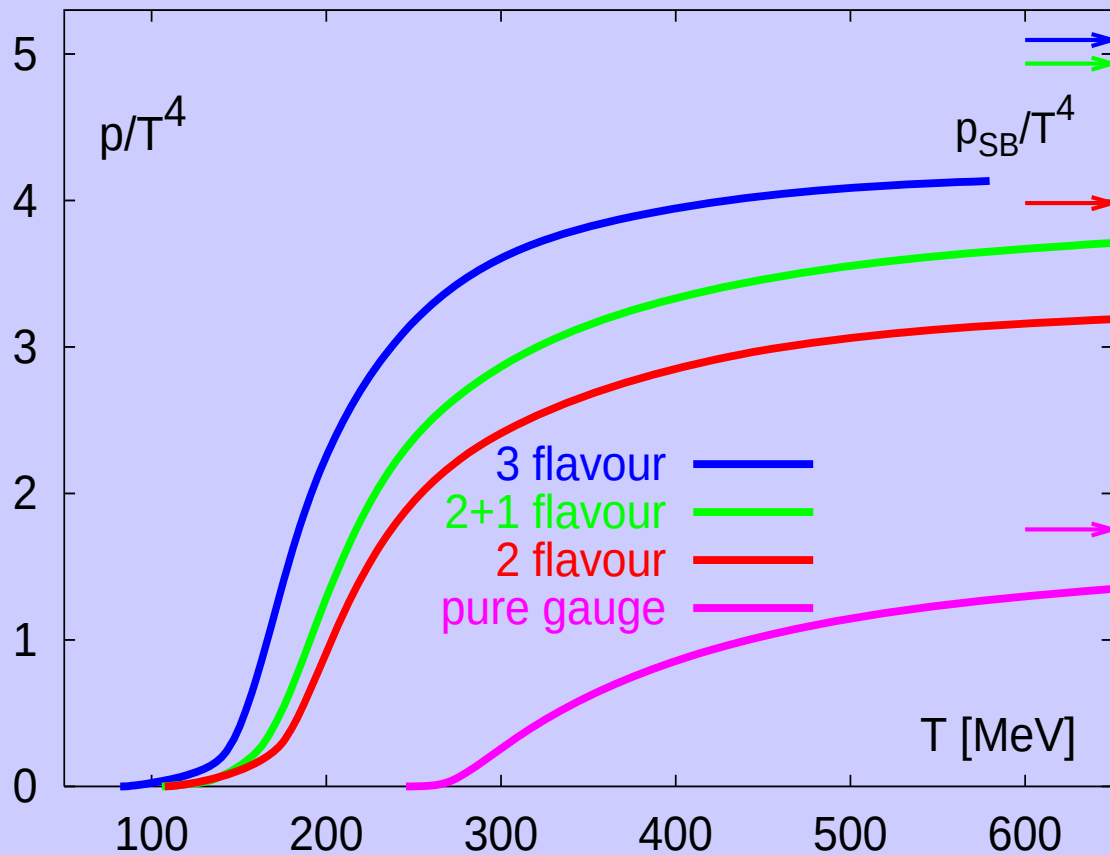
Mark G. Alford hep-lat/0610046; C. Schmidt hep-lat/0610116; Urs M. Heller hep-lat/061011;
M.A. Stephanov hep-lat/0701002

Talks at Lattice 2007!

G. Aarts hep-lat/0710.0739; Z. Fodor hep-lat/0710.0739; F. Karsch hep-lat/0711/0661

Quark-Gluon Plasma at Finite Temperature

Plasma thermodynamics, example: pressure



F. Karsch (2001-2005)



Quantum Monte Carlo method

Canonical ensemble

- Binary mixture of N_e electrons and N_i protons
- Partition function:

$$Z(N_e, N_i, V, \beta) = Q(N_e, N_i, \beta) / N_e! N_i!$$

$$Q(N_e, N_i, \beta) = \sum_{\sigma} \int_V dr \rho(r, \sigma; \beta)$$

- N-particle density matrix:

$$\rho = \exp(-\beta H) = \underbrace{\exp(-\Delta\beta H) \times \dots \times \exp(-\Delta\beta H)}_{n+1}$$

$$\beta = 1/kT$$

$$\Delta\beta = \beta / (n+1)$$



ACCURACY OF DIRECT PIMC

$$\hat{\rho} = e^{-\beta \hat{H}} = \underbrace{e^{-\Delta\beta \hat{H}} \times \dots \times e^{-\Delta\beta \hat{H}}}_{n+1}$$

$\beta = 1/k_B T$ $\hat{H} = \hat{K} + \hat{U}$ $\Delta\beta = \beta/(n+1)$

$$\hat{\rho}_{\Delta\beta} = e^{-\Delta\beta \hat{H}} = e^{-\Delta\beta \hat{K}} e^{-\Delta\beta \hat{U}} e^{-\frac{(\Delta\beta)^2}{2} [\hat{K}, \hat{U}]}$$

Error $\sim (\beta/n)^2$ for every multiplier

Total error $\Delta\rho \sim \beta^2/n \rightarrow 0$ at $n \rightarrow \infty$

$1 + O(1/n)^2$ for every multiplier
at $n \rightarrow \infty$

$$\rho_{\Delta\beta} = \rho_{\text{free}} \rho_{\text{pot}}(\Delta\beta)$$

High-temperature
pseudopotential



Quark-gluon plasma in canonical ensemble

- High temperature partition function [Phys. Rev. C, **74**, 044909, (2006)]
- **NEW**: Mixture of quasiparticles: N_q quarks, $N_{q'}$ antiquarks, and N_g gluons,
- $\vec{Q}$ – color coordinates of each quasiparticle - vector on unit 3D sphere

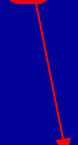
$$\hat{H} = \sum \frac{\hat{p}_\alpha^2}{2m_\alpha} + \sum \frac{g^2 \langle \vec{Q}_\alpha | \vec{Q}_\beta \rangle}{4\pi |r_\alpha - r_\beta|}$$

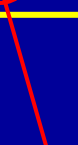
$$Z(N_q, N_{q'}, N_g, V, \beta) = Q(N_q, N_{q'}, N_g, \beta) / N_q! N_{q'}! N_g!$$

$$Q(N_q, N_{q'}, N_g, \beta) = \sum_{\sigma} \int_V dr d\vec{Q} \rho(r, \vec{Q}, \sigma; \beta)$$

- **Our modification** of [Phys.Rev. C, **74**, 044909, (2006)] :
temperature decomposition of N-particle density matrix:

$$\rho = \exp(-\beta \hat{H}) = \underbrace{\exp(-\Delta\beta \hat{H}) \times \dots \times \exp(-\Delta\beta \hat{H})}_{n+1}$$


 $\beta = 1/kT$


 $\Delta\beta = \beta / (n+1)$



$$\rho(r, Q, \sigma; \beta) = \frac{1}{\lambda_{\Delta q}^{3N_q} \lambda_{\Delta q'}^{3N_{q'}} \lambda_{\Delta g}^{3N_g}} \sum_{P=P_q, P_{q'}, P_g} (\pm 1)^{\kappa_P} \int_V dr^{(1)} \dots dr^{(n)} dQ^{(1)} \dots dQ^{(n)} \times$$

$$\rho(r, Q; r^{(1)}, Q^{(1)}; \Delta\beta) \dots \rho(r^{(n)}, Q^{(n)}; \hat{P}r^{(n+1)}, \hat{P}Q^{(n+1)}; \Delta\beta) S(\sigma, \hat{P}\sigma')$$

$$\rho(r^{(l)}, Q^{(l)}; r^{(l+1)}, Q^{(l+1)}) \approx \delta(Q^{(l)} - Q^{(l+1)}) \rho(r^{(l)}, Q^{(l)}; r^{(l+1)}, Q^{(l+1)})$$

spin matrix

Density matrix

$$\sum_{\sigma} \rho(r, Q, \sigma; \beta) = \frac{1}{\lambda_{\Delta}^{3N_q} \lambda_{\Delta}^{3N_{q'}} \lambda_{\Delta}^{3N_g}} \sum_{s=0}^{N_q} \sum_{s'=0}^{N_{q'}} \sum_{s''=0}^{N_g} \rho_{ss's''}([rQ], \beta)$$

$$\rho_{ss's''}([rQ], \beta) = \frac{C_{N_q}^s}{2^{N_q}} \frac{C_{N_{q'}}^{s'}}{2^{N_{q'}}} \frac{C_{N_g}^{s''}}{2^{N_g}} \exp\{-\beta U([rQ], \beta)\} \times$$

$$\times \prod_{l=1}^n \prod_{p=1}^{N_e} \phi_{pp}^l \det \left| \psi_{ab}^{n,1} \right|_s \prod_{p=1}^{N_i} \tilde{\phi}_{pp}^l \det \left| \tilde{\psi}_{ab}^{n,1} \right|_{s'} \prod_{p=1}^{N_i} \tilde{\phi}_{pp}^l \det \left| \tilde{\psi}_{ab}^{n,1} \right|_{s''}$$

$$U([rQ], \beta) = \sum_{l=0}^n \frac{U_l^{qq'g}([r^{(l)}Q], \beta)}{n+1}$$

**Kelbg
potentials**

Exchange matrix $\left\| \psi_{ab}^{n,1} \right\|_s \equiv \left\| \exp \left\{ -\frac{\pi}{\lambda_{\Delta}^2} |(r_a - r_b) + y_a^n|^2 \right\} \right\|_s$

KELBG PSEUDOPOTENTIAL

First order perturbation theory solution of two-particle Bloch equation for density matrix in the limit of weak coupling

$$\Phi^{ab}(\mathbf{r}_{ab}, \mathbf{r}'_{ab}, \Delta\beta) = e_a e_b \int_0^1 \frac{d\alpha}{d_{ab}(\alpha)} \operatorname{erf}\left(\frac{d_{ab}(\alpha)}{2\lambda_{ab}\sqrt{\alpha(1-\alpha)}}\right)$$

$$d_{ab}(\alpha) = |\alpha \mathbf{r}_{ab} + (1-\alpha) \mathbf{r}'_{ab}|$$

$$\lambda_{ab} = \hbar^2 \beta / 2\mu_{ab}$$

$$\mu_{ab}^{-1} = m_a^{-1} + m_b^{-1}$$

Diagonal Kelbg potential:

$$\Phi^{ab}(\mathbf{r}_{ab}, \Delta\beta) = \frac{e_a e_b}{\lambda_{ab} x_{ab}} \left\{ 1 - e^{-x_{ab}^2} + \sqrt{\pi} x_{ab} [1 - \operatorname{erf}(x_{ab})] \right\}$$

$$|\mathbf{r}_{ab}| \rightarrow 0$$

$$|\mathbf{r}_{ab}| \gg \lambda_{ab}$$

$$\frac{\sqrt{\pi} e_a e_b}{\lambda_{ab}}$$

$$\frac{e_a e_b}{|\mathbf{r}_{ab}|}$$

$$x_{ab} = |\mathbf{r}_{ab}| / \lambda_{ab}$$

Color Coulomb or Color Kelbg potential ?

Richardson, Gelman, Shuryak, Zahed, Harmann, Donko, Leval, Kalman (r=0 ?)

$$x_{ab} = |\mathbf{r}_{ab}| / \lambda_{ab}$$

$$\lambda_{ab} = 2\pi\hbar^2 \varepsilon / \mu_{ab}$$

Our suggestion: Color Kelbg potential

$$\Phi^{ab}(x_{ab}, \varepsilon) = \frac{\langle \vec{Q}_a | \vec{Q}_b \rangle g^2}{\lambda_{ab} x_{ab}} \left\{ 1 - e^{-x_{ab}^2} + \sqrt{\pi} x_{ab} [1 - \text{erf}(x_{ab})] \right\}$$

Objects Q are color coordinates of quarks and gluons

There is **no divergence** at small interparticle distances and it has a true asymptotics (T, x_{ab})

$$|\mathbf{r}_{ab}| \rightarrow 0$$

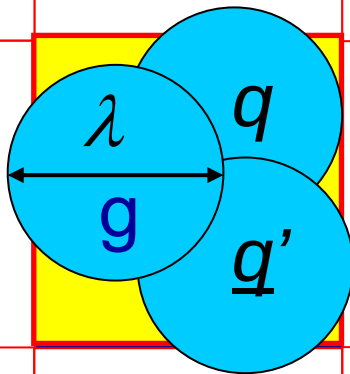
$$|\mathbf{r}_{ab}| \gg \lambda_{ab}$$

$$\frac{\sqrt{\pi} e_a e_b}{\lambda_{ab}}$$

$$\frac{e_a e_b}{|\mathbf{r}_{ab}|}$$

$$\begin{aligned} \text{Ha} &\rightarrow k_B T_c, & T_c &= 175 \text{ MeV}, \\ T_c &< T, & m_a &\sim 5 k_B T_c / c^2, \\ L_0 &\sim \hbar c / k_B T_c, & r_s &= \langle r \rangle / L_0 < 0.1, \\ L_0 &\sim 7 \cdot 10^{-15} \text{ m}, & x_{ab} &\sim 1 \end{aligned}$$

PERIODIC BOUNDARY CONDITIONS TREATMENT OF EXCHANGE EFFECTS



Inside main cell –
exchange matrix (exact)

Accuracy control of sign problem
– comparison with ideal
degenerate gas

$$n_e \lambda_e^3 \sim 30$$

Filinov V.S. // J. Phys. A: Math. Gen. 34, 1665 (2001)

Filinov V.S. et al. // J. Phys. A: Math. Gen. 36, 6069 (2003)



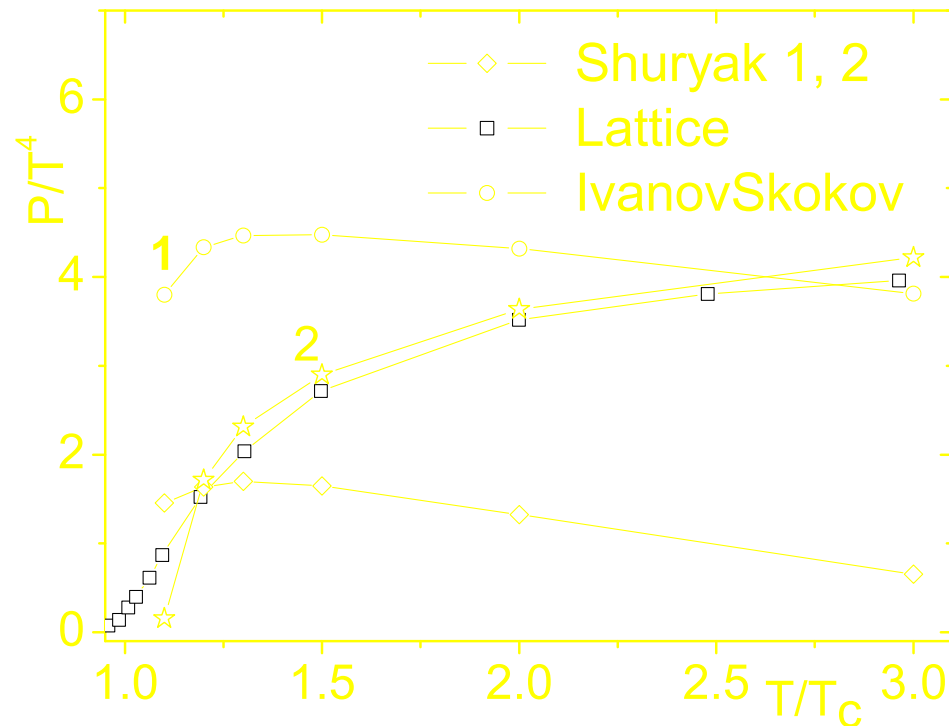
EQUATION OF STATE

Three models for $M_{\text{all}}(T)$, $n(T)$, $g_2(T)$:

1) Shuryak, 2) Ivanov, Skokov, 3) Modified Shuryak

Shuryak 2 -

$\langle r \rangle = 0.42$ fm





Pair distribution functions

Color correlation functions

$$\hat{H} = \sum \frac{\hat{p}_\alpha^2}{2m_\alpha} + \sum \frac{g^2 \langle \vec{Q}_\alpha | \vec{Q}_\beta \rangle}{4\pi |r_\alpha - r_\beta|}$$

$$Z(N_q, N_{q'}, N_g, V, \beta) = Q(N_q, N_{q'}, N_g, \beta) / N_q! N_{q'}! N_g!$$

$$Q(N_q, N_{q'}, N_g, \beta) = \sum_{\sigma} \int_V dr dQ \rho(r, Q, \sigma; \beta)$$

$$g_{ab}(R_1 - R_2) = g_{ab}(R_1, R_2) = \frac{1}{Q(N_q, N_{q'}, N_g)} \times$$

$$\sum_{\sigma} \int_V dr dQ \delta(R_1 - r^a_1) \delta(R_2 - r^b_2) \rho(r, Q, \sigma; \beta),$$

$$c_{ab}(R_1 - R_2)_{Def} = \frac{1}{Q(N_q, N_{q'}, N_g)} \sum_{\sigma} \int_V dr dQ \times$$

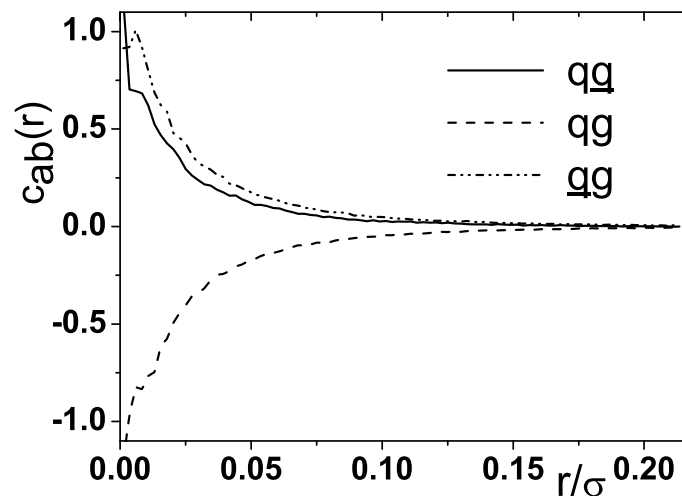
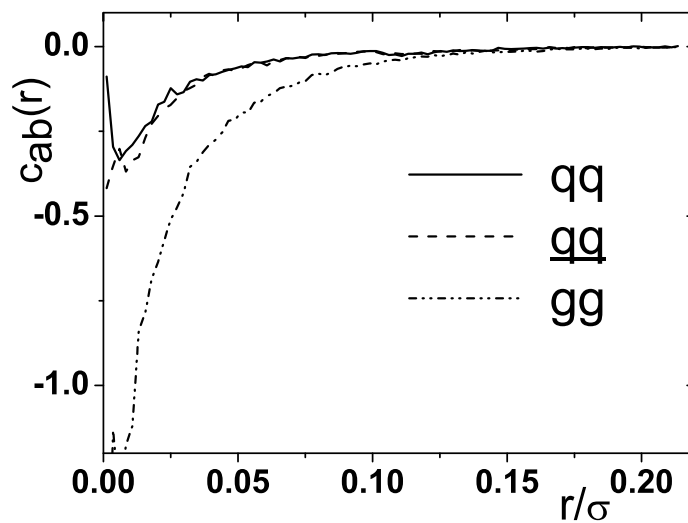
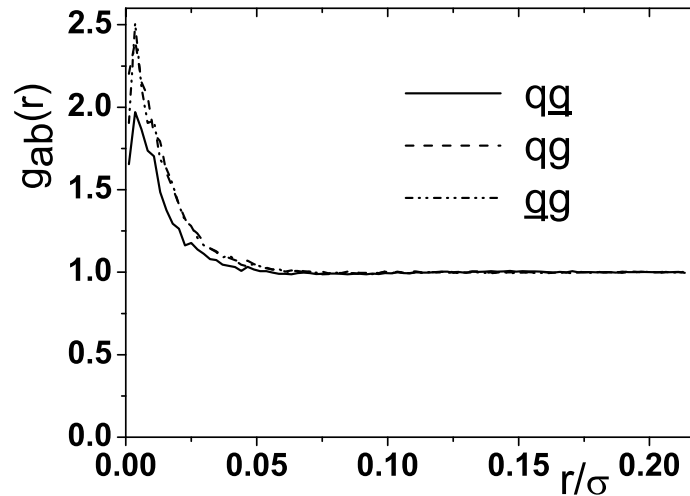
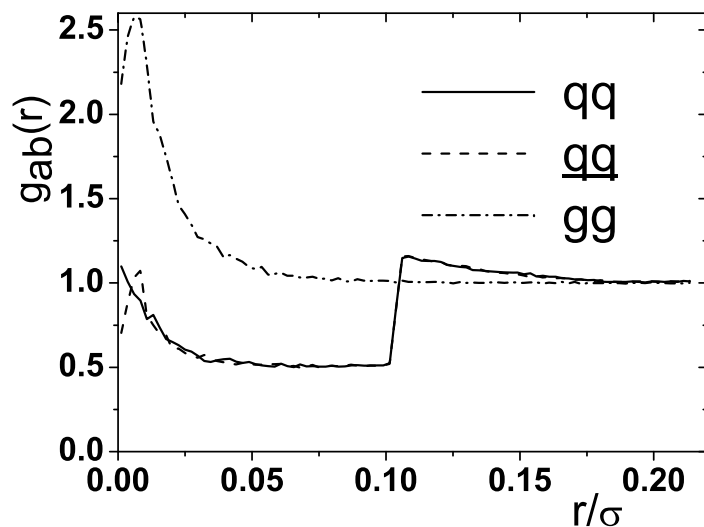
$$\delta(R_1 - r^a_1) \delta(R_2 - r^b_2) \langle Q^1_a | Q^2_b \rangle \rho(r, Q, \sigma; \beta)$$



PAIR DISTRIBUTION FUNCTIONS

$$T = 3 T_c$$

COLOR CORRELATION FUNCTIONS



Thank you for attention.

Contact E-mails:

vs_filinov@hotmail.com

Vladimir_Filinov@mail.ru