

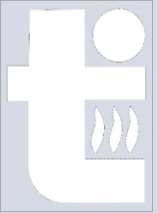
**Stochastic Simulations of Thermodynamic and Kinetic Properties
of Strongly Coupled Quark-Gluon Plasmas
in Feynman and Wigner Representation
of Quantum Statistical Mechanics.**

V. Filinov¹, M. Bonitz², Y. Ivanov³,
P. Levashov¹, V. Fortov¹

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

²Institut für Theoretische Physik und Astrophysik, Kiel, Germany

³Gesellschaft für Schwerionenforschung, Darmstadt, Germany



OUTLINE

- Phase diagram of strongly coupled quantum Coulomb systems
- Basic assumptions of **semi-classical** theory for non-Abelian plasma and limits of applicability
- Simulation of thermodynamics of quantum many-particle systems by Feynman path integral Monte Carlo method
- Wigner approach to simulations of quantum dynamics
- Applications to the semi-classical models of quark-gluon plasma
- Applications to the strongly coupled electromagnetic plasma

Interaction and quantum effects in strongly coupled Coulomb systems with different masses of particles.

Coulomb interaction:

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

Classical one-component plasma - COCP

Quantum one-component plasma - QOCP

Classical two-component plasma - CTCP

Quantum two-component plasma model - QTCP

— Nonideality boundary:

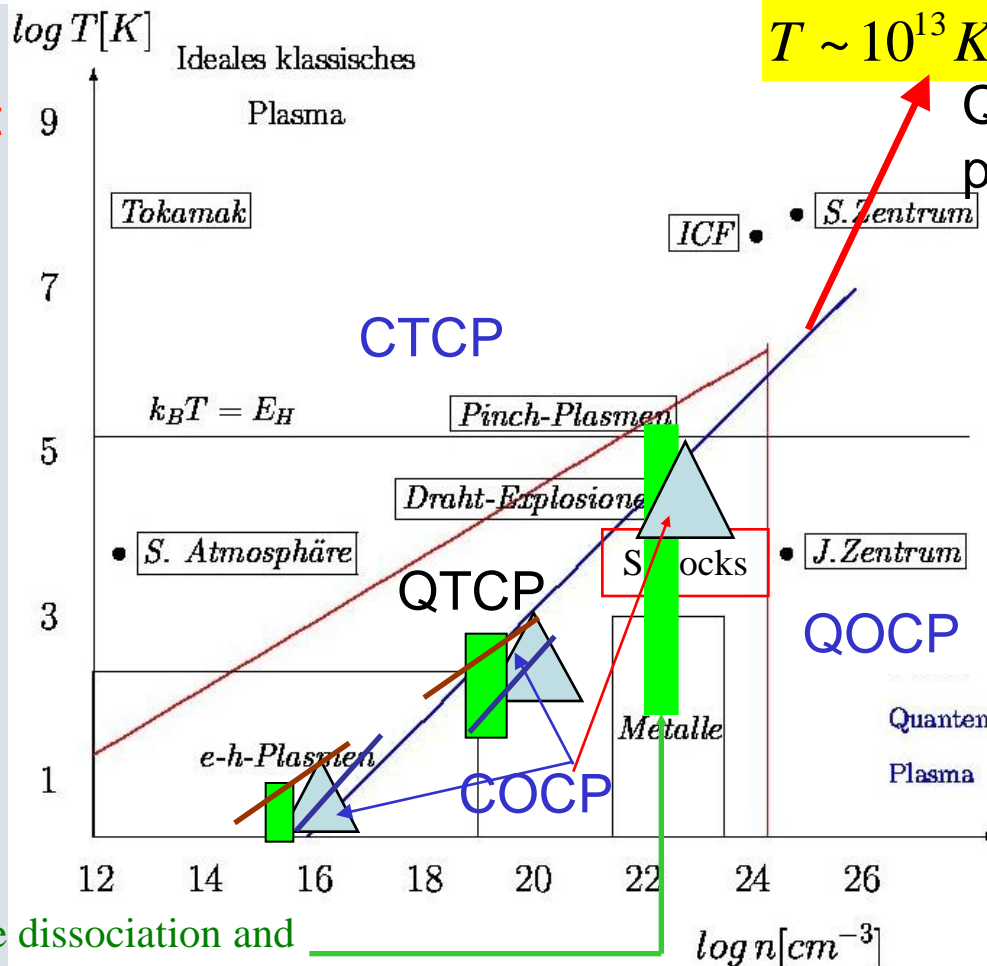
$$\langle U_{Coul} \rangle = \langle E_{Kin} \rangle$$

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

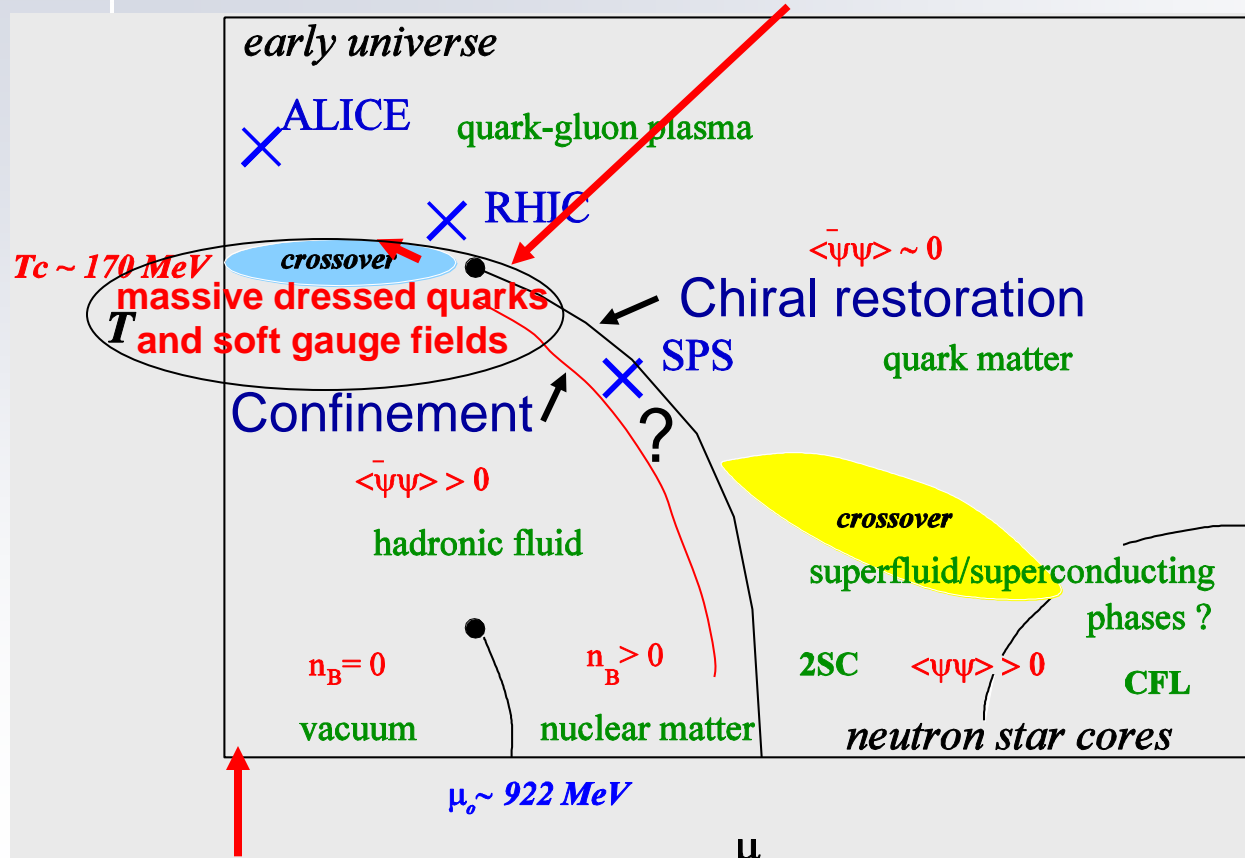


Pressure dissociation and ionization, Mott effect

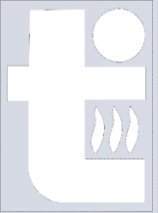
Semi-classical theory for non-Abelian system of color Coulomb quasi-particles

is based on resummation technique and lattice simulations allowing for consideration of quark-gluon plasma as system of dressed quark, antiquark and gluon presented by color Coulomb quasiparticles with T-dependent dispersion curves and width

Litim, Manuel, Stoecker, Bleicher, Feinberg, Richardson, Bonasera, Maruyama, Hatsuda, Shuryak, Fukushima,



Phase diagram
(F.Karsch)



Basic assumptions of the **semi-classical** quasiparticle model of quark – gluon plasma

is based on resummation technique and lattice simulations allowing for consideration of quark-gluon plasma as system of dressed quark, antiquark and gluon presented by **color Coulomb quasiparticles** with T-dependent dispersion curves and width.

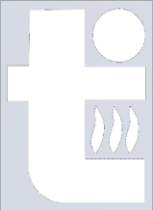
(Phys.Lett.B478,161(2000), Phys. Rev. C, **74**, 044909, (2006))

- All color **quasiparticles** are massive ($m > T$) and move non-relativistically
- Interparticle interaction is dominated by a **color Coulomb** potential with distance dependent coupling constant.
- The color operators are substituted by their average values
– **classical color vectors in SU(3) (8D vectors with 2 Casimirs condit.)**.

The model input requires :

- The temperature dependence of the quasiparticle mass.
- The temperature dependence of the coupling constant.

All the input quantities should be deduced from lattice QCD calculations and substituted in quantum Hamiltonian.



Thermodynamics of quark - gluon plasma in grand canonical ensemble within Feynman formulation of quantum mechanics

$$H_\beta = K_\beta + U_C = \sum_a \sqrt{p_a^2 + m_a^2(\beta)} + U_C \approx$$

$$\approx \sum_a \left(N_a m_a(\beta) + \frac{p_a^2}{2m_a(\beta)} \right) + \sum_{a,b} \frac{g^2 (|r_a - r_b|, \beta) \langle \vec{Q}_a | \vec{Q}_b \rangle}{4\pi |r_a - r_b|}, m_a \gg T$$

Grand canonical partition function

$$\Omega(\mu, \mu_g = 0, V, \beta) =$$

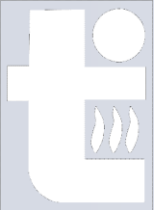
$$= \sum_{N_q, N_{\underline{q}}, N_g} \exp(\beta\mu(N_q - N_{\underline{q}})) Q(N_q, N_{\underline{q}}, N_g, \beta) / N_q! N_{\underline{q}}! N_g!$$

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

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

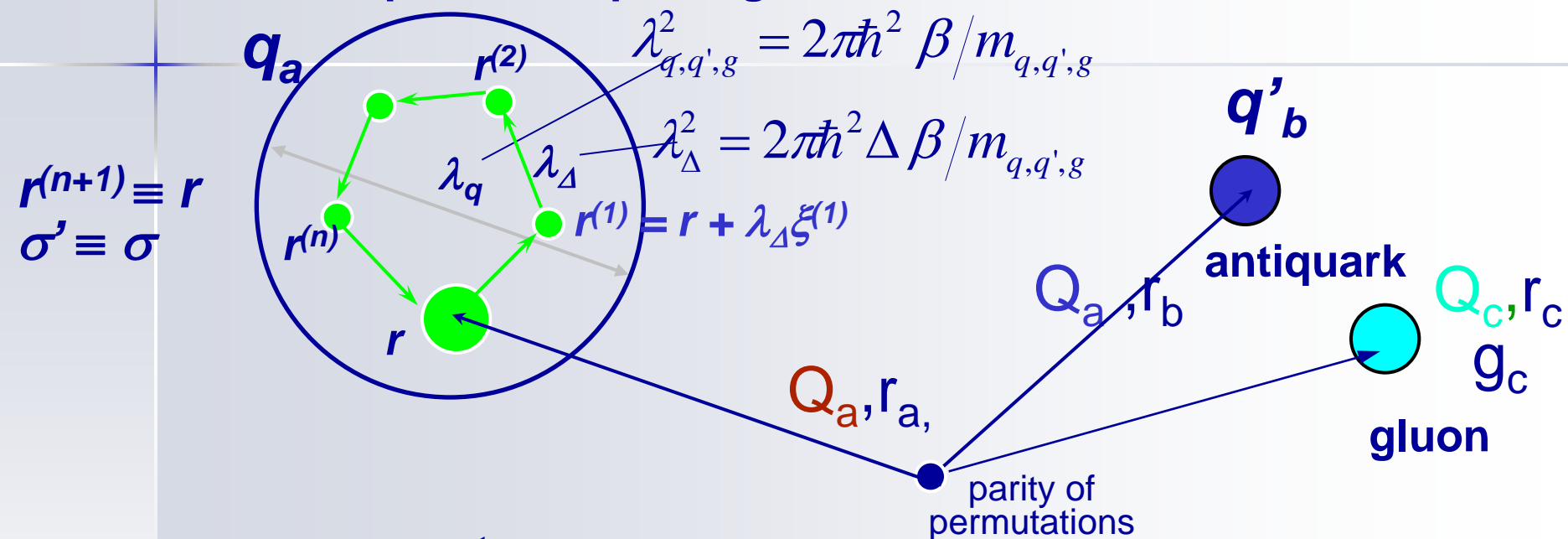
$$\beta = 1/kT$$

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



PATH INTEGRALS MONTE-CARLO METHOD

quark, antiquark, gluon

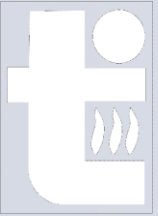


$$\rho(r, Q, \sigma; \beta) = \frac{1}{\lambda_{\Delta q}^{3N_q} \lambda_{\Delta q'}^{3N_{q'}} \lambda_{\Delta g}^{3N_g}} \sum_{P=P_q, P_{q'}, P_g} (\pm 1)^{K_P} \int_V dr^{(1)} \dots dr^{(n)} dQ^{(1)} \dots dQ^{(n)} \times$$

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

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

spin matrix



Density matrix

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

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

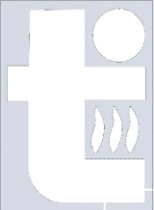
$$\times \prod_{l=1}^n \prod_{p=1}^{N_e} \phi_{pp}^l \det \left| \psi_{ab}^{n,1} \right|_s \prod_{p=1}^{N_i} \tilde{\phi}_{pp}^l \det \left| \tilde{\psi}_{ab}^{n,1} \right|_{s'} \prod_{p=1}^{N_i} \tilde{\phi}_{pp}^l \text{per} \left| \tilde{\psi}_{ab}^{n,1} \right|_{s''}$$

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

Pairwise sum of Kelbg potentials for each $l=0, \dots, n$

Exchange matrix

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



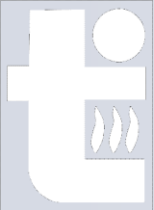
First studies and **testing** method within **simplified** quasiparticle model of quark – gluon plasma.

- All color quasiparticles are massive ($m > T$) and move non-relativistically
- All quasiparticle masses are the same.
- We do not distinguish between quark flavors.
- Interparticle interaction is dominated by a color Coulomb potential with interparticle distance dependent coupling constant.
- The color operators are substituted by their average values
 - classical color vectors in $SU(2)$ (3D vec. with 1 Cas.) instead of $SU(3)$.
- Canonical ensemble instead of grand canonical ensemble.
- Numbers of quarks, antiquarks and gluons are equal.

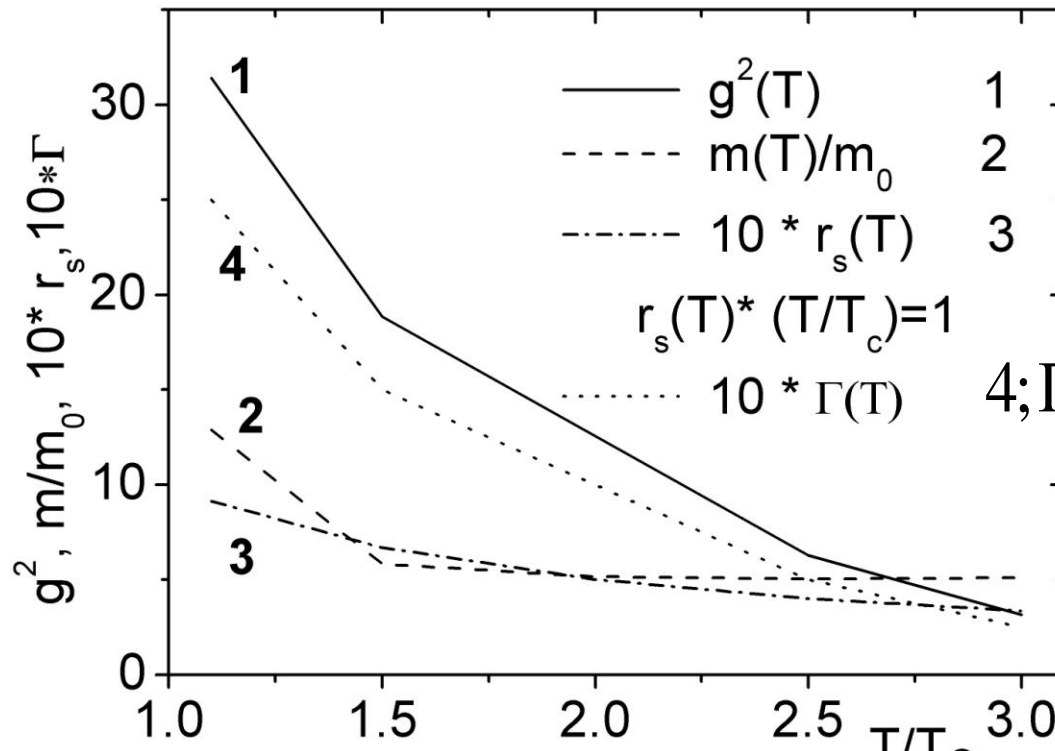
The model input requires :

- The temperature dependence of the quasiparticle mass.
- The temperature dependence of the coupling constant.
- The temperature dependence of the quasiparticle density.

All the input quantities should be deduced from lattice QCD calculations.



Input quantities from lattice calculations in **simplified** version



Coupling constant

$$\alpha(T) = g^2(T) / 4\pi \sim 1$$

Ratio of potential to kinetic energy per quasiparticle

$$\langle Q_a | Q_b \rangle g^2$$

SU(3)

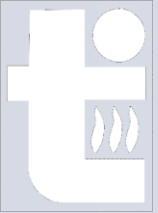
SU(2)

Quasiparticle masses:

$$m(T)/T_c \approx \frac{0.9}{(T/T_c - 1)} + 3.45 + 0.4T/T_c$$

Density: $n\sigma^3 \approx 0.24(T/T_c)^3$ $4\pi r_s^3 n\sigma^3 / 3 = 1$ $\sigma \approx 1.1 \text{ fm}$ $r_s(T) = \langle r \rangle / \sigma \approx 1 / (T/T_c)$

[Phys. Rev. C, 74, 044909, (2006), Phys. Rev. D, 73, 014509, (2006)]



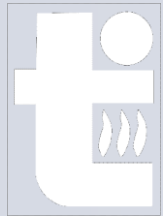
Snapshots of typical configurations

$$T=1.1T_0$$

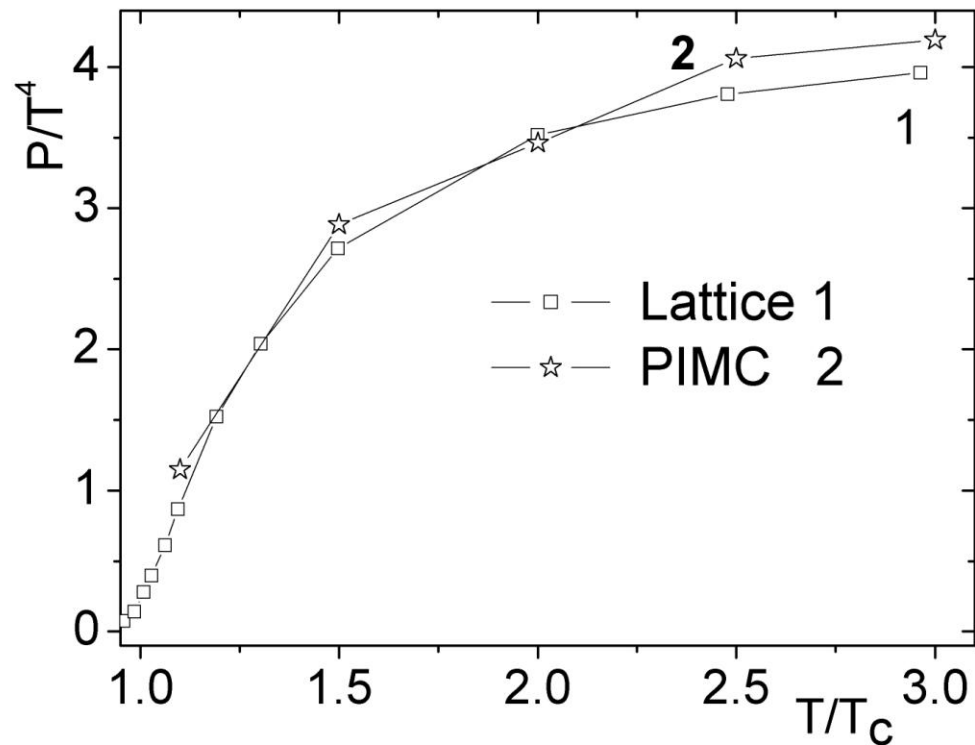
Gas-like rarefied system
of 3-4 quasiparticle clusters

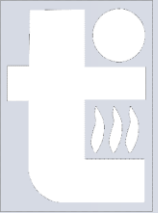
$$T=3T_0$$

Liquid-like dense system
of individual quasiparticles



Equation of State. Comparison path integral results with lattice (2+1) QCD





Pair distribution functions in canonical ensemble

Color correlation functions

$$H_\beta \approx \sum_a \left(N_a m_a(\beta) + \frac{p_a^2}{2m_a(\beta)} \right) + \sum_{a,b} \frac{g^2(|r_a - r_b|, \beta) C_{ab} \langle \vec{Q}_a | \vec{Q}_b \rangle}{4\pi |r_a - r_b|}$$

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

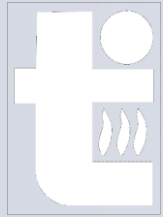
$$Q(N_q, N_{q'}, N_g, \beta) = \sum_{\sigma} \int_V dr d\mathbf{Q} \rho(r, \mathbf{Q}, \sigma; \beta)$$

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

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

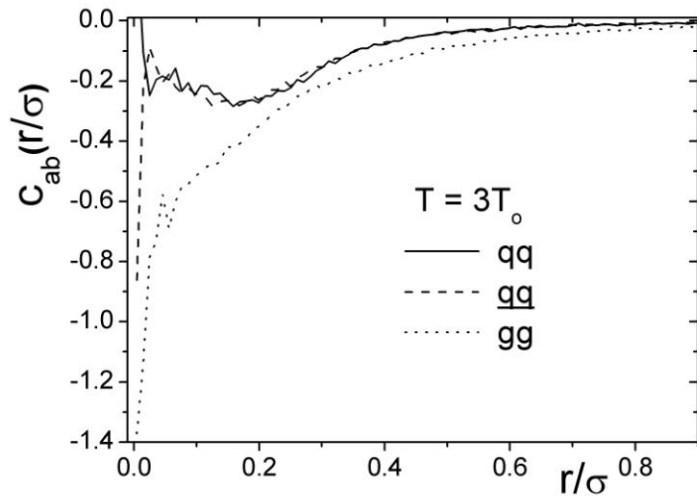
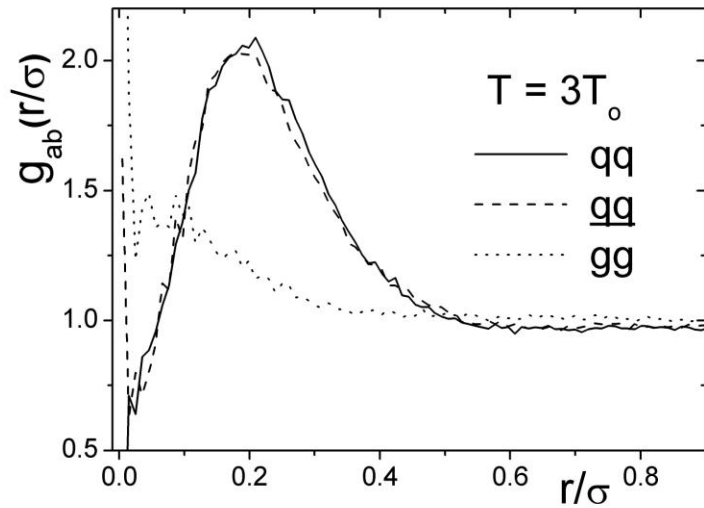
$$c_{ab}(R_1 - R_2)_{Def} = \frac{1}{Q(N_q, N_{q'}, N_g)} \sum_{\sigma} \int_V dr d\mathbf{Q} \times$$

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

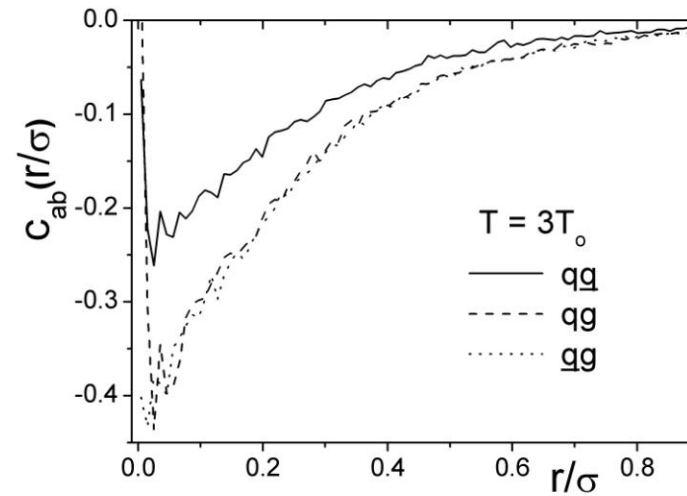
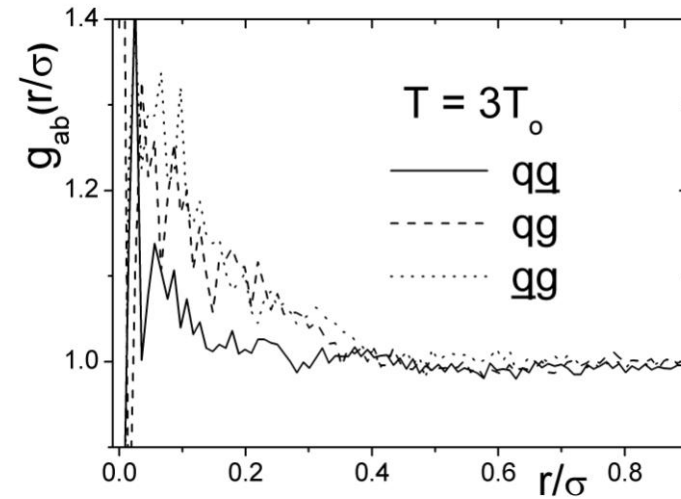


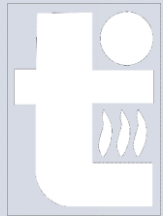
PAIR DISTRIBUTION AND COLOR CORRELATION FUNCTIONS

Similar quasiparticles



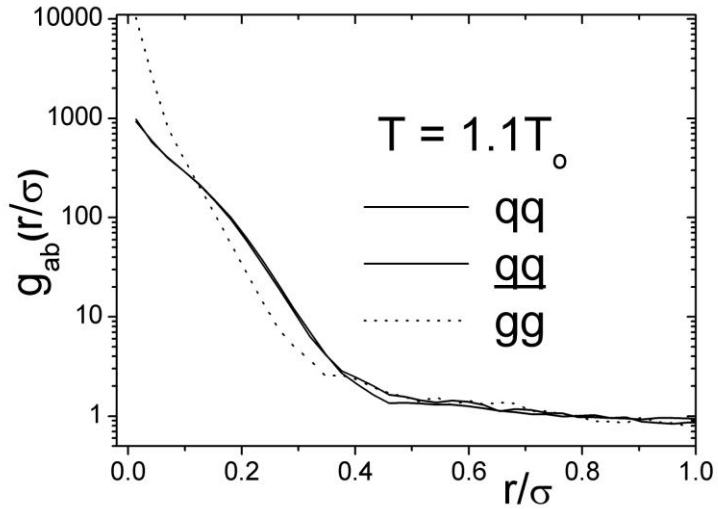
Different quasiparticles



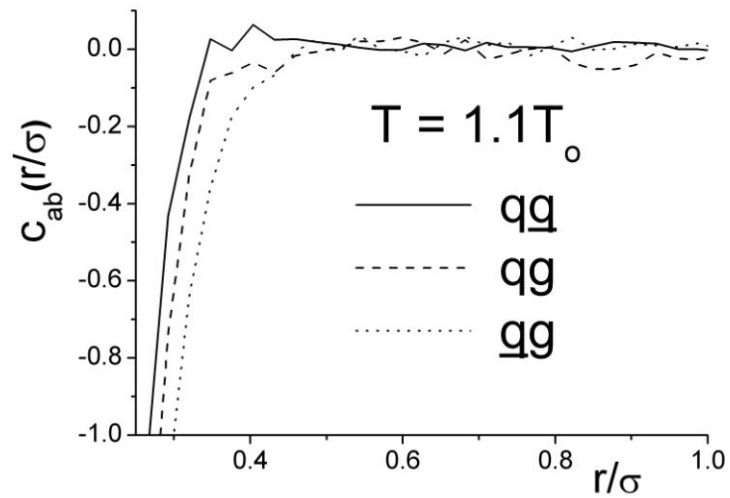
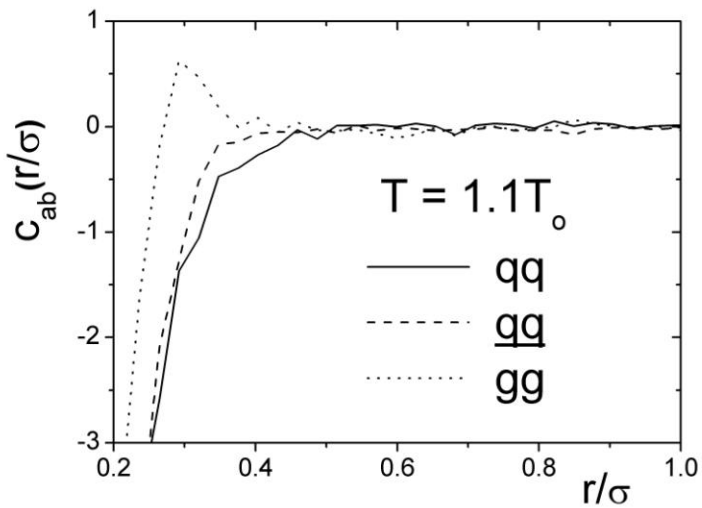
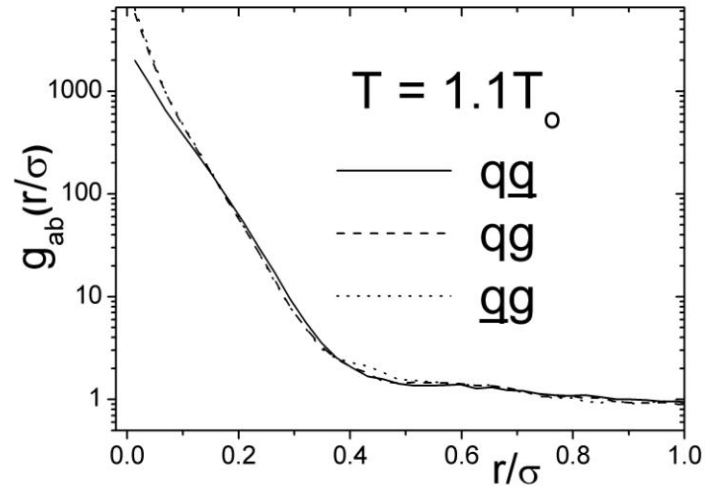


PAIR DISTRIBUTION AND COLOR CORRELATION FUNCTIONS

Similar quasiparticles



Different quasiparticles





Estimation of the quasiparticle bound states

The product $r^2 g_{ab}(r)$ has the physical meaning of a probability to find an two quasiparticles at a distance $|r|$ from each other.

On the other hand, the corresponding quantum mechanical probability is the product of r^2 and the two-particle Slater sum \sum_{ab}

$$\sum_{ab}^2 = 8\pi^{3/2} \lambda_{ab}^3 \sum_{E_\alpha}^\infty |\Psi_\alpha(r)|^2 \exp(-\beta E_\alpha) = \sum_{ab}^d + \sum_{ab}^c$$

$$\sum_{ab}^d = 8\pi^{3/2} \lambda_{ab}^3 \sum_{E_\alpha}^{E'} |\Psi_\alpha(r)|^2 \exp(-\beta E_\alpha)$$

$$r^2 g(r) \sim r^2 \left(\sum_{ab}^d + \sum_{ab}^c \right)$$

$$r^2 g(r) \sim r^2 \sum_{ab}^d > r^2, r < a_b$$

$$r^2 g(r) \sim r^2 \sum_{ab}^c \sim r^2, r > a_b$$

$$\sum_{ab}^c \gg \sum_{ab}^d \Rightarrow r^2 * \sum_{ab}^c \sim r^2$$

$$\sum_{ab}^c \ll \sum_{ab}^d \Rightarrow r^2 * \sum_{ab}^d \gg r^2$$

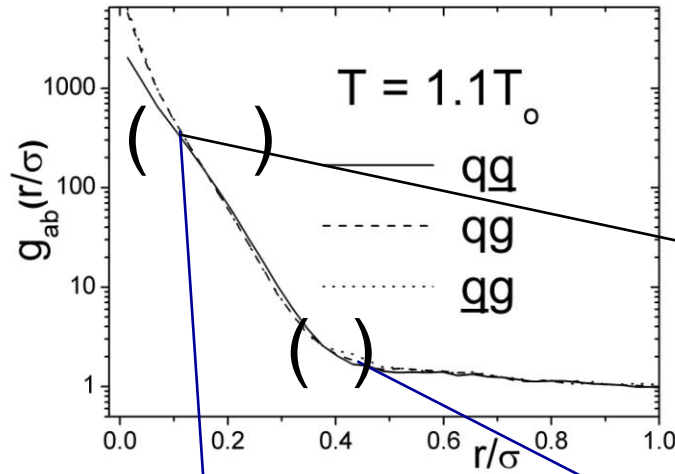
Peak related to bound states at interparticle distances of order one Bohr radius exists if discrete bound states in **electron-hole** or **hydrogen** plasma are well populated (low temperatures and small densities)

For low densities it is reasonable to choose $E' > -1/\beta$ while for high densities is appropriate $E' = -Ry / r_s$ since the quasiparticle in states with energy $E_\alpha > E'$ can be considered as free particles.

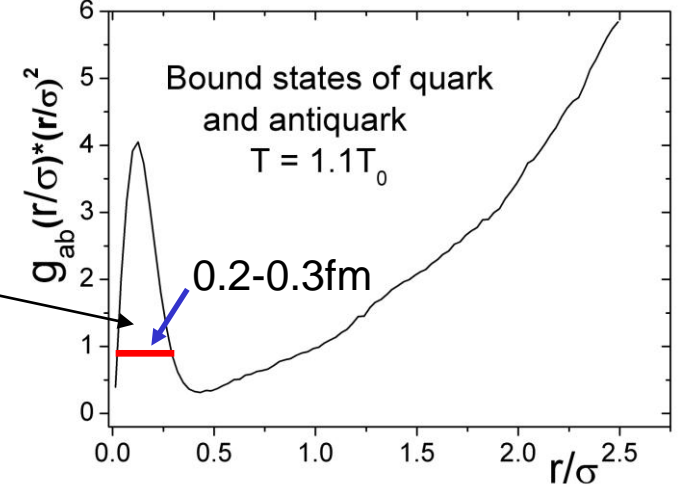


Color bound states and mean force potential ($T=1.1T_c$)

Distribution functions



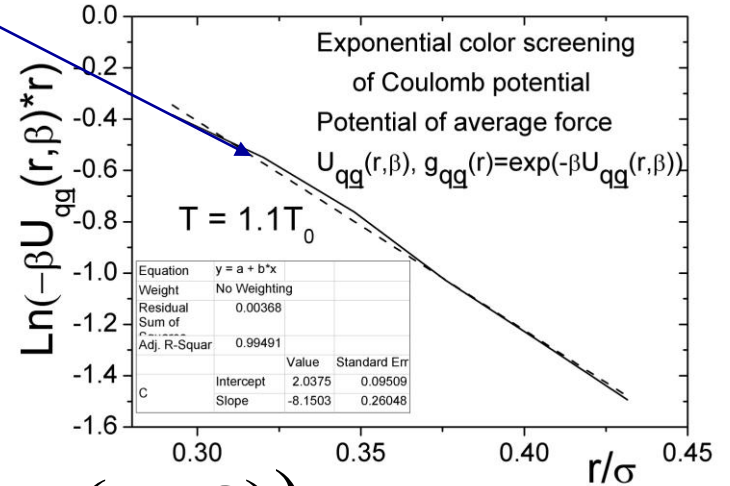
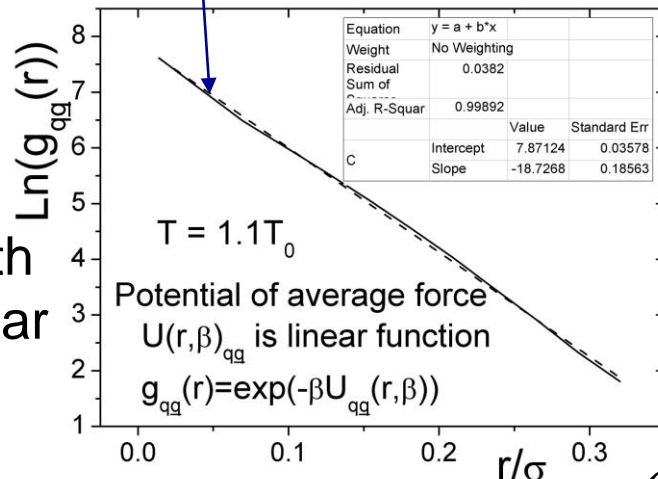
r^2 * Distribution function



Linear part of the mean force potential

Color screening part of mean force potential

Depth $U > 1$ GeV agree with lattice near T_c

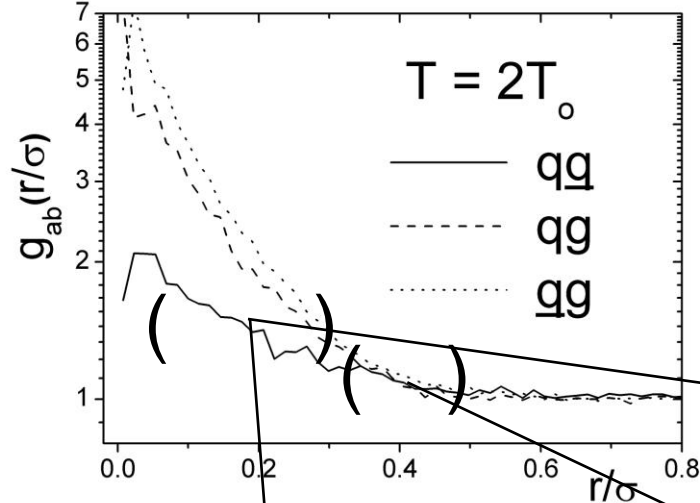


$$g_{q\bar{q}}(r) = \exp(-\beta U_{q\bar{q}}(r, \beta))$$

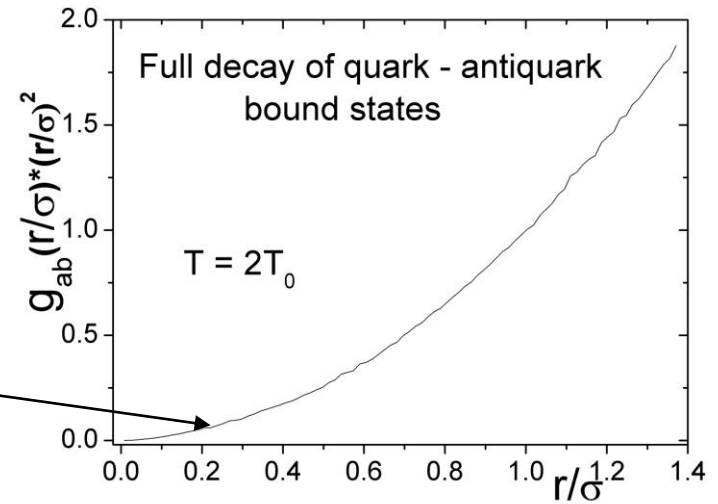


Decay of color bound states and mean force potential ($T=2T_c$)

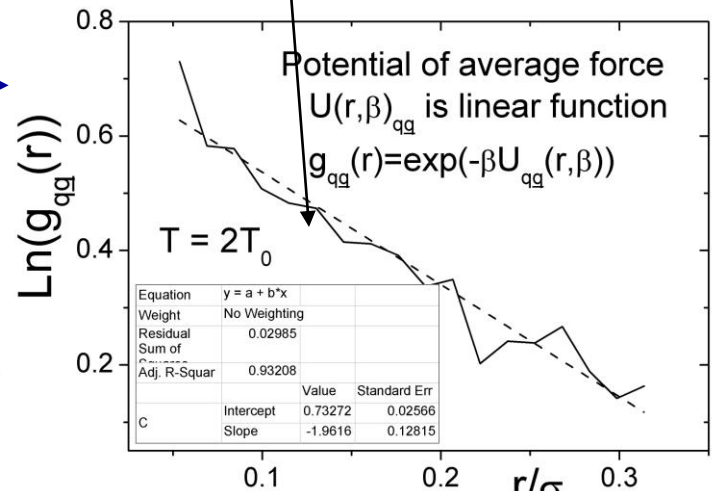
Distribution functions



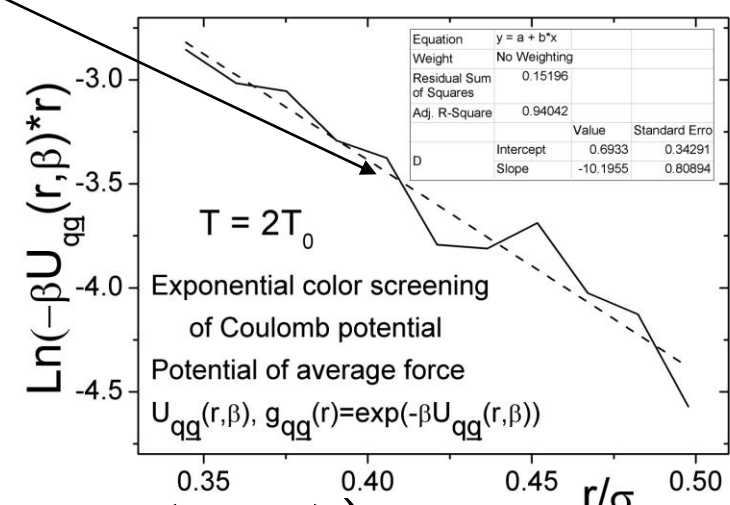
r^2 * Distribution function



Linear part of the mean force potential



Color screening part of mean force potential



Depth ~ 175 MeV

$$g_{qq}(r) = \exp(-\beta U_{qq}(r, \beta))$$



Kinetic properties of quark – gluon plasma in canonical ensemble

$$C_{FA}(t) = Z^{-1} \text{Tr} \left\{ F \exp\left(i \frac{Ht_c}{h}\right) A \exp\left(-i \frac{Ht_c}{h}\right) \right\};$$

$$H = K + V(qQ), t_c = t - i \frac{\beta h}{2}, \beta = \frac{1}{kT},$$

$$Z = \text{Tr} \{ \exp(-\beta H) \}$$

$$C_{FA}(t) = \frac{1}{(2\pi h)^{2v}} \iint dQ_1 dp_1 dq_1 dp_2 dq_2 F(p_1, q_1) A(p_2, q_2) \times$$

In this model we use approximation

$$W(p_1, q_1, Q_1; p_2, q_2, Q_1; t; i\beta h),$$

$$\delta(Q_1 - Q_1') \delta(Q_2 - Q_2') \delta(Q_1 - Q_2)$$

$$A(p, q) = \iint d\xi \exp\left(-i \frac{p\xi}{h}\right) \left\langle q - \frac{\xi}{2} \left| A \right| q + \frac{\xi}{2} \right\rangle$$

Weil symbols of operators

$$W(p_1, q_1, Q_1; p_2, q_2, Q_1; t; i\beta h) = Z^{-1} \iint d\xi_1 d\xi_2 \exp\left(i \frac{p_1 \xi_1}{h}\right) \exp\left(i \frac{p_2 \xi_2}{h}\right) \times$$

$$\left\langle q_1 + \frac{\xi_1}{2} \left| \exp\left(i \frac{Ht_c}{h}\right) \right| q_2 - \frac{\xi_2}{2} \right\rangle \left\langle q_2 + \frac{\xi_2}{2} \left| \exp\left(-i \frac{Ht_c}{h}\right) \right| q_1 - \frac{\xi_1}{2} \right\rangle$$



Integral equation

$$W(p_1, q_1, Q_1; p_2, q_2, Q_2; t; i\beta h) = \bar{W}(p_1^0, q_1^0, Q_1^0; p_2^0, q_2^0, Q_2^0; 0; i\beta h) +$$

$$+ \int_0^t d\tau \iint ds \iint d\eta W(p_1^\tau - s, q_1^\tau, Q_1^\tau; p_2^\tau - \eta, q_2^\tau, Q_2^\tau; \tau; i\beta h) \gamma(s, q_1^\tau, Q_1^\tau; \eta, q_2^\tau, Q_2^\tau),$$

$$\gamma(s, q_1^\tau, Q_1^\tau; \eta, q_2^\tau, Q_2^\tau) = \frac{1}{2} \{ \omega(s, q_1^\tau, Q_1^\tau) \delta(\eta) - \omega(\eta, q_2^\tau, Q_2^\tau) \delta(s) \}, F(q, Q) = -\nabla_q V(q, Q)$$

$$\omega(\eta, q, Q) = \frac{4}{(2\pi h)^v h} \iint dq' V(q - q', Q) \text{Sin}\left(\frac{2sq'}{h}\right) + F(q, Q) \square \frac{d\delta(s)}{ds}$$

$$\frac{dq_1^t}{dt} = \frac{1}{2m} p_1^t, \frac{dp_1^t}{dt} = \frac{1}{2} F(q_1^t, Q_1^t),$$

$$\frac{dQ_{1,i}^{t,a}}{dt} = \frac{1}{2} \sum_{b,c} f^{abc} Q_{1,i}^b \nabla_{Q_{1,i}^c} V(q_1^t, Q_1^t),$$

$$p_1^t(t, p_1, q_1, Q_1) = p_1, q_1^t(t, p_1, q_1, Q_1) = q_1, Q_1^t(t, p_1, q_1, Q_1) = Q_1$$

$$\frac{dq_2^t}{dt} = -\frac{1}{2m} p_2^t, \frac{dp_2^t}{dt} = -\frac{1}{2} F(q_2^t, Q_2^t),$$

$$\frac{dQ_{2,i}^{t,a}}{dt} = -\frac{1}{2} \sum_{b,c} f^{abc} Q_{2,i}^b \nabla_{Q_{2,i}^c} V(q_2^t, Q_2^t),$$

$$p_2^t(t, p_2, q_2, Q_1) = p_2, q_2^t(t, p_2, q_2, Q_1) = q_2, Q_2^t(t, p_2, q_2, Q_1) = Q_1$$

Positive time direction

Color dynamics in SU(2) or SU(3)

Initial conditions

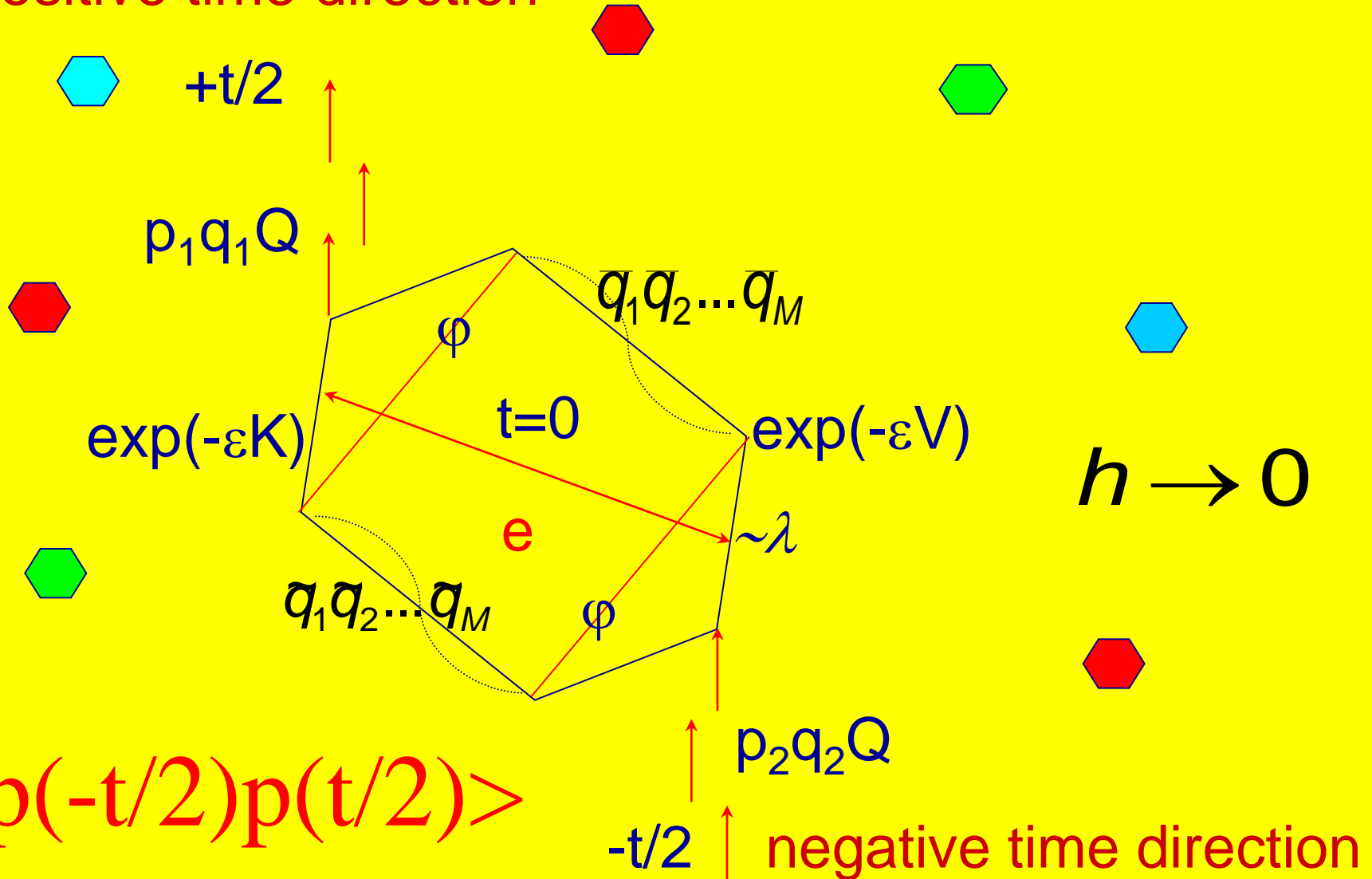
Hamiltonian equations

Negative time direction



Schematic snapshot for color phase space dynamics

positive time direction



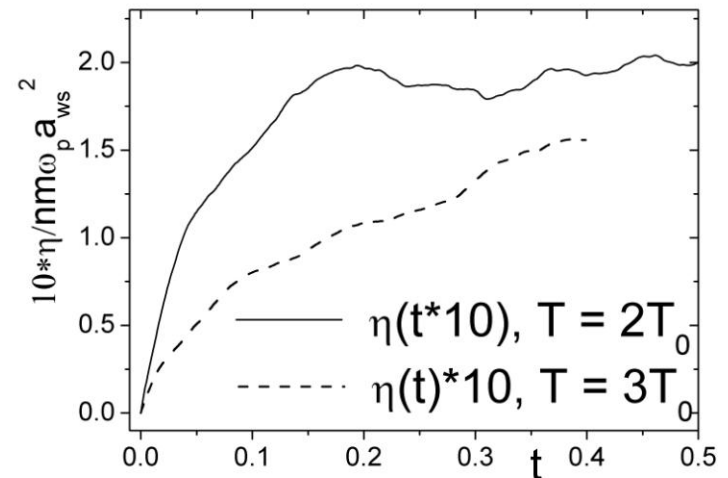
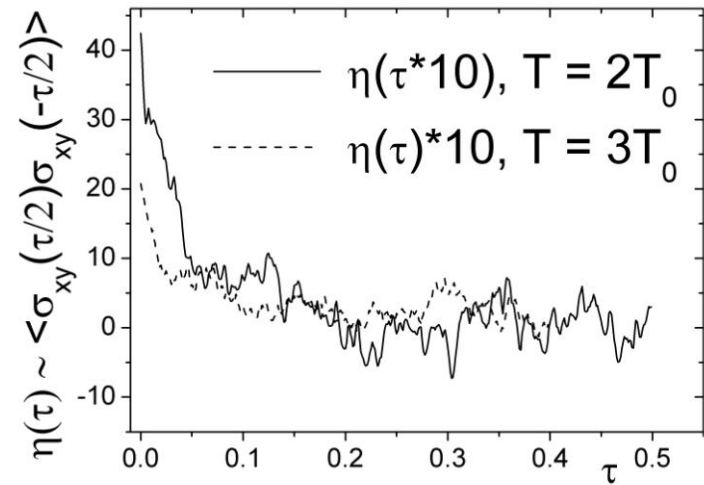


Time autocorrelation function of the stress energy tensor and shear viscosity of quark –gluon plasma

$$\eta(\tau) = \frac{n}{3k_B T} \left\langle \sum_{X < Y} \sigma_{XY}(\tau/2) \sigma_{XY}(-\tau/2) \right\rangle$$

$$\sigma_{XY}(\tau) = \frac{1}{N} \left(\sum_{i=1}^N m_i v_{ix} v_{iy} + \frac{1}{2} \sum_{i \neq j} r_{ij,x} F_{ij,y} \right)$$

$$\eta = \lim_{t \rightarrow \infty} \eta(t) = \lim_{t \rightarrow \infty} \int_0^t d\tau \eta(\tau)$$



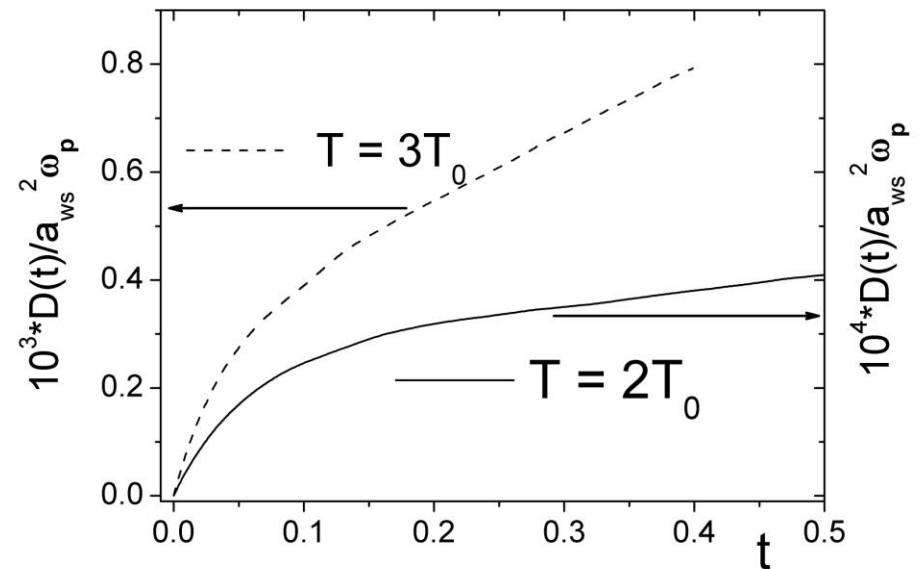
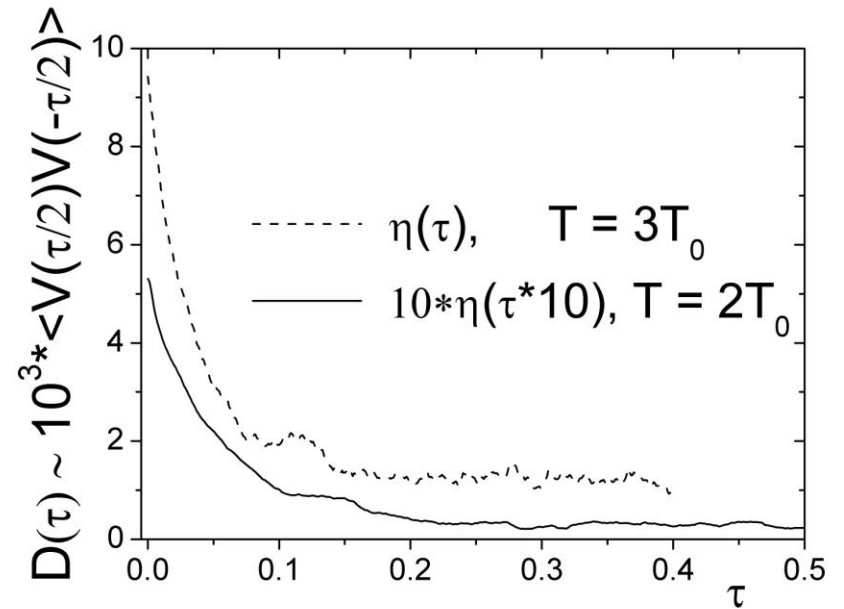


Velocity autocorrelation function and diffusion constant QGP

$$D(\tau) = \langle v(\tau/2)v(-\tau/2) \rangle =$$

$$= \frac{1}{3N} \langle \sum_{i=1}^N \vec{v}_i(\tau/2) \cdot \vec{v}_i(-\tau/2) \rangle$$

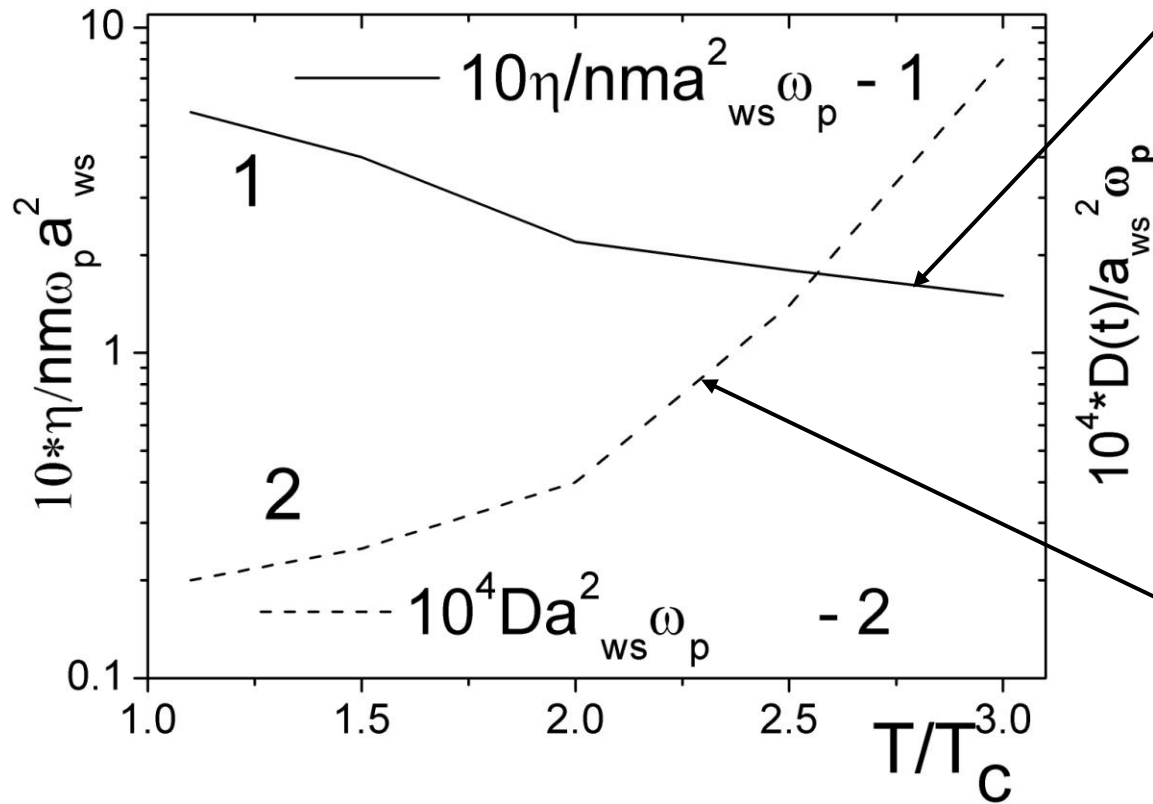
$$D = \lim_{t \rightarrow \infty} D(t) = \lim_{t \rightarrow \infty} \int_0^t d\tau D(\tau)$$





Diffusion coefficient and shear viscosity

Shear viscosity agrees with Gelman et al., 2006



Diffusion coefficient is $\sim 10^3$ lower in comparison with Gelman et al., 2006



**Electromagnetic plasma
Crystallization of protons**

HYDROGEN, PIMC-SIMULATION,

$n = 10^{25} \text{ cm}^{-3}$, $T = 10\,000 \text{ K}^\circ$

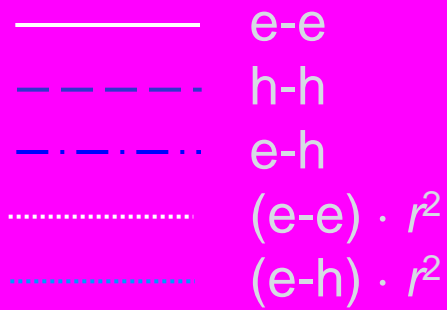
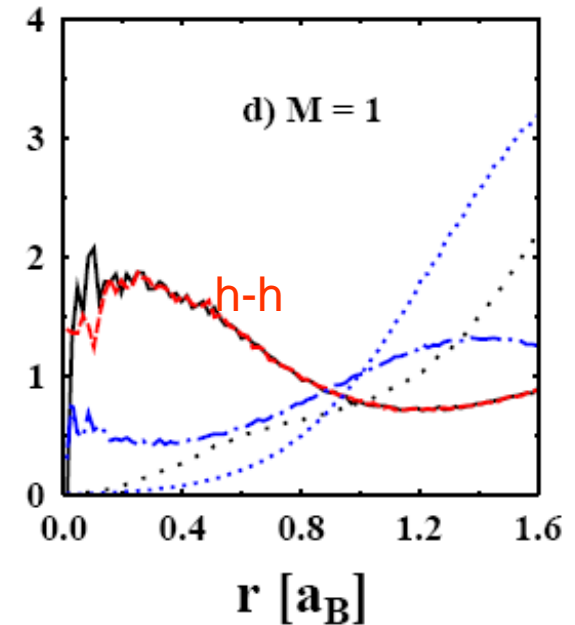
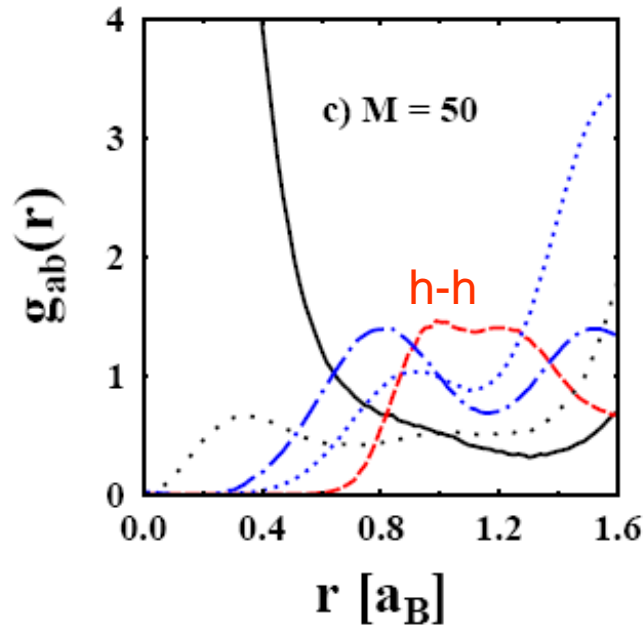
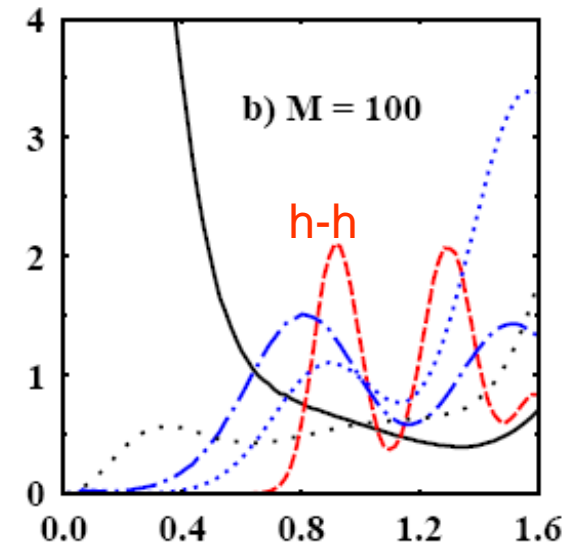
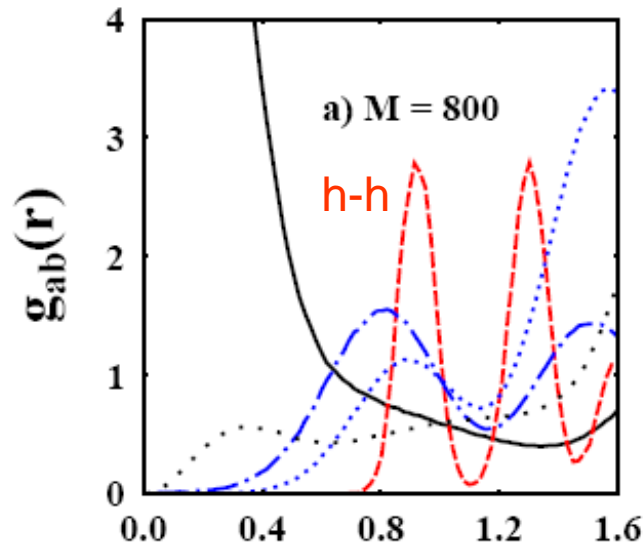
**Bloch oscillation of electron density
in periodic potential**

HOLE CRYSTALLIZATION AND QUANTUM MELTING

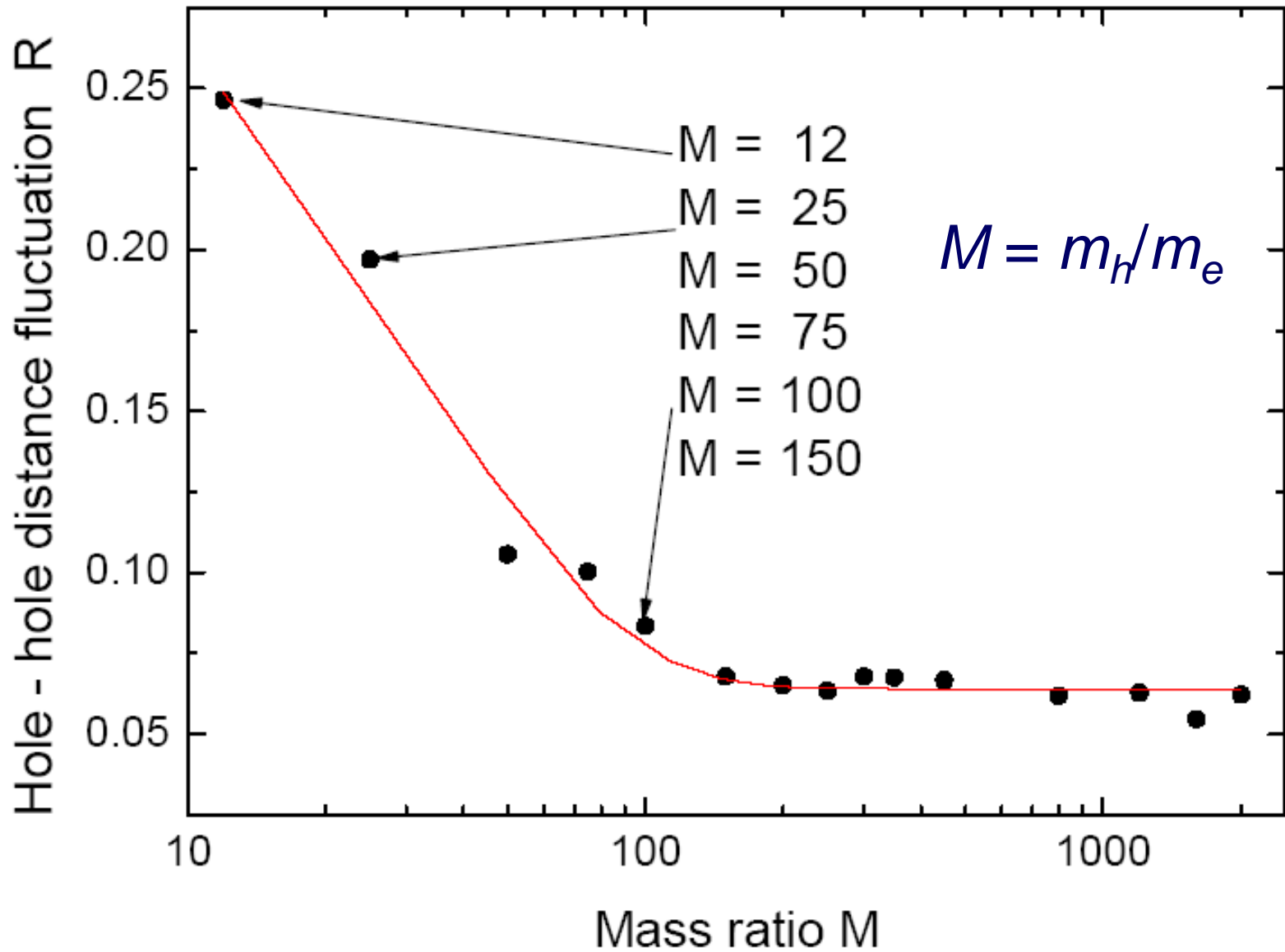
$$\langle r \rangle / a_B = 0.63$$

$$T = 0.064 E_b$$

$$M = m_h / m_e$$



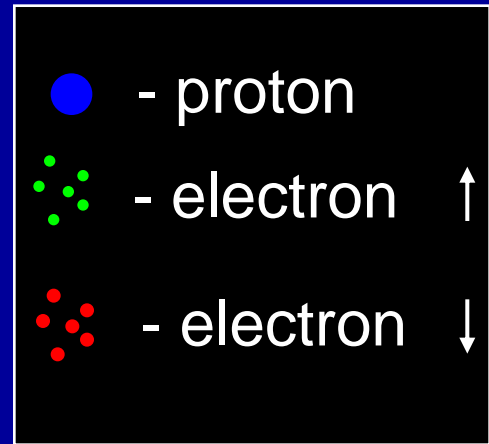
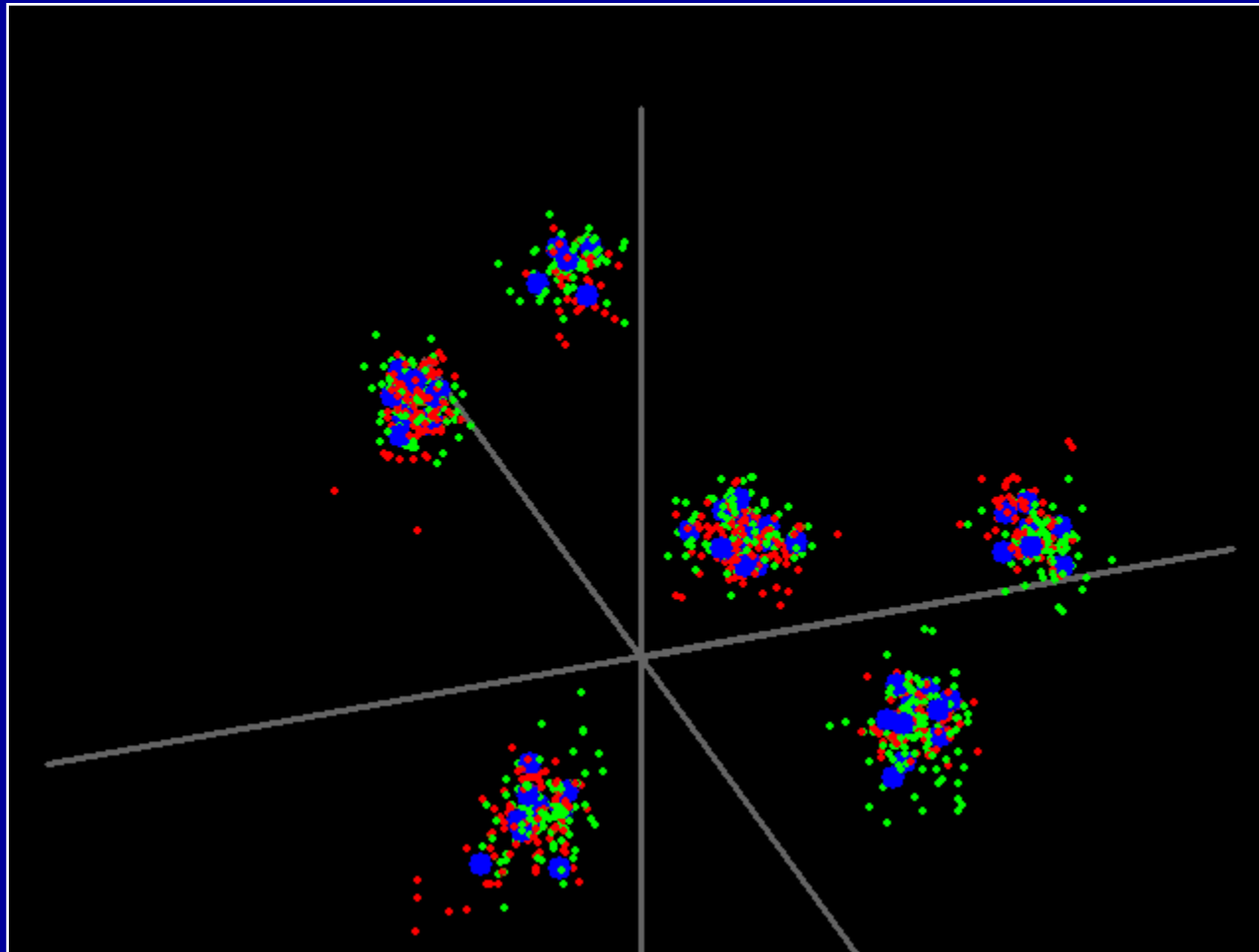
HOLE-HOLE DISTANCE FLUCTUATIONS



Phase transition to metallic state

Metallic drops and many particle clusters in hydrogen plasma

3D quantum two-component plasma.



$T = 10000 \text{ K}, n = 10^{22} \text{ cm}^{-3}, \rho = 0.0167 \text{ g/cm}^3$



CONCLUSIONS

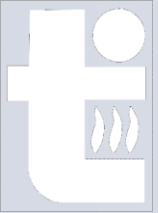
- Path integral Monte Carlo is a reliable and very fast method of simulation thermodynamic properties in a wide range of plasma parameters
- Quantum dynamics can be constructed on the basis of Feynman and Wigner formulation of quantum mechanics
- The developed numerical approach can be applied to consideration of EM and QG plasmas.
- Results of simulations agree with available theoretical and experimental data.

Thank you for attention.

Contact E-mails:

vs_filinov@hotmail.com

Vladimir_Filinov@mail.ru



Quantum simulations of strongly coupled electromagnetic and quark-gluon plasmas.

V. Filinov¹, M. Bonitz², Y. Ivanov³,
P. Levashov¹, V. Fortov¹

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

²Institut für Theoretische Physik und Astrophysik, Kiel, Germany

³Gesellschaft für Schwerionenforschung, Darmstadt, Germany