Quantum dynamics of charged fermions in the Wigner formulation of quantum mechanics

V. S. Filinov[1], A. S. Larkin[1,2],

[1]*Joint Institute for High Temperatures, RAS, Moscow, Russia*
[2]*Moscow Institute for Physics and Technology, Moscow Region, Russia*

OUTLINE

- Feynman path integral approach to quantum mechanics.

- New path integral representation of the Wigner function.

- Explicit analytical approximations of quantum Wigner function.

- Solution of fermion 'sign' problem based on Pauli blocking of fermions and effective phase space pair pseudopotential.

- Influence of the interparticle interaction on the high energy asymptotic
- of the momentum distribution functions ('quantum tails').

- Equation of states, internal energy, pair correlation, momentum distribution functions

- Quantum generalization of classical molecular dynamic method in the Wigner formulation quantum mechanics and calculations of the electron conductivity of strongly coupled plasma media.

Basic ideas of path integrals

Partition function:

$$Z(V,T) = Tr\left(e^{-\beta \hat{H}}\right) \qquad \left(\beta = 1/kT\right)$$

Hamiltonian:

$$\hat{H} = \sum_{a=1}^{N} \frac{\hat{p}_a^{\,2}}{2m_a} + U(\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_N)$$

$$[\hat{p}_i, \hat{q}_j] = -i\hbar \delta_{ij} \implies [\hat{K}, \hat{U}] \neq 0$$

Operators of kinetic and potential energy do not commutate :

$$e^{-\beta\left(\hat{K}+\hat{U}\right)} \neq e^{-\beta \hat{K}} \cdot e^{-\beta \hat{U}}$$

1. High temperature decomposition :

$$e^{-\beta\hat{H}} = e^{-\frac{\beta}{M}\hat{H}} \cdot e^{-\frac{\beta}{M}\hat{H}} \cdot \ldots \cdot e^{-\frac{\beta}{M}\hat{H}}$$

2. Discrete representation :

$$Tr\left[e^{-\beta\hat{H}}\right] = Tr\left[e^{-\varepsilon\hat{H}} \cdot 1 \cdot e^{-\varepsilon\hat{H}} \cdot \ldots \cdot 1 \cdot e^{-\varepsilon\hat{H}}\right] \qquad \hat{1} = \int d^{3N}q \, |q\rangle\langle q|$$

$$\Downarrow$$

$$Z(V,T) = \int d^{3N}q \, d^{3N}q^1 \ldots d^{3N}q^{M-1} \langle q|e^{-\frac{\beta}{M}\hat{H}}|q^1\rangle \cdot \langle q^1|e^{-\frac{\beta}{M}\hat{H}}|q^2\rangle \cdot \ldots \cdot \langle q^{M-1}|e^{-\frac{\beta}{M}\hat{H}}|q\rangle$$

3. High temperature density matrix:

$$\langle q^m|e^{-\frac{\beta}{M}\hat{H}}|q^{m+1}\rangle = M^{3N/2}\lambda^{-3N} \cdot \exp\left\{-\frac{\pi}{\lambda^2/N}\sum_{a=1}^{N}\left(q_a^{m+1} - q_a^m\right)^2 - \frac{\beta}{M}U(q^m)\right\} + O\left(M^{-2}\right)$$

$$\lambda = \sqrt{\frac{2\pi\hbar^2\beta}{m}}$$ - thermal wave length

$$Z(V,T) = \int d^{3N}q\, d^{3N}q^1 \ldots d^{3N}q^{M-1}\, \lambda^{-3NM}\, \exp\left\{ -\sum_{m=0}^{M-1}\left[\frac{\pi}{\lambda^2}\sum_{a=1}^{N}\left(q_a^{\,m+1} - q_a^{\,m}\right)^2 + \frac{\beta}{M}U\left(q^m\right) \right] \right\}_{q_0 = q_M = q}$$

- Discrete representation

Limit $\quad M \to: \infty$

$\quad m/M \to \tau \qquad\qquad$ - «time»

$\quad q_a^{\,m} \to q(\tau) \qquad\qquad$ - path

$\quad \dfrac{\vec{q}_a^{\,m+1} - \vec{q}_a^{\,m}}{1/M} \to \dot{\vec{q}}_a(\tau) \qquad$ - «velocity on the path

$\int d^{3N}q^1 \int d^{3N}q^2 \ldots \int d^{3N}q^{M-1} \to \int\limits_{q(0)=q(1)=q} D^{3N}q(\tau) \quad$ - The Wiener path integral measure

Path integral representation

electron

e_b

$r^{(2)}$

$\lambda_e^2 = 2\pi\hbar^2\,\beta/m_e$

$\lambda_\Delta^2 = 2\pi\hbar^2\Delta\,\beta/m_e$

λ_e λ_Δ

$r^{(n+1)} \equiv r$
$\sigma' \equiv \sigma$

$r^{(n)}$

$r^{(1)} = r + \lambda_\Delta\xi^{(1)}$

r

P_a

proton

q_a

r_b

parity of
permutations
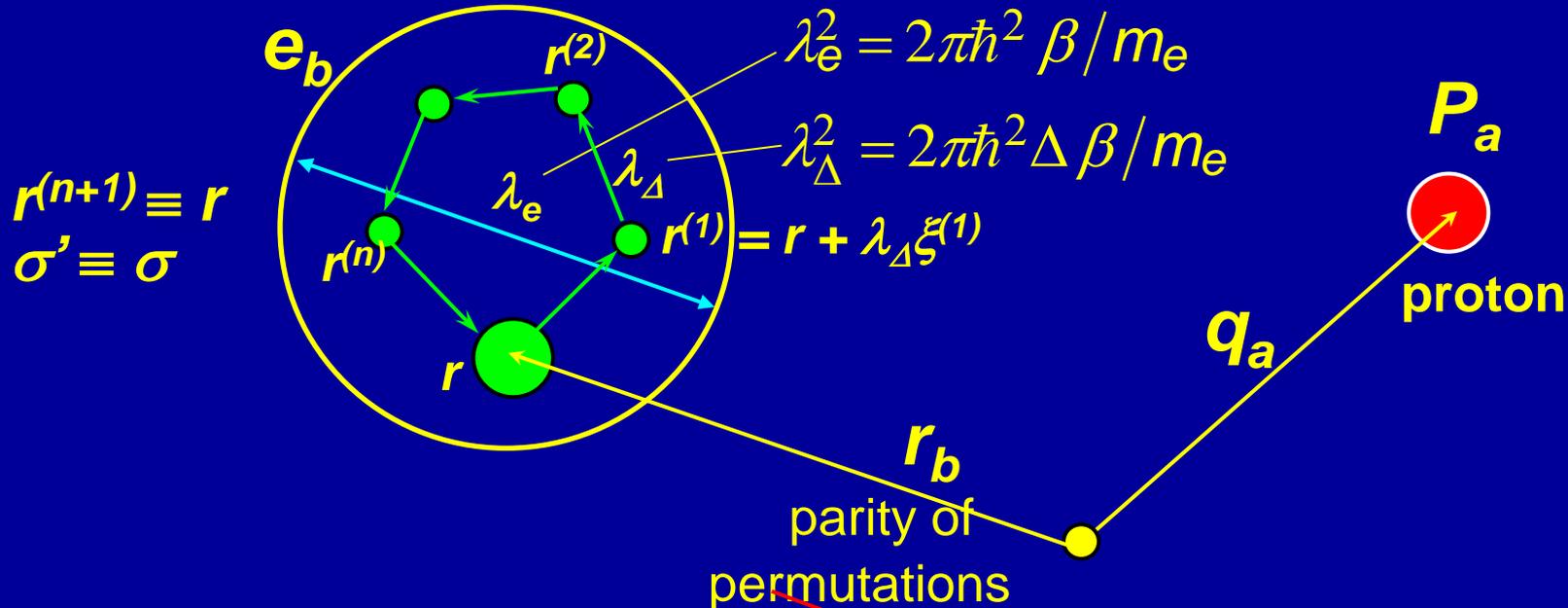
$$\rho(q,r,\sigma;\beta) = \frac{1}{\lambda_i^{3N_i}\,\lambda_\Delta^{3N_e}} \sum_P (-1)^{\kappa_P} \int\limits_V dr^{(1)}\dots dr^{(n)} \times$$

Thermal wave
lengths

$$\rho\!\left(q,r,r^{(1)};\Delta\beta\right)\dots\rho\!\left(q,r^{(n)},P\,r^{(n+1)};\Delta\beta\right) S(\sigma,P\sigma'),$$

N-particle exchange
operator

Spin matrix

PIMC simulations

$N_e = N_i = 50$, $n = 20$
Hydrogen atoms
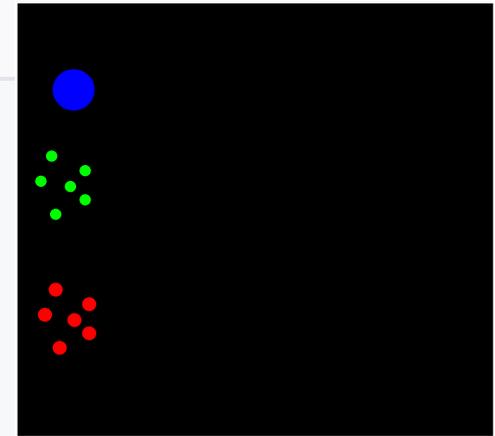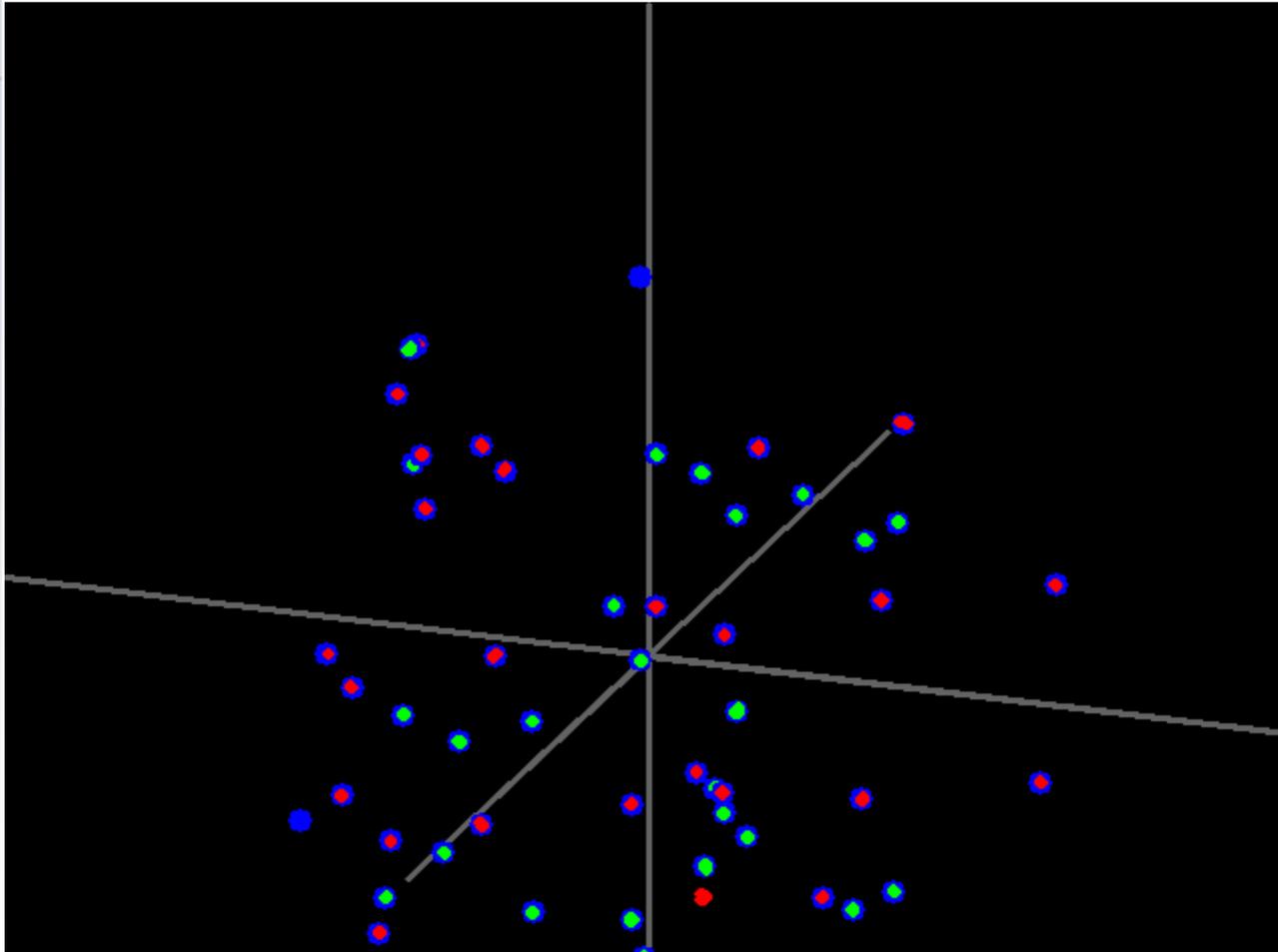
T = 10000 K, n = 10^{18} cm^{-3}, ρ = 1.67·10^{-6} g/cm^3

PIMC simulations

$N_e = N_i = 50$, $n = 20$

Hydrogen molecular
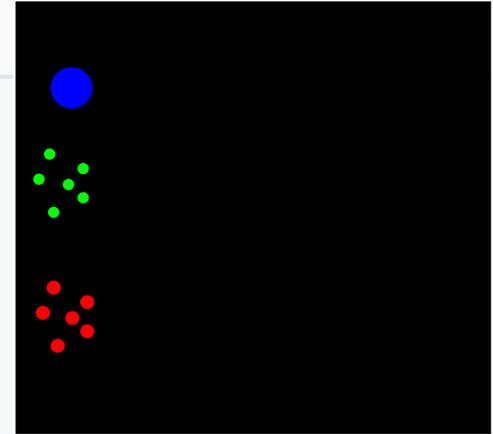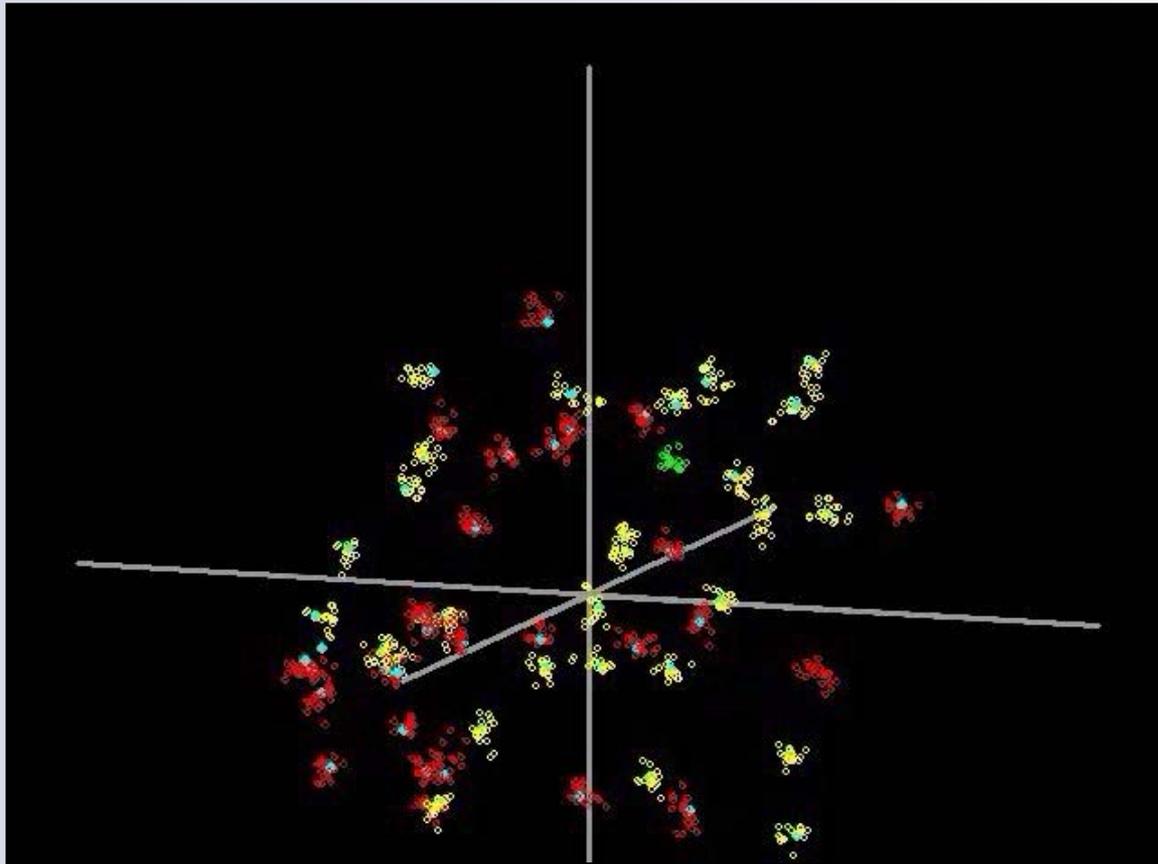
T = 10000 K, n = 10^{21} cm^{-3}, ρ = 1.67·10^{-3} g/cm^3
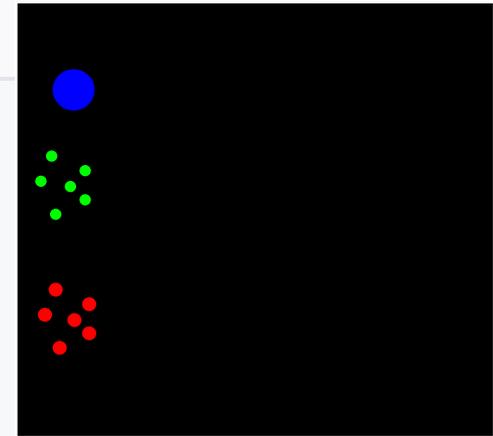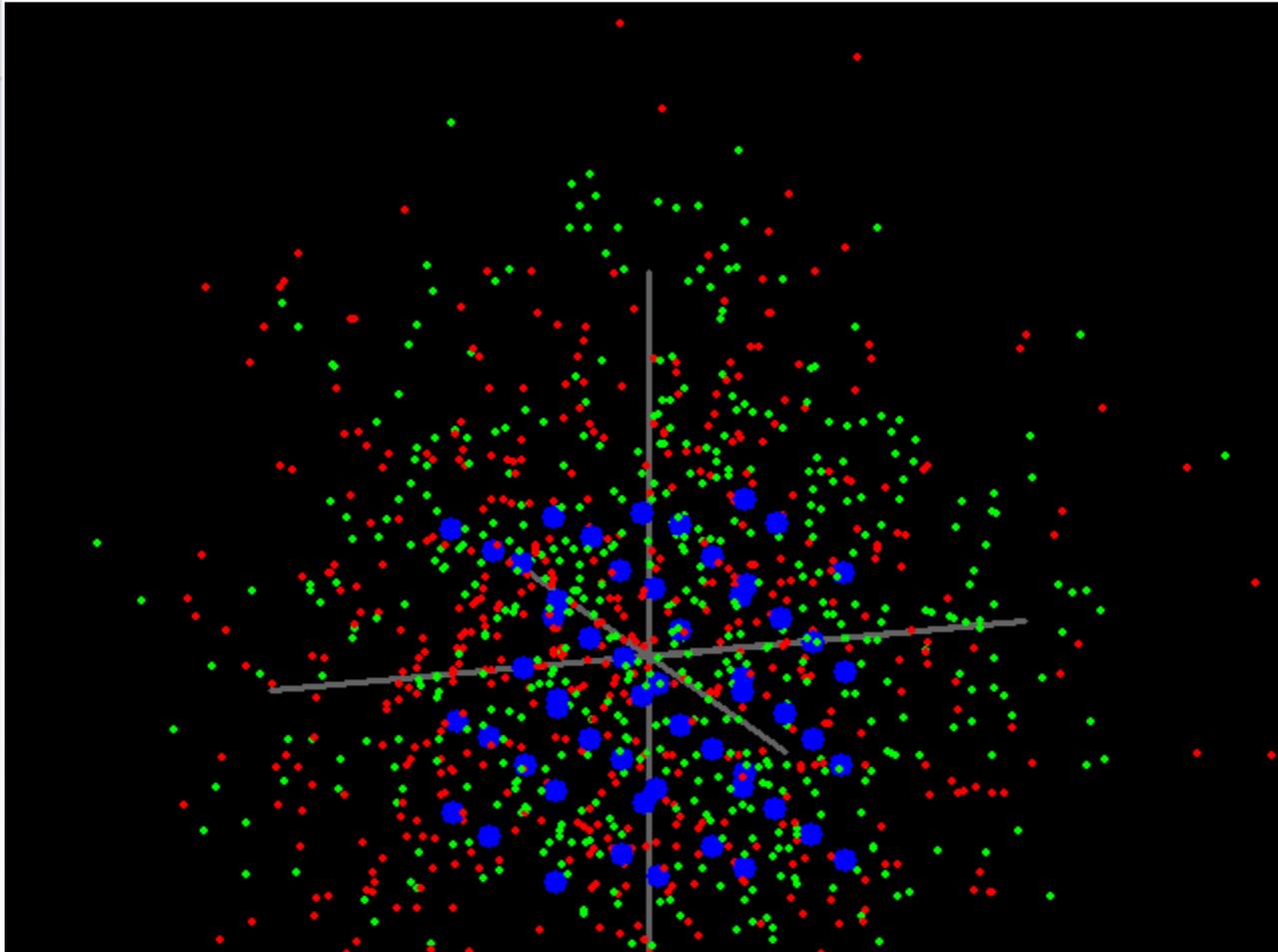
DPIMC simulation

$N_e = N_i = 50$, $n = 20$
Phase transition in hydrogen plasma
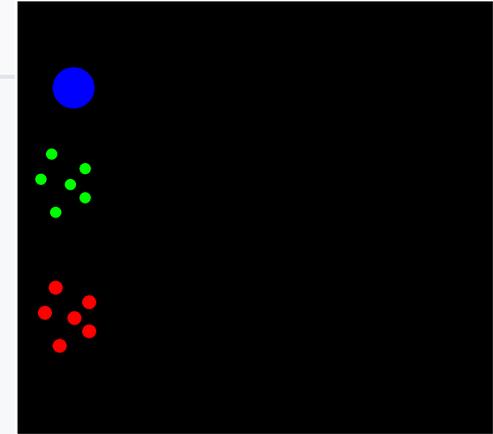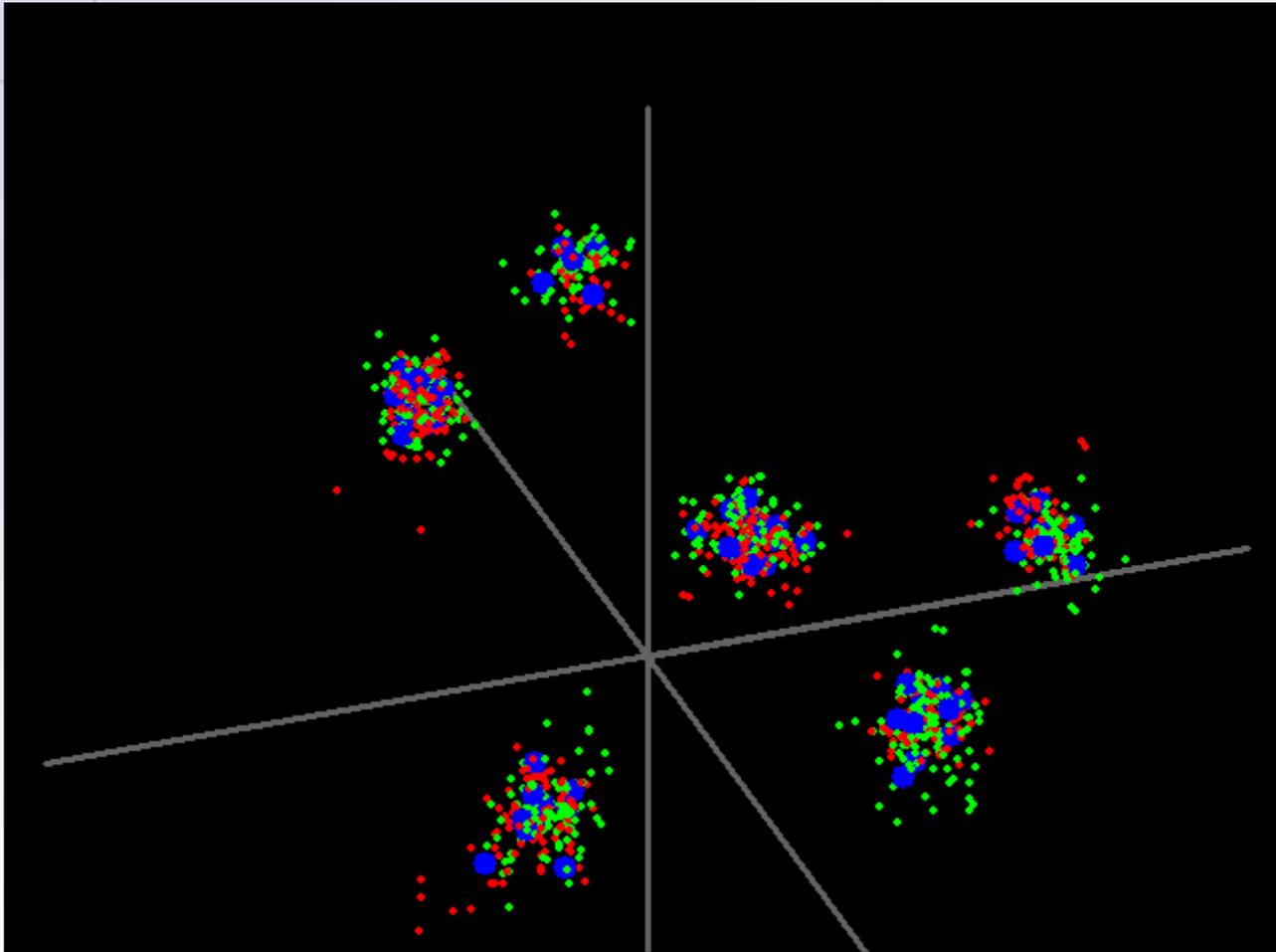
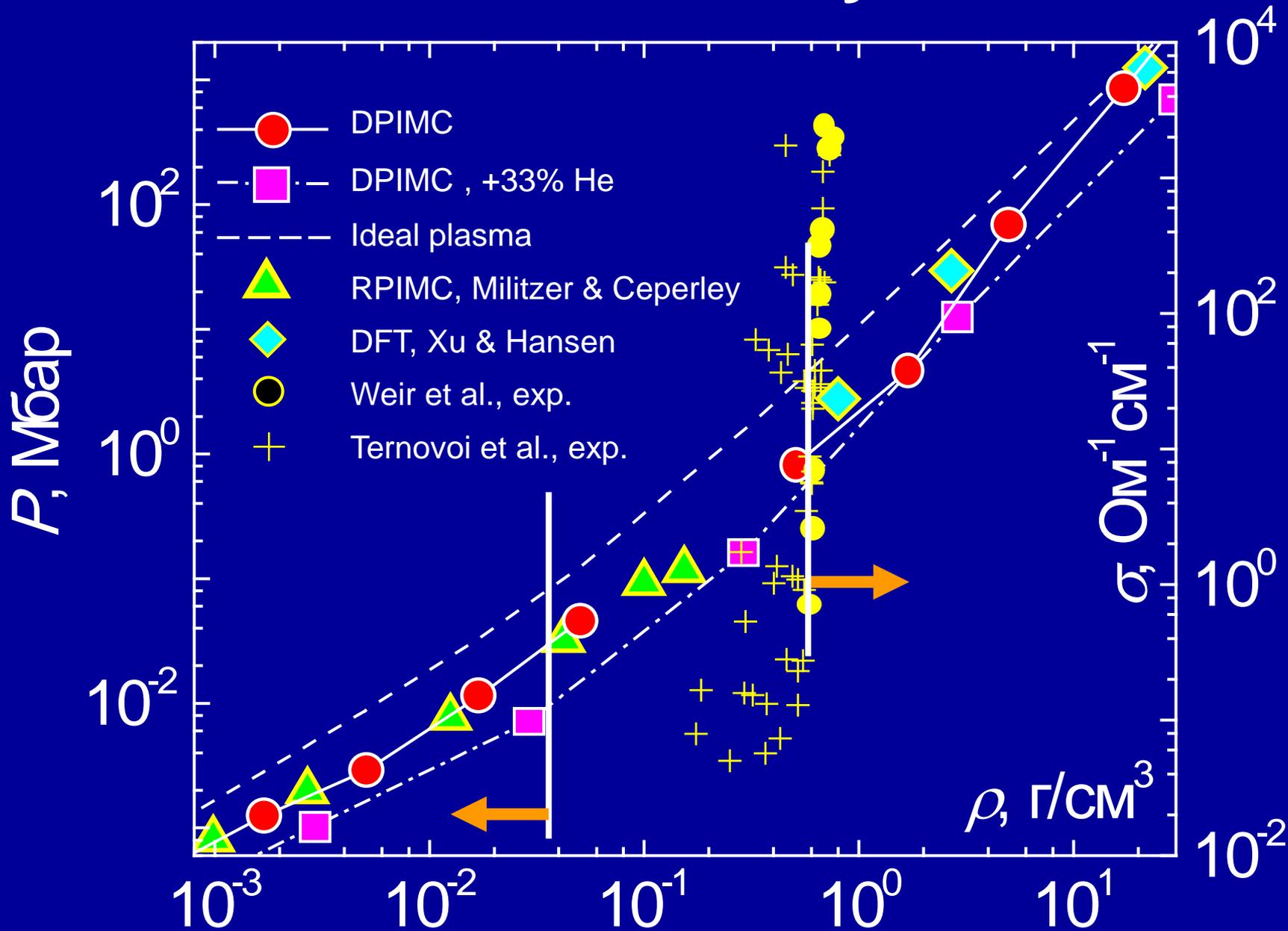$T = 10000$ K, $n = 10^{22}$ cm^{-3}, $\rho = 0.0167$ g/cm^3

PIMC simulation

$N_e = N_i = 50$, $n = 20$
Ordering of protons

$T = 10000$ K, $n = 3 \cdot 10^{25}$ cm^{-3}, $\rho = 50.2$ g/cm^3

Pressure and Conductivity $T = 10000$ K

Wigner functions in thermodynamics

Aim is to calculate:

– Average values of quantum operators

– Momentum distributions and pair correlation functions

Average value of arbitrary quantum operator:

$$\langle A \rangle = Tr\{\hat{A}\hat{\rho}\} = \int \frac{d^{3N}p \, d^{3N}q}{(2\pi\hbar)^{3N}} A(p,q) \cdot W(p,q)$$

Wigner function:

$$W(p,q,\beta) = Z^{-1} \int d^{3N}\xi \langle q - \xi/2 | e^{-\beta\hat{H}} | q + \xi/2 \rangle \cdot \exp\left(\frac{i}{\hbar} \langle p | \xi \rangle \right)$$

Weyl's symbol of operator A(p,x) :

$$A(p,q) = \int d^{3N}s \langle p + s/2 | \hat{A} | p - s/2 \rangle \cdot \exp\left(\frac{i}{\hbar} \langle q | s \rangle \right)$$

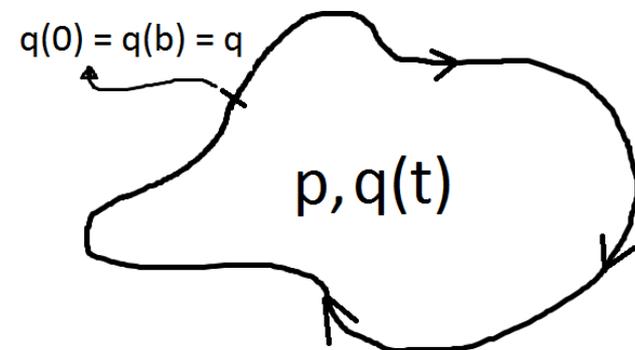# Path integral representation of Wigner function.

$$W(p,q) = Z^{-1} \int d^{3N}\xi \exp\left(\frac{i}{\hbar}\langle p|\xi\rangle\right) \cdot \sum_P (-1)^P \langle q - \xi/2 | e^{-\beta\hat{H}} | P(q+\xi/2)\rangle$$

$$W(p,q) = Z^{-1} \int d^{3N}\xi \exp\left\{\frac{i}{\hbar}\langle p|\xi\rangle\right\} \sum_P (-1)^P \exp\left\{-\frac{\pi}{\lambda^2}|Pq - q|^2\right\}$$

$$\times \int_{q=q(0)}^{Pq(\beta)} D^{3N}q(\tau) \exp\left(-\int_0^1 d\tau\left[\frac{\pi}{\lambda^2}\sum_{a=1}^N \dot{q}_a^2(\tau) + \beta U\left(q(\tau) + \xi(\tau - 1/2)\right)\right]\right)$$

$$\times \exp\left\{-\frac{\pi}{2\lambda^2}\langle\xi|P+E|\xi\rangle\right\}$$

q(0) = q(b) = q

p, q(t)

Problem: (*3N)D* Fourier transform

Harmonic and linear approximation of interparticle potential.

$$U(q + \xi(\tau - 1/2)) \approx U(q) + (\tau - 1/2)\xi_{a,i} \cdot \frac{\partial U}{\partial q_{a,i}} +$$

$$+ \frac{1}{2}(\tau - 1/2)^2 \xi_{a,i}\xi_{b,j} \cdot \frac{\partial^2 U}{\partial q_{a,i}\partial q_{b,j}}$$

$$W(p,q) = \exp(-\beta V(p,q)) \int_{q=q(0)}^{q(\beta)} D^{3N}q(\tau)\exp\left(-\int_0^1 d\tau\left[\frac{\pi}{\lambda^2}\sum_{a=1}^{N}\dot{q}_a{}^2(\tau) + \beta U(q(\tau))\right]\right)$$

$$\times \left(\det\left|\chi_{ai,bj}\right|\right)^{-1/2}\exp\left(-\frac{\beta}{2}\frac{p_{ai}\chi_{ai,bj}p_{bj}}{\sqrt{m_a m_b}} + \pi J_{ai}\chi_{ai,bj}J_{bj}\right)\times\cos\left(\frac{p_{ai}\chi_{ai,bj}J_{bj}}{\hbar}\right)$$

$$J_{ai}[q(\tau)] = \frac{\lambda}{2\pi}\int_0^\beta d\tau(\tau - \beta/2)\cdot\frac{\partial U(q(\tau))}{\partial q_{ai}} \qquad \chi_{ai,bj}[q(\tau)] = \delta_{ai,bj} + \frac{\lambda^2}{2\pi}\int_0^\beta d\tau(\tau - \beta/2)^2\cdot\frac{\partial^2 U(q(\tau))}{\partial q_{ai}\partial q_{bj}}$$
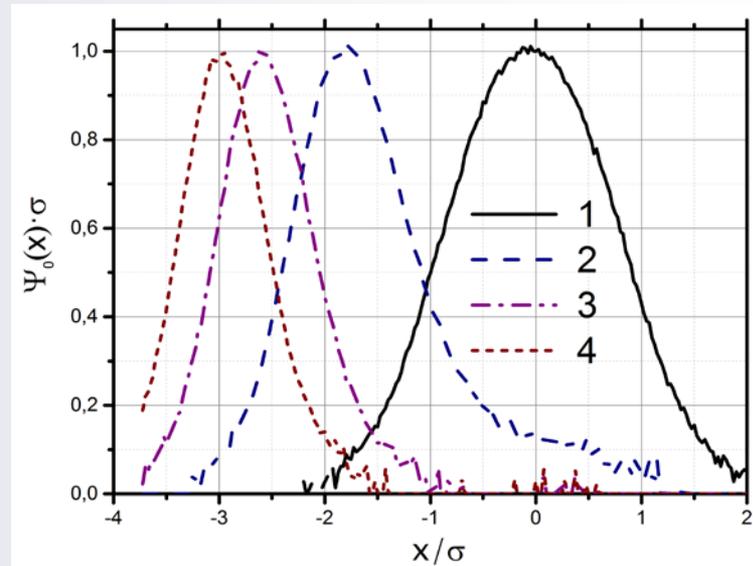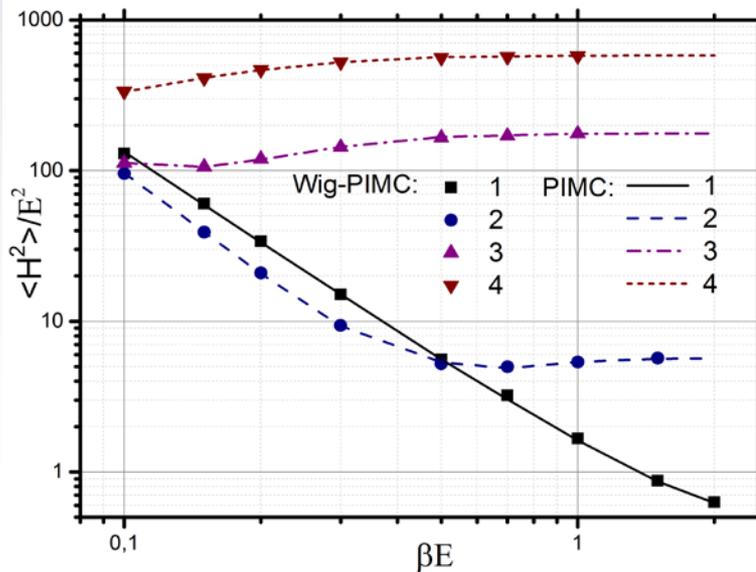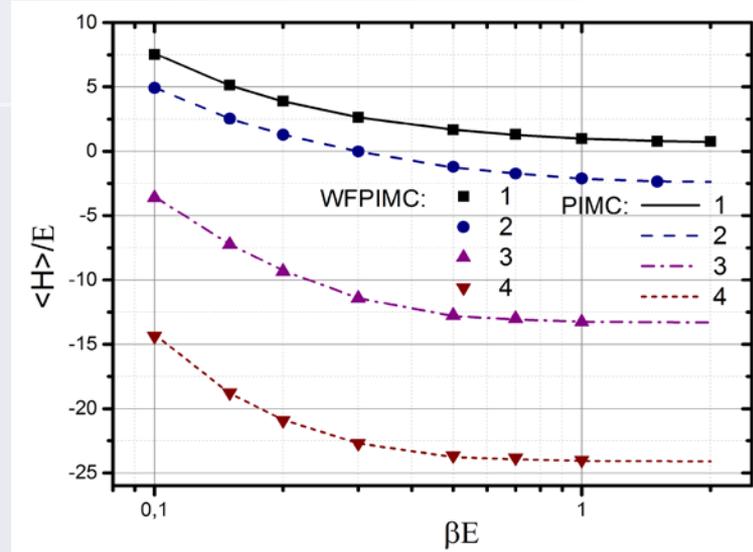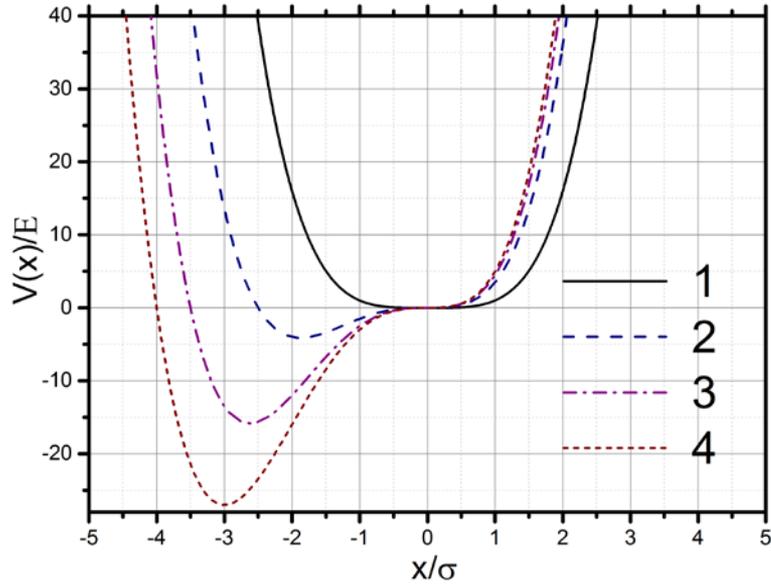
$$V(p,q) = \sum_{l<t} v_{lt} \qquad v_{lt} = -kT\ln\left\{1 - \exp\left(-\frac{2\pi|q_l - q_t|^2}{\lambda^2}\right)\exp\left(-\frac{\lambda^2|(p_l + J_l) - (p_t + J_t)|^2}{(2\pi h)^2\alpha(n\lambda^3)}\right)\right\}$$

Test Calculations. Energy and ground state of 1D anharmonic oscillator

$$V_{3-4}(x) = cx^3 + bx^4$$

c=0, 5/3, 7/3, 6
b=const=1

Pauli blocking by pair repulsive exchange pseudopotential in phase space

Here Fermi statistical effects defined by pair permutations are allowed for by pair exchange pseudopotential in phase space depending on coordinates, momenta and degeneracy parameter of particles and taking into account Pauli blocking of fermions.

$$v_{lt} = -kT \ln \left\{ 1 - \exp\left(-\frac{2\pi |q_l - q_t|^2}{\lambda^2} \right) \exp\left(-\frac{\lambda^2 |(p_l + J_l) - (p_t + J_t)|^2}{(2\pi h)^2 \alpha(n\lambda^3)} \right) \right\} \qquad V(p,q) = \sum_{l<t} v_{lt}$$

$$W(p,q) = \exp(-\beta V(p,q)) \int_{q=q(0)}^{q(\beta)} D^{3N} q(\tau) \exp\left(-\int_0^1 d\tau \left[\frac{\pi}{\lambda^2} \sum_{a=1}^N \dot{q}_a^{\,2}(\tau) + \beta U(q(\tau)) \right] \right)$$

$$\times \left(\det |\chi_{ai,bj}| \right)^{-1/2} \exp\left(-\frac{\beta}{2} \frac{p_{ai} \chi_{ai,bj} p_{bj}}{\sqrt{m_a m_b}} + \pi J_{ai} \chi_{ai,bj} J_{bj} \right) \times \cos\left(\frac{p_{ai} \chi_{ai,bj} J_{bj}}{\hbar} \right)$$

$$J_{ai}[q(\tau)] = \frac{\lambda}{2\pi} \int_0^\beta d\tau (\tau - \beta/2) \cdot \frac{\partial U(q(\tau))}{\partial q_{ai}} \qquad \chi_{ai,bj}[q(\tau)] = \delta_{ai,bj} + \frac{\lambda^2}{2\pi} \int_0^\beta d\tau (\tau - \beta/2)^2 \cdot \frac{\partial^2 U(q(\tau))}{\partial q_{ai} \partial q_{bj}}$$
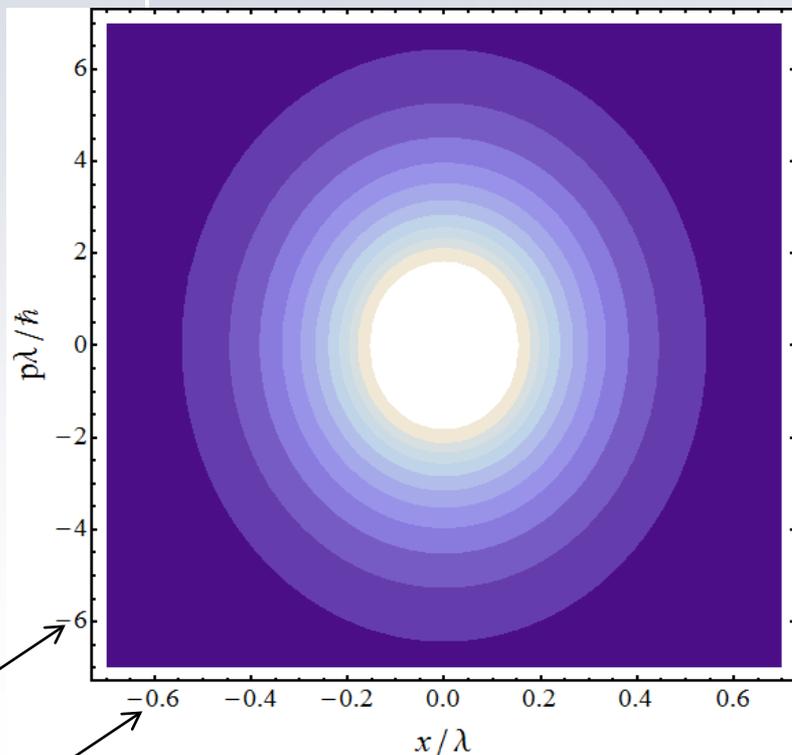
Contour plots of the repulsive effective exchange pair pseudopotentials in phase space.
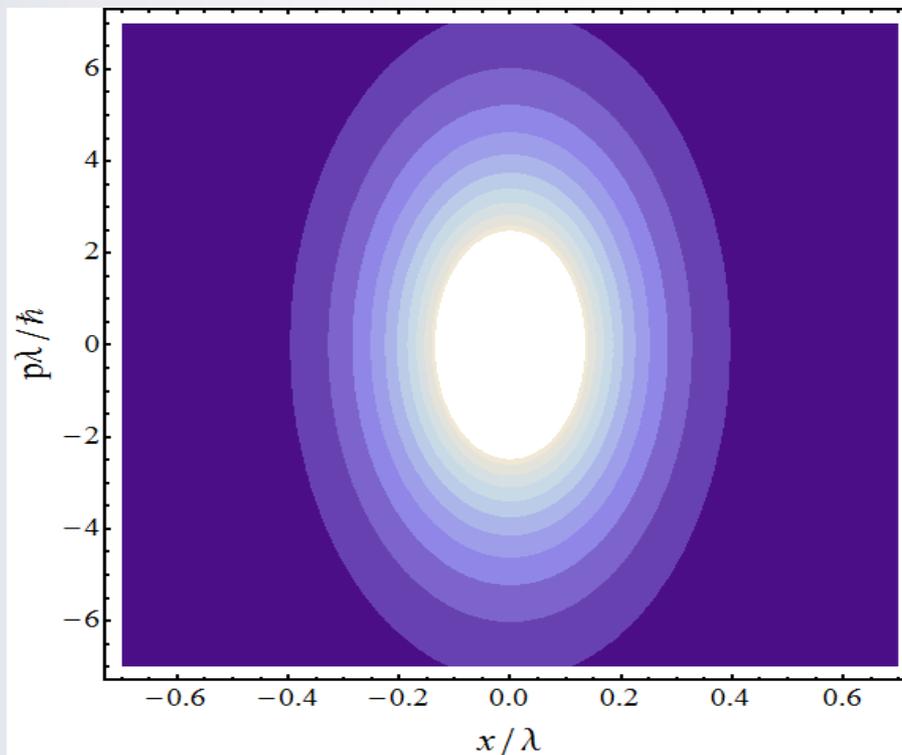
$$\chi = N\lambda^3_e /V = 5.6$$

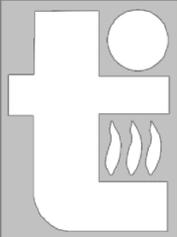In dark area pseudopotential is less than 0.1. $\beta v_{lt} < 0.1$
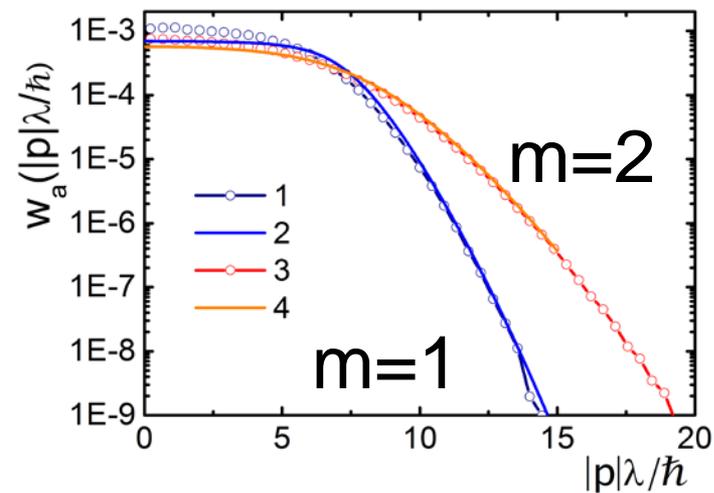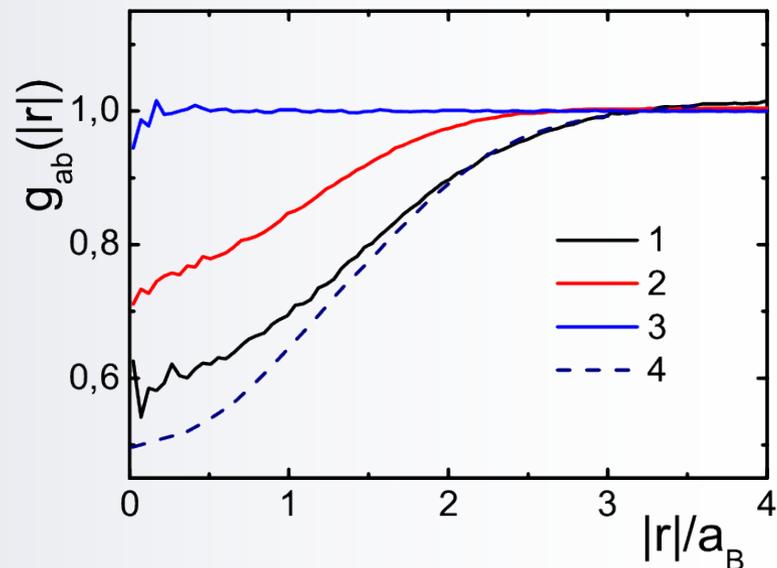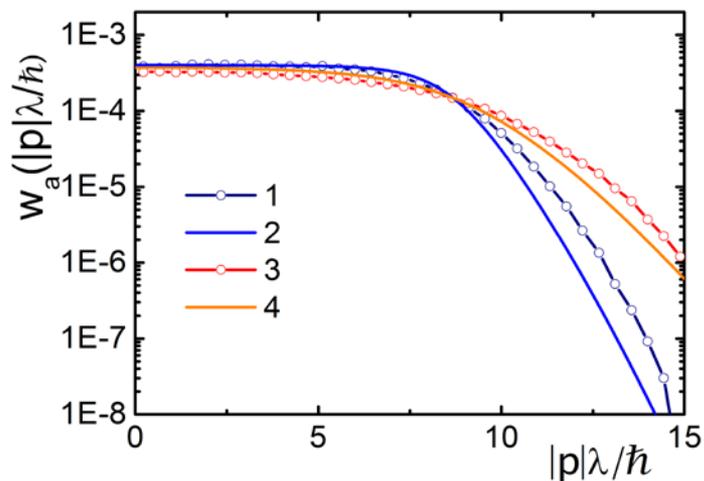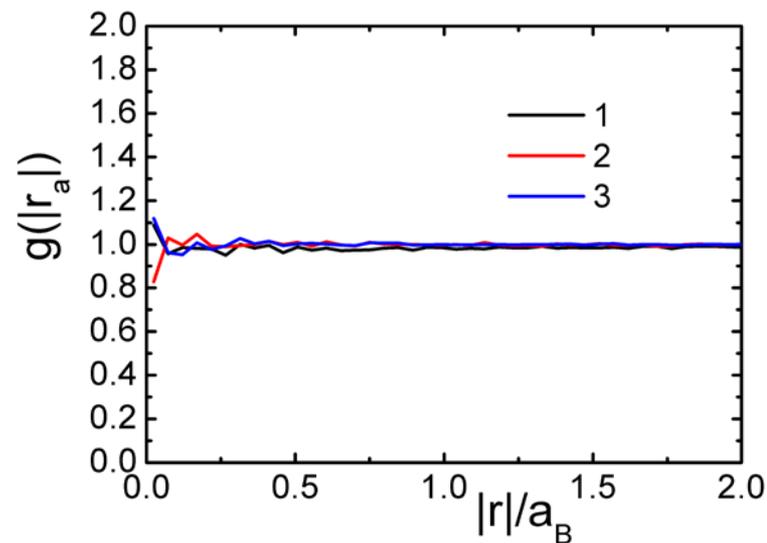In white area pseudopotential is larger than 1.9. $\beta v_{lt} > 1.9$

m=1

m=2

Test Calculations. The momentum distributions and pair correlation functions for ideal electron - hole plasma.

$\chi = N\lambda_e^3/V = 10$

$\chi = N\lambda_e^3/V = 5.6$

PIMC momentum distributions functions for non ideal electron - hole plasma.

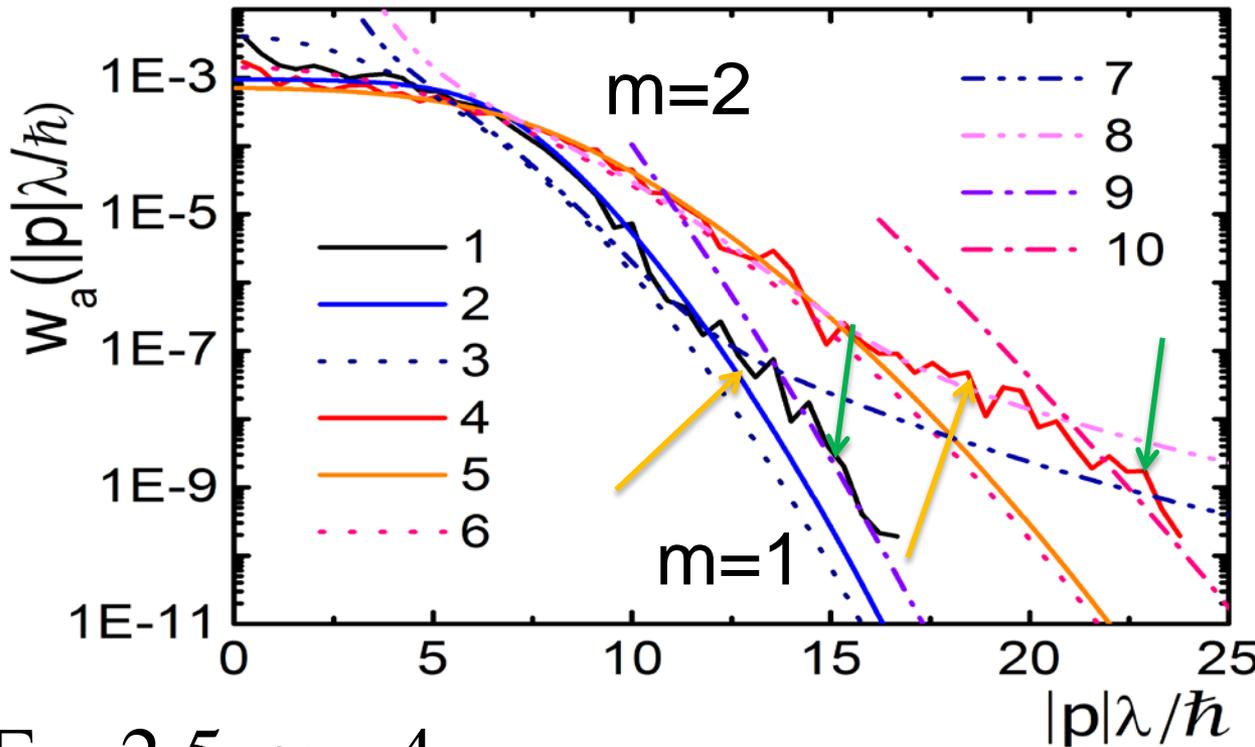$$\Gamma = \beta e^2 \sqrt[3]{N/V}; \chi = N\lambda^3{}_e/V$$

$1,4 - PIMC$

$2,5 - FD$

$$3,6 - MD \sim \exp(-\frac{(p\lambda)^2}{4\pi})$$

Asymptotics

$7,8 - MD + const/p^8$

$9,10 - MD + MD' \times const/p^8$

$$\Gamma = 2.5, \chi = 4$$

Galitskii V M and Yakimets V V 1966
Zh. Eksp. Teor. Fiz., 51} 957

Kimball J C 1975 J. Phys. A : Math. Gen., 8 1513

Starostin A N, Mironov A B, Aleksandrov N L, Fischc N J, Kulsrudc R M 2002 Physica A 305 287

Eletskii A V, Starostin A N and Taran M D 2005 Physics – Uspekhi 48 281

Emelianov A V, Eremin A V, Petrushevich Yu V, Sivkova E E, Starostin A N, Taran M D, Fortov V E 2011 ETP Letters 94:7 530

Kochetov I V, Napartovich A P, Petrushevich Yu V, Starostin A N, Taran M D 2016 High Temperature 54:4} 563
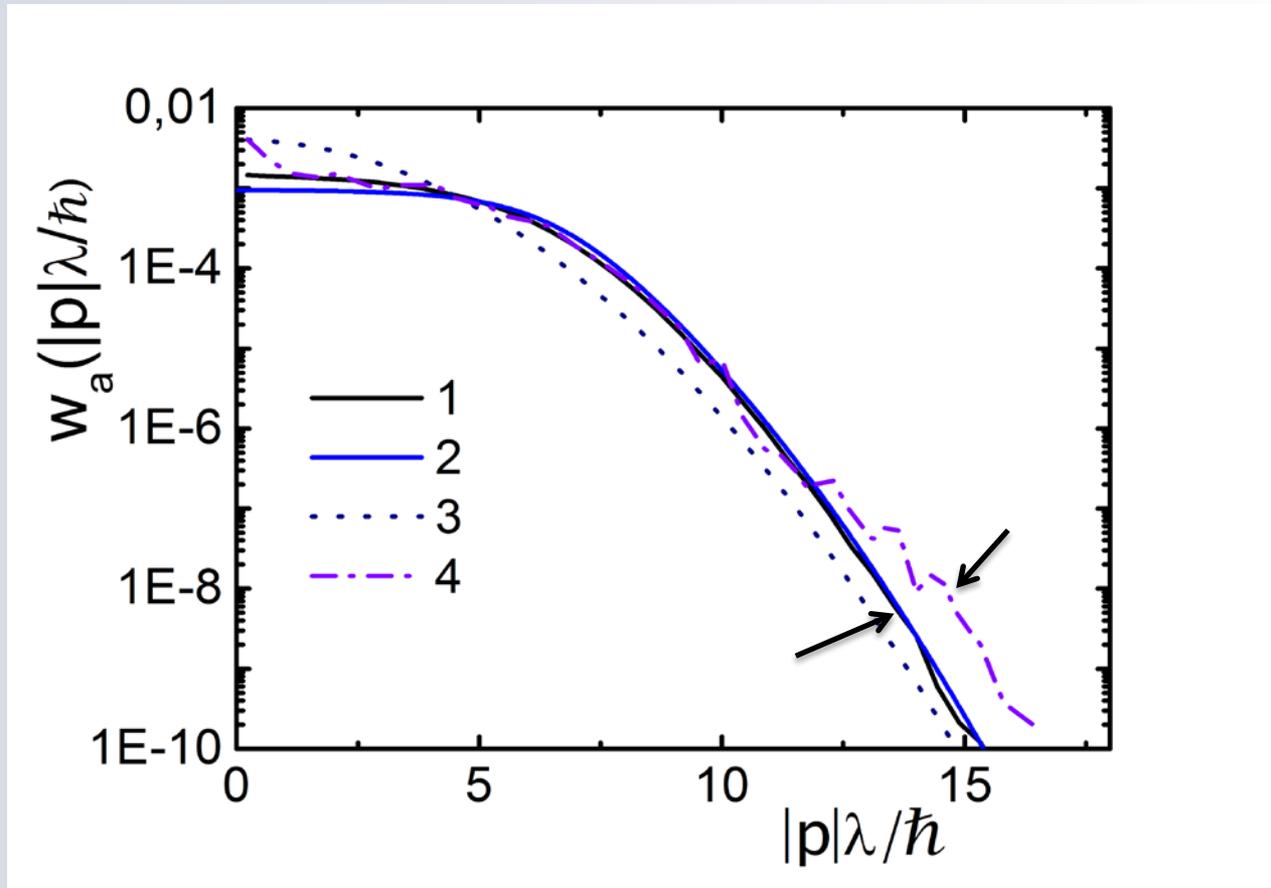
Starostin A N, Petrushevich Yu V 2016 Abstracts Scientific-Coordination Workshop on Non-Ideal Plasma Physics December 7-8, 2016, Moscow, Russia, http://www.ihed.ras.ru/npp2016/program/
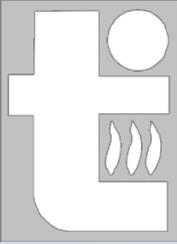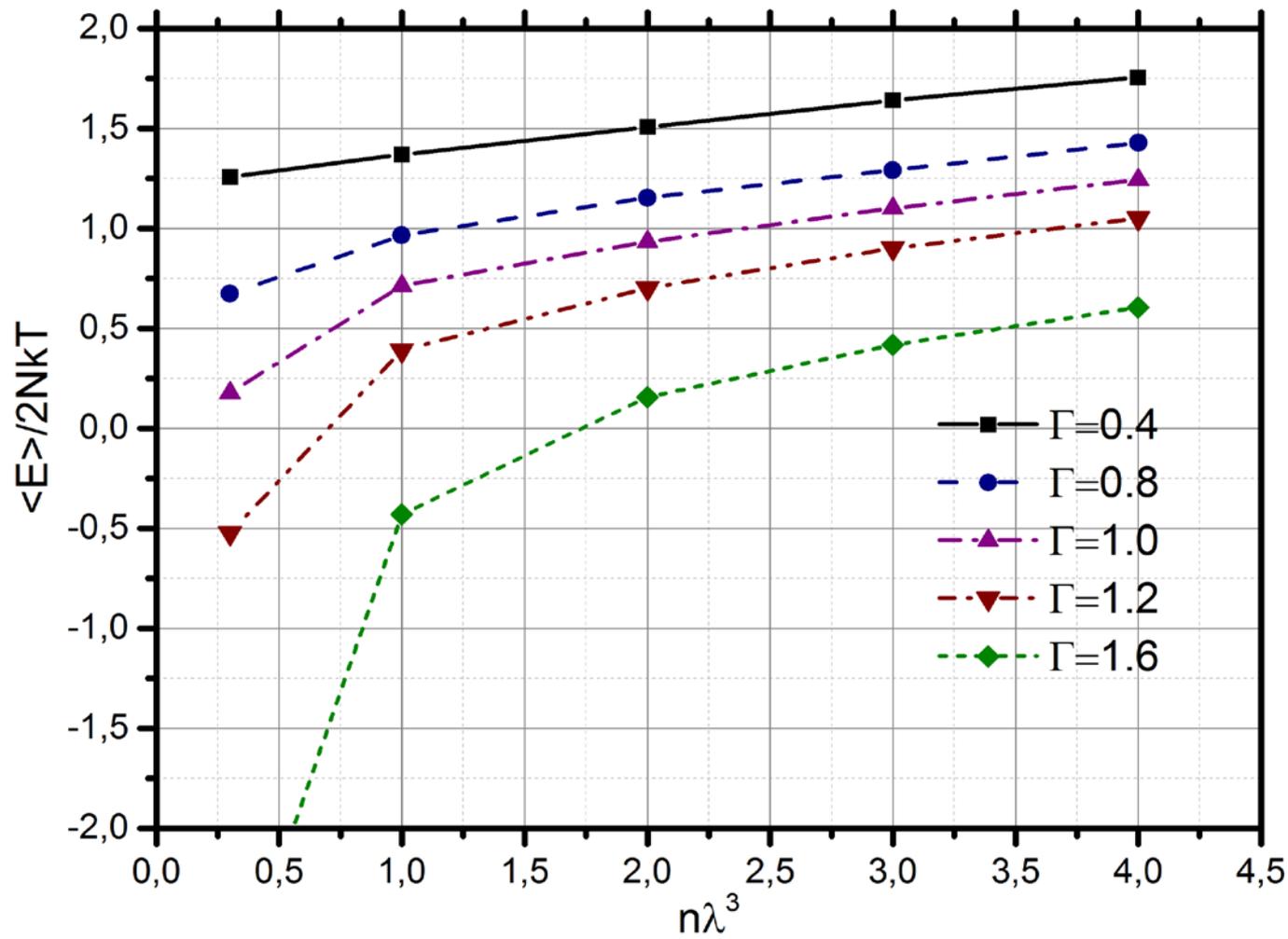
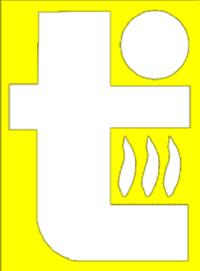# Momentum distribution of quantum uniform electronic gas

$$\Gamma = 2.5,\ \chi = 4$$

Internal energy of the two component Coulomb system of particles :

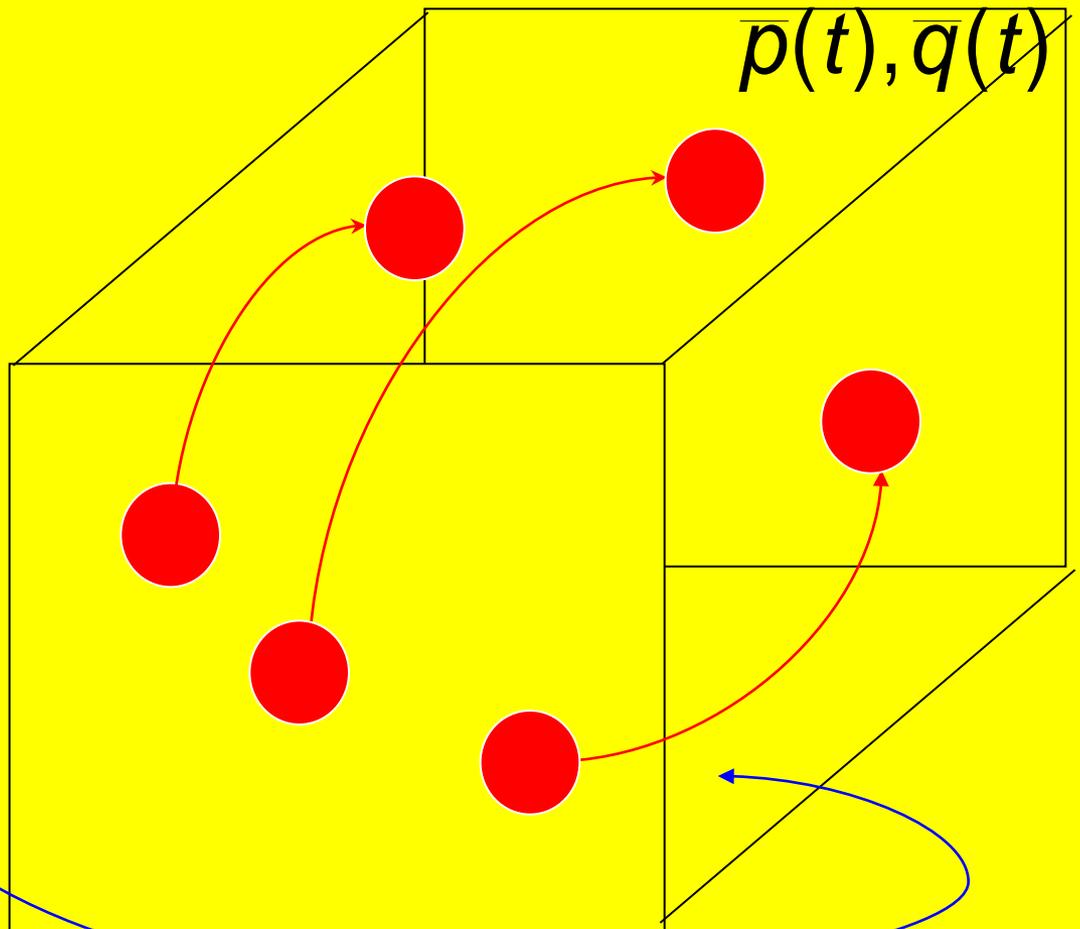$$m_h = 9m_e$$

Classical dynamics in phase space

$$W(\overline{p}(0), \overline{q}(0)) \sim \exp(-\beta H(\overline{p}(0), \overline{q}(0))$$

$$\frac{d\overline{p}}{dt} = \overline{F}(q(t))$$

$$\frac{d\overline{q}}{dt} = \frac{\overline{p}(t)}{m}$$

$$< \overline{p}(t)\overline{p}(0) >$$

$\overline{p}(t), \overline{q}(t)$

$\overline{p}(0), \overline{q}(0)$
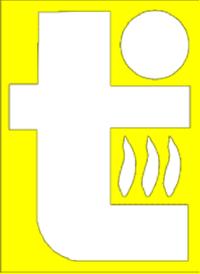
Wigner approach to quantum mechanics

$$ih\frac{\partial \Psi(\overline{Q},t)}{\partial t} = \tilde{H}\Psi(\overline{Q},t);$$

$$\Psi(\overline{Q},0) = \Psi_o(\overline{Q});$$

N-particle functions

$$\tilde{H} = \frac{h^2}{2m}\Delta + V(\overline{Q})$$

$$\rho(\overline{Q},\overline{Q}',t) = \Psi(\overline{Q},t)\Psi^*(\overline{Q}',t)$$

$$f(\overline{q},\overline{p},t) = \int \Psi(\overline{q}-\frac{\overline{\xi}}{2},t)\Psi^*(\overline{q}+\frac{\overline{\xi}}{2},t)\exp(i\frac{\overline{\xi}\overline{p}}{h})d\overline{\xi}$$

$$\overline{q} = \frac{\overline{Q}+\overline{Q}'}{2}, \overline{\xi} = \overline{Q}-\overline{Q}'$$
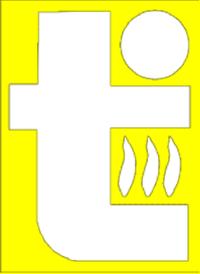
Wigner – Liouville equation

3N-dimensional vectors

$$\frac{\partial f}{\partial t} + \frac{\overline{p}}{m}\frac{\partial f}{\partial \overline{q}} + \overline{F}\frac{\partial f}{\partial \overline{q}} = \int f(\overline{p} - \overline{s})\omega(\overline{s}, \overline{q})d\overline{s}, h \to 0$$

$$\omega(\overline{s}, \overline{q}) = \frac{4}{(\pi h)^\nu h}\int V(\overline{q} - \overline{q}')Sin(\frac{2\overline{s}\overline{q}'}{h})d\overline{q}' + \overline{F}\frac{\partial \delta(\overline{s})}{\partial \overline{s}}, \overline{F} = -\nabla V$$

$$\frac{d\overline{q}}{dt} = \frac{\overline{p}}{m}, \overline{q}_t(t, \overline{p}, \overline{q}) = \overline{q}$$

$$\frac{d\overline{p}}{dt} = \overline{F}(\overline{q}), \overline{p}_t(t, \overline{p}, \overline{q}) = \overline{p}$$

$$f(\overline{p}, \overline{q}, t) = f_0(\overline{p}_0, \overline{q}_0, 0) + \int_0^t d\tau \int d\overline{s} f(\overline{p}_\tau - \overline{s}, \overline{q}_\tau, \tau)\omega(\overline{s}, \overline{q}_\tau)$$

$$f_0(\overline{q}, \overline{p}, t) = \int \Psi_0(\overline{q} - \frac{\overline{\xi}}{2}, t)\Psi_0^*(\overline{q} + \frac{\overline{\xi}}{2}, t)\exp(i\frac{\overline{\xi}\overline{p}}{h})d\overline{\xi}$$
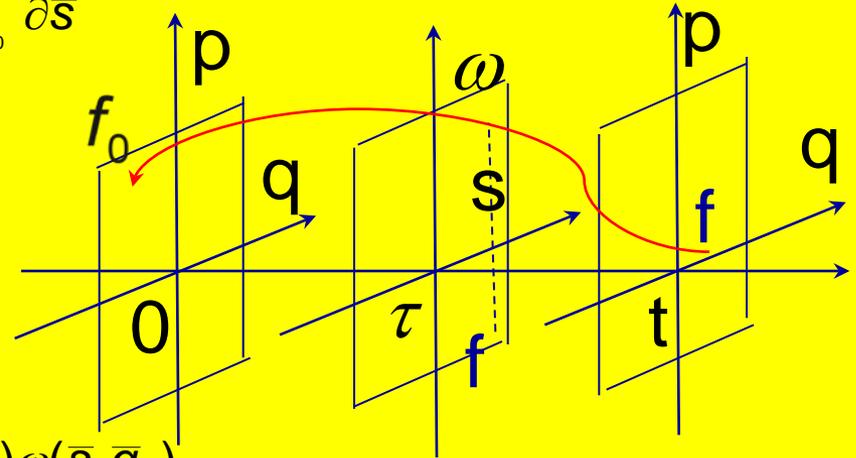
Klimontovich equation
or Tatarskii condition

Iteration series. Quantum averages.

$$f(\overline{p}, \overline{q}, t) = f_0(\overline{p}_0, \overline{q}_0, 0) + \int\limits_0^t d\tau \int d\overline{s}\, f_0(\overline{p}^\tau{}_\varsigma - \overline{s}, \overline{q}^\tau{}_\varsigma, \varsigma\mid_{\varsigma=0})\omega(\overline{s}, \overline{q}^\tau) + \ldots.$$

$$\mid \int\limits_0^t d\tau \int d\overline{s}\, f_0(\overline{p}^\tau{}_\varsigma - \overline{s}, \overline{q}^\tau{}_\varsigma, \varsigma\mid_{\varsigma=0})\omega(\overline{s}, \overline{q}^\tau)\mid \leq \frac{t^n Q`}{n!}\mid_{n=1}$$
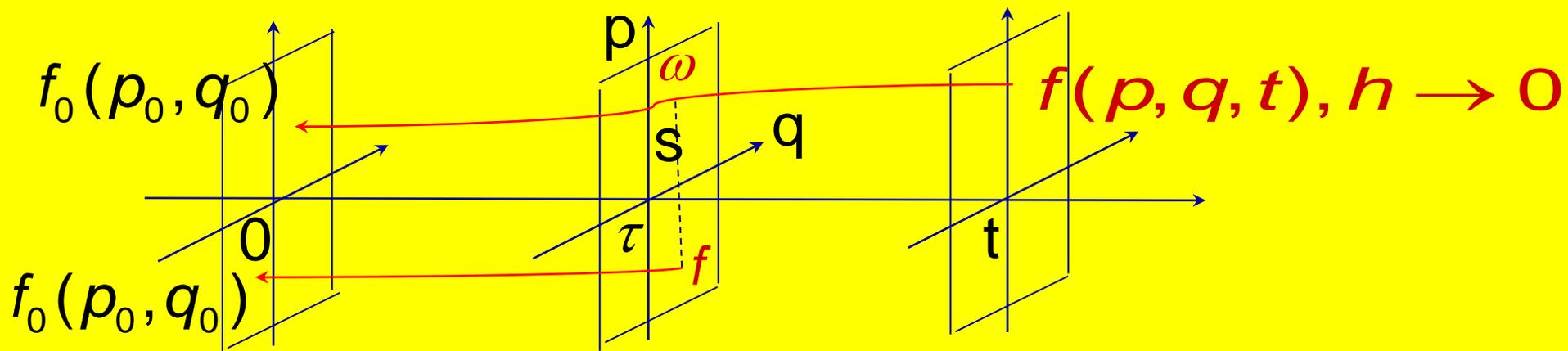
$$<\Psi_t\mid A\mid\Psi_t> = \int dp\,dq\, A(p,q) f(p,q,t)$$

$$A(p,q) = \int d\xi \exp(i\frac{p\xi}{h}) < q - \frac{\xi}{2}\mid A\mid q + \frac{\xi}{2}>$$
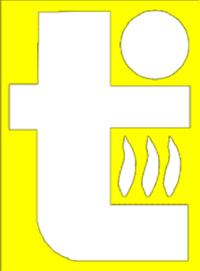
Quantum dynamics in the phase space

$$P \sim \left| W^L(\overline{p}(0), \overline{q}(0)) \right|$$

$$weight = \text{sign}\left(W^L(\overline{p}(0), \overline{q}(0)) \right)$$

$$\frac{d\overline{p}}{dt} = \overline{F}(q(t))$$

$$\frac{d\overline{q}}{dt} = \frac{\overline{p}(t)}{m}$$

Average values of quantum operator Weyl's symbol

$$< \overline{p}(t)\overline{p}(0) >$$

Virtual quantum trajectories

$\overline{p}(t), \overline{q}(t)$

Virtual classical trajectories

Random momentum jumps

$\overline{p}(0), \overline{q}(0)$
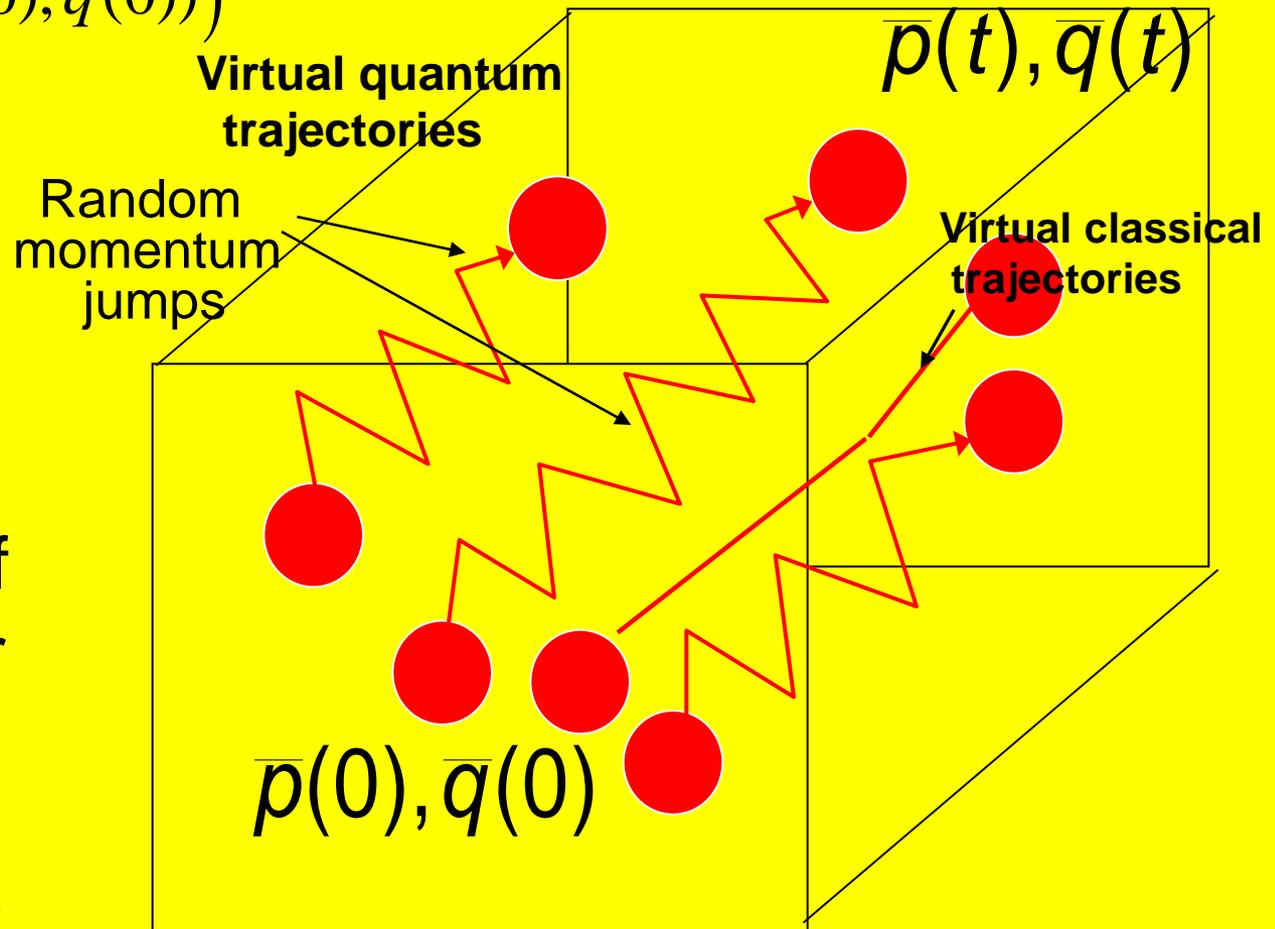
Canonical ensemble

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

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

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

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

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

$$A(p, q) = \iint d\xi \exp(-i\frac{p\xi}{h}) < q - \frac{\xi}{2} | A | q + \frac{\xi}{2} >$$

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

$$< q_1 + \frac{\xi_1}{2} | \exp(i\frac{Ht_c}{h}) | q_2 - \frac{\xi_2}{2} >< q_2 + \frac{\xi_2}{2} | \exp(-i\frac{Ht_c}{h}) | q_1 - \frac{\xi_1}{2} >$$

Integral equation

$$W(p_1, q_1; p_2, q_2; t; i\beta h) = \overline{W}(p^0{}_1, q^0{}_1; p^0{}_2, q^0{}_2; 0; i\beta h) +$$

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

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

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

$$\frac{dp_1^t}{dt} = \frac{1}{2}F(q_1^t), \, p_1^t(t, p_1, q_1) = p_1$$
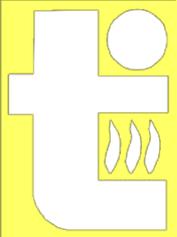
— positive time direction

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

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

— negative time direction

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

Initial conditions

$$\exp(-\frac{\beta}{2}H) = \exp(-\varepsilon H)\exp(-\varepsilon H)...\exp(-\varepsilon H), \varepsilon = \beta/2M$$

$$\exp(-\varepsilon H) = \exp(-\varepsilon K)\exp(-\varepsilon V)\exp(-\frac{\varepsilon^2[K,V]}{2})...,$$

$$\overline{W}(p_1, q_1; p_2, q_2; 0; i\beta h) \approx \iint d\overline{q}_1 d\overline{q}_2 ... d\overline{q}_M d\breve{q}_1 d\breve{q}_2 ... d\breve{q}_M *$$

$$\Psi\{p_1, q_1; p_2, q_2; \overline{q}_1, \overline{q}_2 ... \overline{q}_M; \breve{q}_1, \breve{q}_2 ... \breve{q}_M; i\beta h\},$$

$$\Psi\{p_1, q_1; p_2, q_2; \overline{q}_1, \overline{q}_2 ... \overline{q}_M; \breve{q}_1, \breve{q}_2 ... \breve{q}_M; i\beta h\} =$$

$$Z^{-1} < q_1 | \exp(-\varepsilon K) | \overline{q}_1 > \exp(-\varepsilon V(\overline{q}_1)) < \overline{q}_1 | \exp(-\varepsilon K) | \overline{q}_2 >$$

$$\exp(-\varepsilon V(\overline{q}_2))...\exp(-\varepsilon V(\overline{q}_M)) < \overline{q}_M | \exp(-\varepsilon K) | q_2 > \varphi(p_2, \overline{q}_M, \breve{q}_1) *$$

$$< q_2 | \exp(-\varepsilon K) | \breve{q}_1 > \exp(-\varepsilon V(\breve{q}_1)) < \breve{q}_1 | \exp(-\varepsilon K) | \breve{q}_2 >$$

$$\exp(-\varepsilon V(\breve{q}_2))...\exp(-\varepsilon V(\breve{q}_M)) < \breve{q}_M | \exp(-\varepsilon K) | q_1 > \varphi(p_1, \breve{q}_M, \overline{q}_1)$$

$$\varphi(p, \overline{q}, \breve{q}) = \lambda^\nu \exp(\frac{< \frac{p\lambda}{h} + i\pi \frac{\overline{q} - \breve{q}}{\lambda} | \frac{p\lambda}{h} + i\pi \frac{\overline{q} - \breve{q}}{\lambda} >}{2\pi}), \lambda^2 = \frac{2\pi h^2 \beta}{2Mm},$$
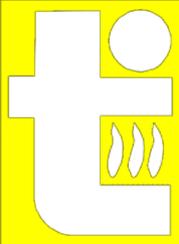
Iteration series

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

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

$$= \frac{1}{(2\pi h)^{2\nu}} \iint dp_1 dq_1 dp_2 dq_2 F(p_1 q_1) A(p_2 q_2) \overline{W}(p_1^0, q_1^0; p_2^0, q_2^0; 0; i\beta h) +$$

$$+ \frac{1}{(2\pi h)^{2\nu}} \iint dp_1 dq_1 dp_2 dq_2 F(p_1 q_1) A(p_2 q_2) \int_0^t d\tau \int ds \int d\eta \gamma(s, q_1^\tau; \eta, q_2^\tau)*$$

$$\overline{W}(p_1^\varsigma - s, q_1^\varsigma; p_2^\varsigma - \eta, q_2^\varsigma; \varsigma|_{\varsigma=0}; i\beta h) + ...$$

$$\overline{W}(p_1, q_1; p_2, q_2; 0; i\beta h) = Z^{-1} \iint d\xi_1 d\xi_2 \exp(i\frac{p_1 \xi_1}{h}) \exp(i\frac{p_2 \xi_2}{h})*$$

$$< q_1 + \frac{\xi_1}{2}|\exp(-\frac{\beta H}{2})|q_2 - \frac{\xi_2}{2} >< q_2 + \frac{\xi_2}{2}|\exp(-\frac{\beta H}{2})|q_1 - \frac{\xi_1}{2} >$$

Schematic shapshot

positive time direction

+t/2

-s

Positive backgroud

-s

$p_1 q_1$

$\bar{q}_1 \bar{q}_2 \ldots \bar{q}_M$

φ

$\exp(-\varepsilon K)$

t=0

$\exp(-\varepsilon V)$

$h \rightarrow 0$

e

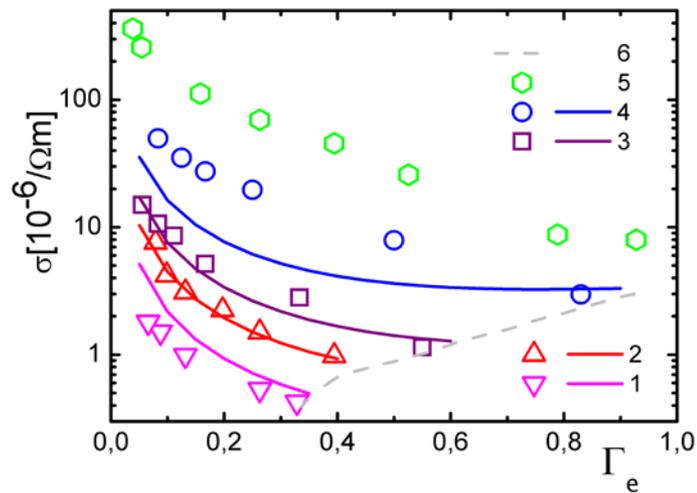$\sim \lambda$

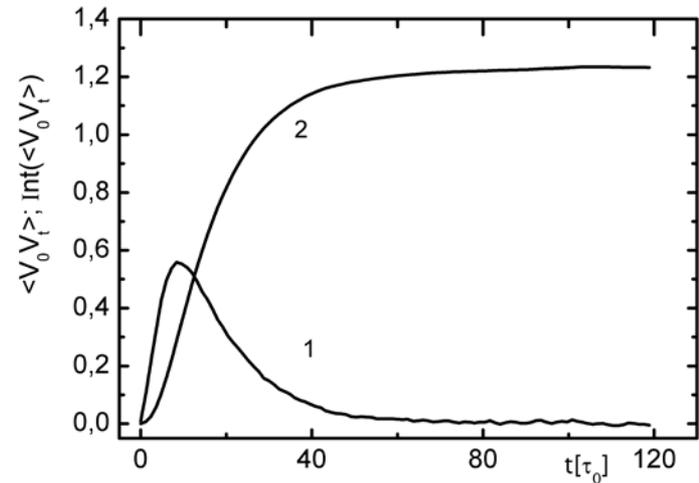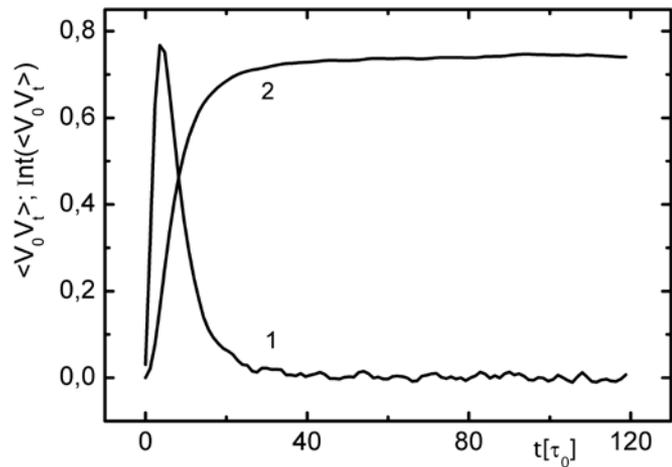$\bar{q}_1 \bar{q}_2 \ldots \bar{q}_M$

φ

$p_2 q_2$
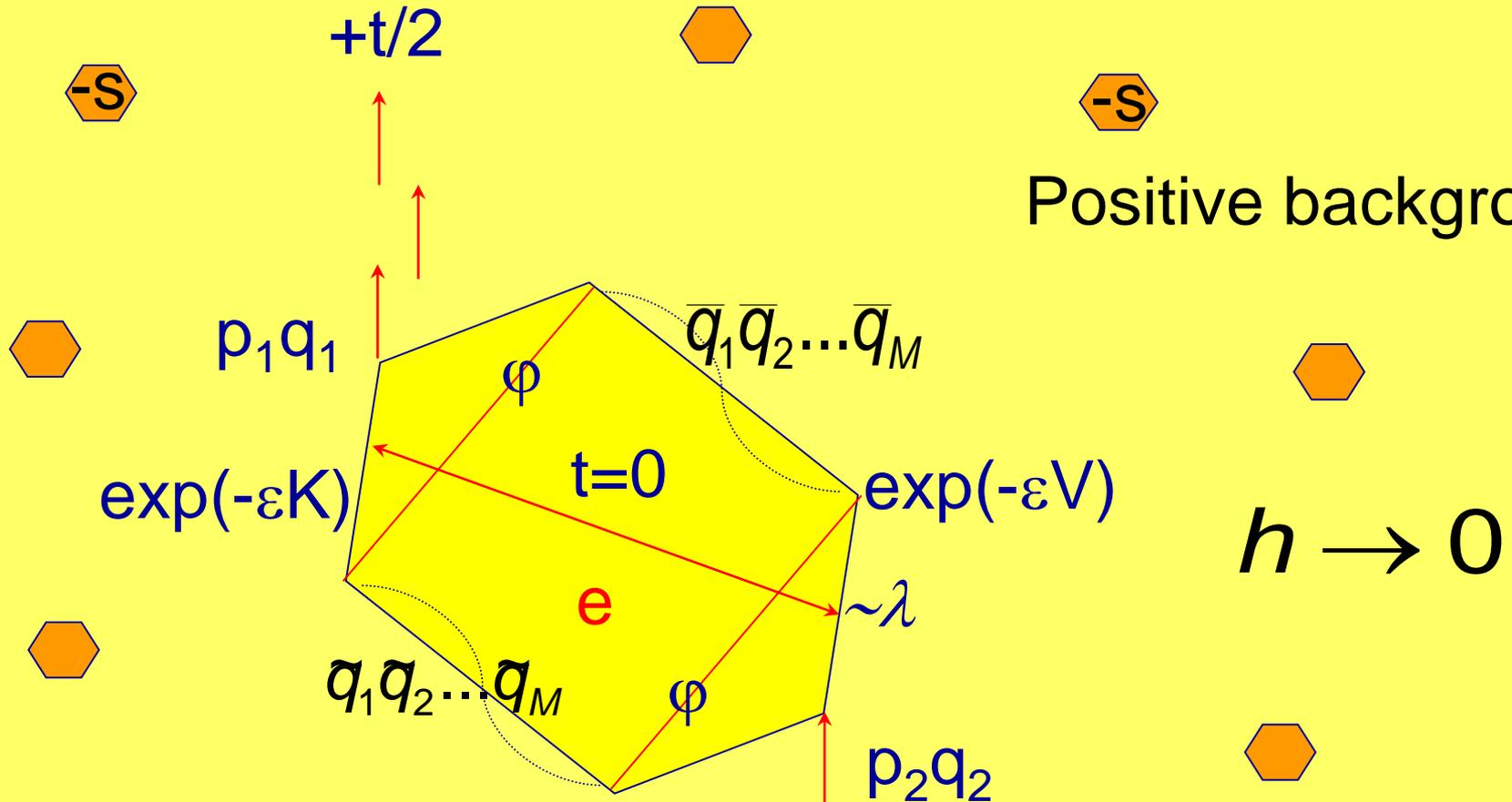
$\langle p(-t/2) p(t/2) \rangle$

-t/2

negative time direction

Electron electrical conductivity of plasma
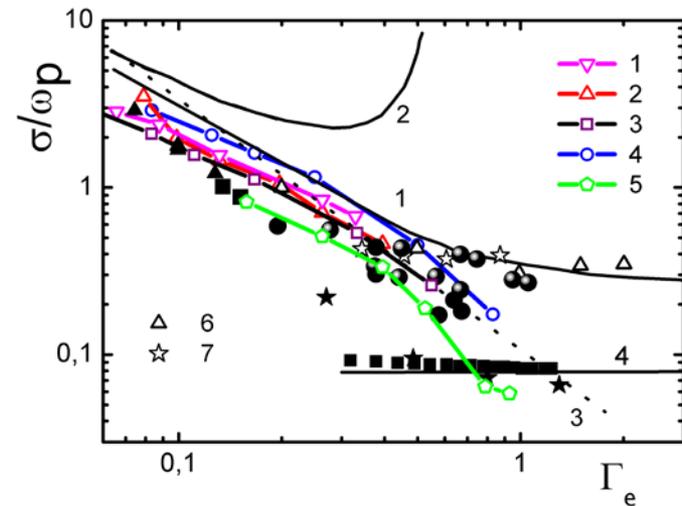
Conclusions two

• We present the new numerical approach for treatment kinetic properties of the quantun many particle systems in Wigner formulation of quantum mechanics.

• We have developed also numerical approach based on path integral formulation of quantum mechanics for treatment thermodynamic properties of strongly coupled particle systems.

• Electricall frequency conductivity has been obtained in wide density – temperature region and agree with avalable analitical and experinetal data.

Springer Series in Plasma Science and Technology
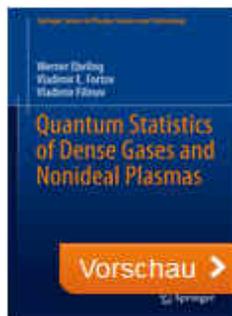
© 2017

Quantum Statistics of Dense Gases and Nonideal Plasmas

Autoren: **Ebeling**, Werner, **Fortov**, Vladimir E., **Filinov**, Vladimir

Quantum Statistics of Dense Gases and Nonideal Plasmas

Vorschau >

Authored by pioneering authors in the field

» Weitere Vorteile

Über dieses Buch   Über den Autor

The aim of this book is the pedagogical exploration of the basic principles of quantum-statistical thermodynamics as applied to various states of matter – ranging from rare gases to astrophysical matter with high-energy density. The reader will learn in this work that thermodynamics and quantum statistics are still the concepts on which even the most advanced research is operating - despite of a flood of modern concepts, classical entities like temperature, pressure, energy and entropy are shown to remain fundamental.

The physics of gases, plasmas and high-energy density matter is still a growing field and even though solids and liquids dominate our daily life, more than 99 percent of the visible Universe is in the state of gases and plasmas and the overwhelming part of matter exists at extreme conditions connected with very large energy densities, such as in the interior of stars.

This text, combining material from lectures and advanced seminars given by the authors over many decades, is a must-have introduction and reference for both newcomers and seasoned researchers alike.

Services zu diesem Buch

» Produkt Flyer herunterladen

» Online-Besprechungsexemplar lesen

» Druckfähiges Cover herunterladen
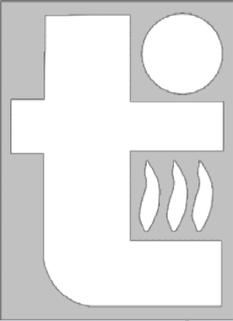
Inhaltsverzeichnis (12 Kapitel)

Thank you for attention.

Contact E-mails:

vladimir_filinov@mail.ru

Kelbg potential

$$x_{ab} = |\mathbf{r}_{ab}| / \lambda_{ab} \qquad \lambda_{ab} = 2\pi\hbar^2 \varepsilon / \mu_{ab}$$

$$\Phi^{ab}(x_{ab}, \varepsilon) = \frac{e_a e_b}{\lambda_{ab} x_{ab}} \left\{ 1 - e^{-x_{ab}^2} + \sqrt{\pi} x_{ab} \left[1 - erf(x_{ab}) \right] \right\}$$
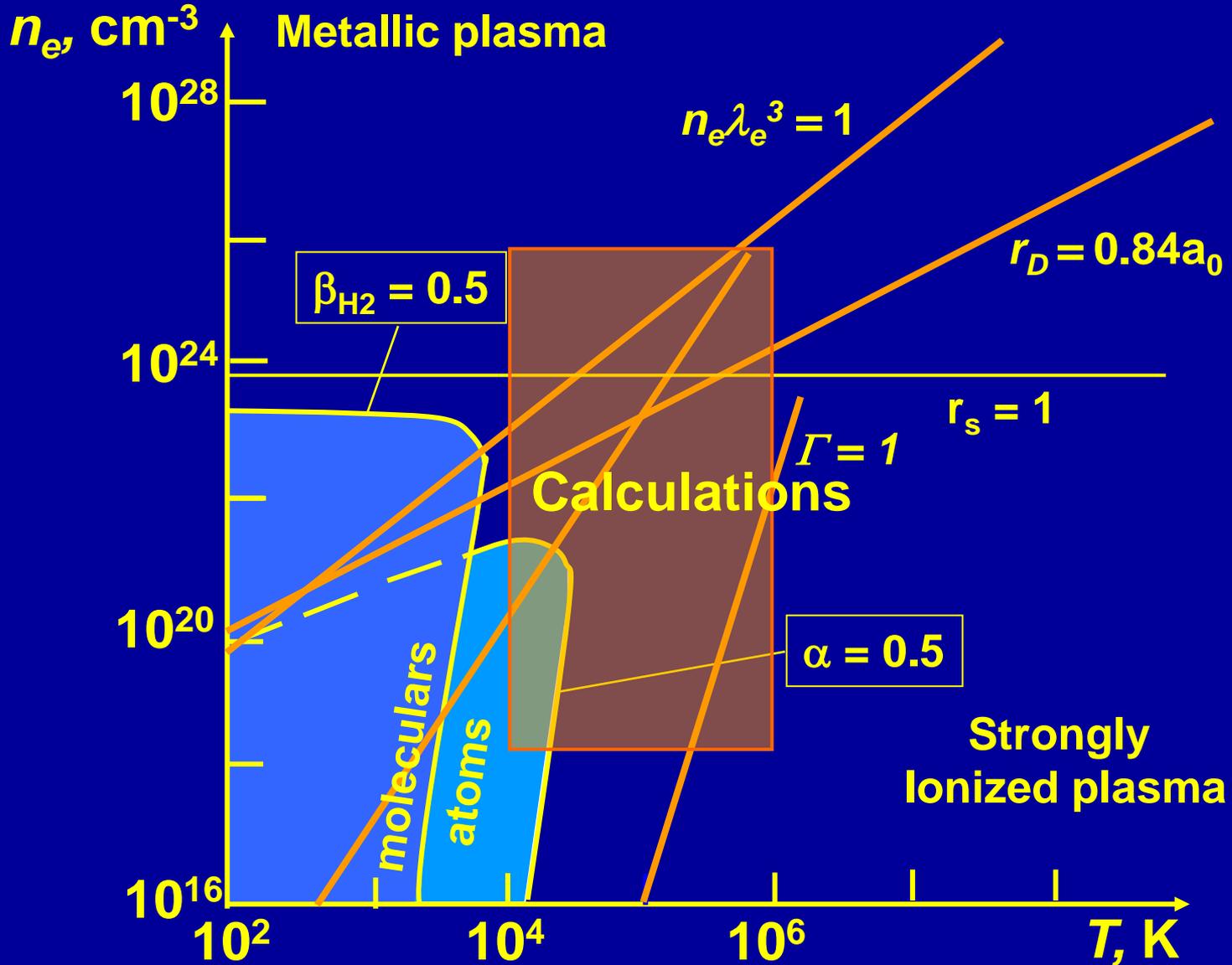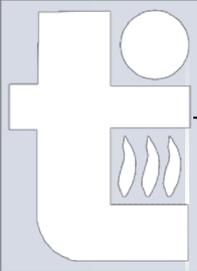
$$|\mathbf{r}_{ab}| \rightarrow 0 \qquad\qquad |\mathbf{r}_{ab}| >> \lambda_{ab}$$

$$\frac{\sqrt{\pi} e_a e_b}{\lambda_{ab}} \qquad\qquad \frac{e_a e_b}{|r_{ab}|}$$

Phase diagram

Metallic plasma

n_e, cm^{-3}

10^{28}

$n_e\lambda_e^3 = 1$

$r_D = 0.84a_0$

$\beta_{H2} = 0.5$

10^{24}

$r_s = 1$

$\Gamma = 1$

Calculations

10^{20}

moleculars

atoms

$\alpha = 0.5$

Strongly
Ionized plasma

10^{16}

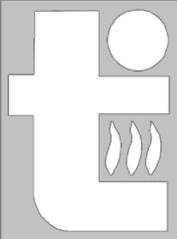10^2 10^4 10^6 T, K

Квантовая динамика кулоновских фермионов в вигнеровском представлении квантовой механики

В.С. Филинов, А.С. Ларкин

[1]*Joint Institute for High Temperatures, RAS, Moscow, Russia*
[2]*Moscow Institute for Physics and Technology, Moscow Region, Russia*
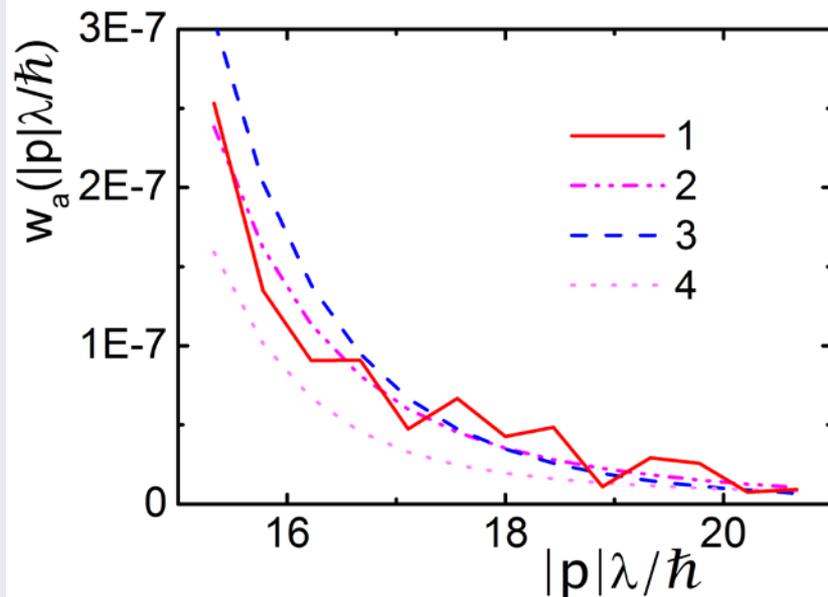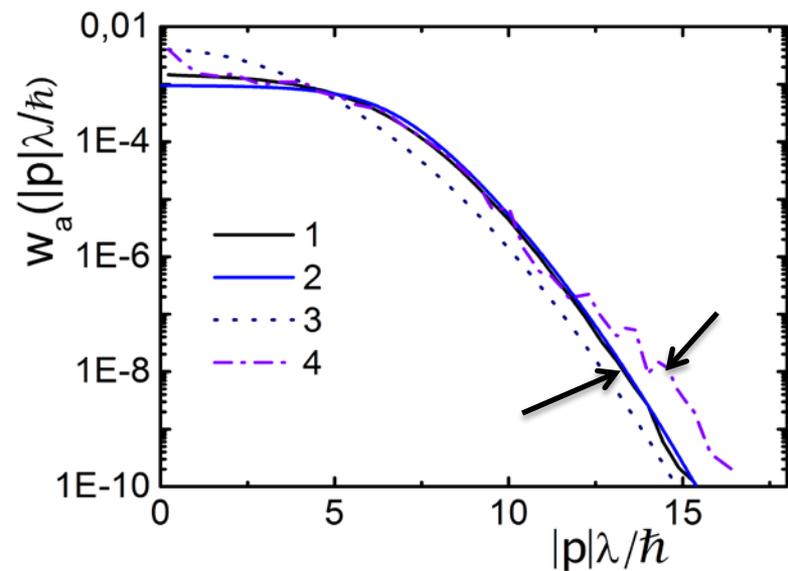
Momentum distribution

Quantum uniform electronic gas

$$\Gamma = 2.5, \chi = 4$$

Power-low approximations

$$\sim 1/p^n, n = 5,8,11$$

- **Strongly coupled systems of quantum particles**
  - Strongly correlated systems $\Gamma \geq 1$
  - Degenerated systems $Ef \sim kT$

Perturbation theories does not work
'Ab initio' numerical methods have to be used.

- **Quantum effects:**
  - Free and bound states
  - Quantum statistics
  - Interaction and uncertainty relation $\delta p \delta x \approx \hbar$

Quantum effects affect thermodynamic values, the shape of momentum and pair distribution functions
.