Theoretical Foundations of Quantum hydrodynamics for dense plasmas

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In collaboration with:

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A brief history of QHD

E. Madelung,
Z. Phys. (1927)

$$\Psi(\mathbf{R},t) = A(\mathbf{R},t)\, e^{\frac{i}{\hbar} S(\mathbf{R},t)}$$

$$i\hbar \frac{\partial \Psi(\mathbf{R},t)}{\partial t} = \hat{H}\Psi(\mathbf{R},t)$$

$$n(\mathbf{r},t) = A^2(\mathbf{r},t), \quad \text{density},$$

$$\mathbf{p}(\mathbf{r},t) = m\mathbf{v}(\mathbf{r},t) = \nabla S(\mathbf{r},t), \quad \text{momentum},$$

$$\frac{\partial n}{\partial t} + \nabla(\mathbf{v}n) = 0,$$

$$\frac{\partial \mathbf{p}}{\partial t} + \mathbf{v}\nabla\mathbf{p} = -\nabla(V+Q),$$

D. Bohm,
Phys. Rev. (1952)

"Bohm potential"

$$Q[n(\mathbf{r},t)] = -\frac{\hbar^2}{2m}\frac{\nabla^2 n^{1/2}}{n^{1/2}},$$

$$m\frac{d}{dt}\vec{v} = -\nabla(V+Q)$$

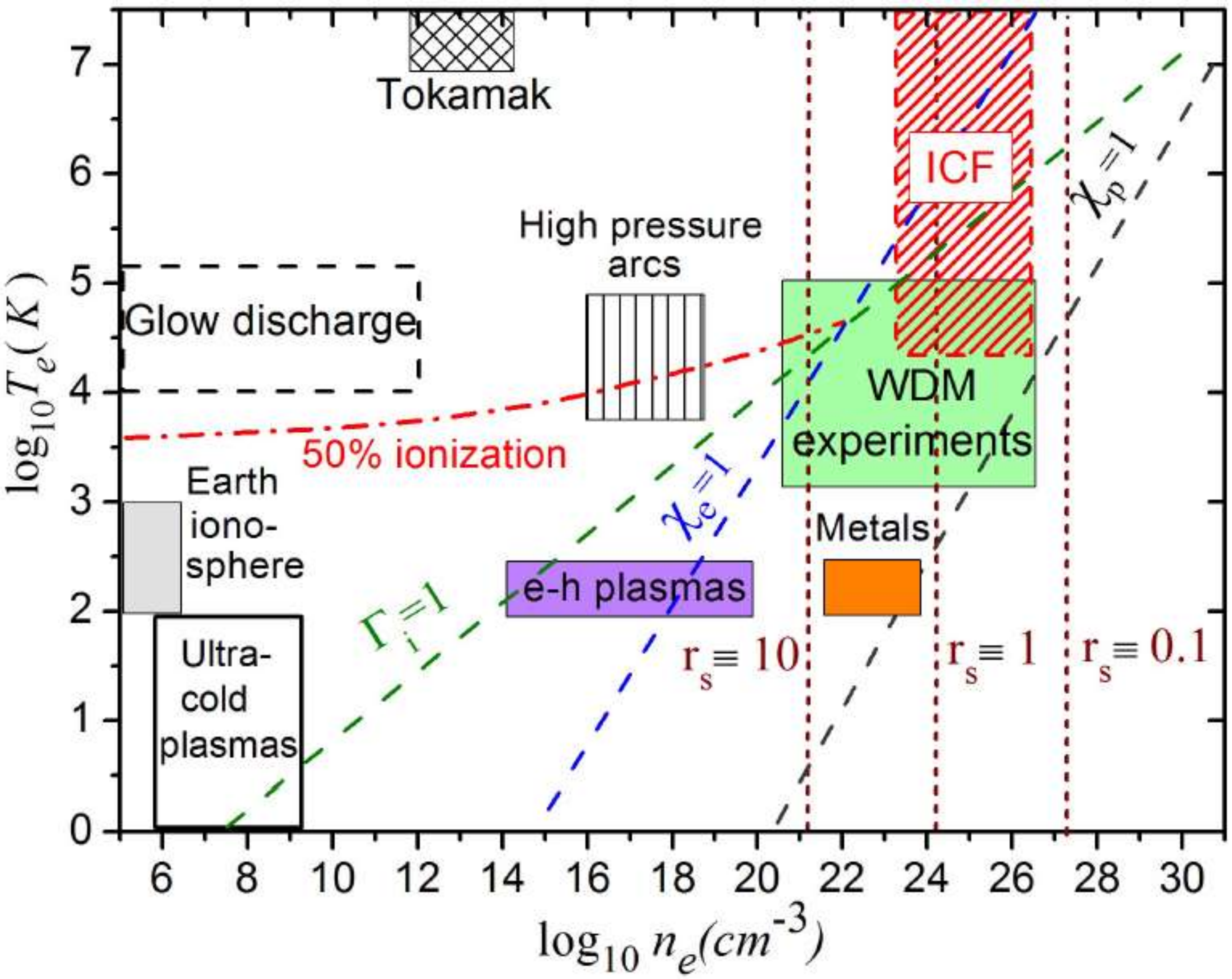
A brief history of QHD

- **Examples of quantum fluid theories**
  - Fermi liquid theory (Landau, Abrikosov...): metals, quasiparticles
  - non-Fermi liquids (Luttinger)
  - quantum spin liquids (magnetic materials)
  - superfluid theory (Bogolyubov)

Is quantum plasma a “quantum fluid” ?

What kind of distinct purely quantum features “quantum plasma fluid” has?

Parameters: $\chi_a = n_a \Lambda_a^3$, $r_s = \bar{r}/a_B$, $\Gamma_i = q_i^2/(\bar{r}_i k_B T_i)$



Different starting points:

- Field theoretical approach => connection to OFDFT
- KSDFT and Bohm trajectories based approach
- Moments of Wigner function [the most consistent with traditional hydrodynamics]

Field theoretical approach

$$H[n(\mathbf{r},t),w(\mathbf{r},t)] = E[n(\mathbf{r},t)] - \int eV_{\text{ext}} n(\mathbf{r},t)\mathrm{d}\mathbf{r} + \int \frac{m_e n(\mathbf{r},t)}{2} \left|\nabla w\left(\mathbf{r},t\right)\right|^2 \mathrm{d}\mathbf{r} + \frac{e^2}{2}\int \frac{n(\mathbf{r},t)n(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'$$

$$E[n] = E_{\text{id}}[n] + E_{\text{xc}}[n]$$

$$\mathbf{v} = -\nabla w$$

$$\frac{\delta H[n(\mathbf{r},t),w(\mathbf{r},t)]}{m_e \delta w(\mathbf{r},t)} = -\frac{\partial n(\mathbf{r},t)}{\partial t}, \qquad \frac{\delta H[n(\mathbf{r},t),w(\mathbf{r},t)]}{\delta n(\mathbf{r},t)} = m_e \frac{\partial w(\mathbf{r},t)}{\partial t}.$$

Field theoretical approach

T=0

continuity equation

$$\frac{\partial}{\partial t} n(\mathbf{r},t) = -\nabla \cdot [n(\mathbf{r},t)\,\mathbf{v}(\mathbf{r},t)],$$

momentum equation

$$m_e \frac{\partial}{\partial t}\mathbf{v}(\mathbf{r},t) + m_e [\mathbf{v}(\mathbf{r},t)\cdot\nabla]\,\mathbf{v}(\mathbf{r},t) = -\nabla\mu(\mathbf{r},t),$$

potential of generalized force

$$\mu[n(\mathbf{r},t)] = \frac{\delta E[n(\mathbf{r},t)]}{\delta n(\mathbf{r},t)} + e\varphi(\mathbf{r},t)$$

$$E[n] = E_{\rm id}[n] + E_{\rm xc}[n] \qquad \varphi(\mathbf{r},t) = e\int \frac{n(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}\mathrm{d}\mathbf{r}' - V_{\rm ext}$$

Field theoretical approach

T=0

continuity equation

$$\frac{\partial}{\partial t} n(\mathbf{r}, t) = -\nabla \cdot [n(\mathbf{r}, t) \mathbf{v}(\mathbf{r}, t)],$$

momentum equation

$$m_e \frac{\partial}{\partial t} \mathbf{v}(\mathbf{r}, t) + m_e [\mathbf{v}(\mathbf{r}, t) \cdot \nabla] \mathbf{v}(\mathbf{r}, t) = -\nabla \mu(\mathbf{r}, t),$$

potential of generalized force

$$\mu[n(\mathbf{r}, t)] = \frac{\delta E[n(\mathbf{r}, t)]}{\delta n(\mathbf{r}, t)} + e\varphi(\mathbf{r}, t)$$

$$E[n] = E_{id}[n] + E_{xc}[n] \qquad \varphi(\mathbf{r}, t) = e \int \frac{n(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' - V_{ext}$$

In the grand canonical ensemble

$$\left\langle \frac{\delta E}{\delta n} \right\rangle = \frac{\delta \Omega}{\delta n}$$

grand potential

$$\Omega[n(\mathbf{r})] = F[n(\mathbf{r})] - \mu_0 N$$

$$\mu[n(\mathbf{r}, t), T] + \mu_0 = \frac{\delta F[n(\mathbf{r}, t)]}{\delta n(\mathbf{r}, t)} + e\varphi(\mathbf{r}, t)$$

$$F = F_{id} + F_{xc}$$

Explicit introduction of temperature

Field theoretical approach

(I) For an equilibrium density profile (that is current free), the Euler-Lagrange equation underlying OF-DFT follows

$$\frac{\delta F[n_0(\mathbf{r})]}{\delta n_0(\mathbf{r})} + e\varphi_0(\mathbf{r}) = \mu_0$$

$$\frac{\delta F[n(\mathbf{r},t)]}{\delta n(\mathbf{r},t)} = ?$$

Field theoretical approach

(II) The equilibrium system is subject to an external perturbation

$$n(\mathbf{r},t) = n_0(\mathbf{r}) + n_1(\mathbf{r},t) \quad w(\mathbf{r},t) = w_1(\mathbf{r},t) \quad \varphi(\mathbf{r},t) = \varphi_0(\mathbf{r}) + \varphi_1(\mathbf{r},t)$$

$$\frac{\delta F[n]}{\delta n(\mathbf{r})} = \left.\frac{\delta F[n]}{\delta n(\mathbf{r})}\right|_{\mathrm{n=n_0}} + \int \mathrm{d}\mathbf{r}' \left.\frac{\delta^2 F[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}')}\right|_{\mathrm{n=n_0}} n_1(\mathbf{r}') + \dots.$$

⇒ **QHD equations**

Field theoretical approach

(II) The equilibrium system is subject to an external perturbation

$$n(\mathbf{r},t) = n_0(\mathbf{r}) + n_1(\mathbf{r},t) \quad w(\mathbf{r},t) = w_1(\mathbf{r},t) \quad \varphi(\mathbf{r},t) = \varphi_0(\mathbf{r}) + \varphi_1(\mathbf{r},t)$$

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⇒ **QHD equations**

The electronic polarization function $\Pi^{-1}_{\mathrm{QHD}}(k,\omega) = e\tilde{\varphi}_1/\tilde{n}_1$

$$\Pi^{-1}_{\mathrm{QHD}}(k,\omega) = \frac{m_e\omega^2}{n_0 k^2} - \mathfrak{F}\left[\left.\frac{\delta^2 F[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t)}\right|_{\mathrm{n=n_0}}\right]$$

↑

?

Field theoretical approach

(II) The equilibrium system is subject to an external perturbation

$$n(\mathbf{r},t) = n_0(\mathbf{r}) + n_1(\mathbf{r},t) \quad w(\mathbf{r},t) = w_1(\mathbf{r},t) \quad \varphi(\mathbf{r},t) = \varphi_0(\mathbf{r}) + \varphi_1(\mathbf{r},t)$$

$$\frac{\delta F[n]}{\delta n(\mathbf{r})} = \frac{\delta F[n]}{\delta n(\mathbf{r})}\bigg|_{\mathrm{n=n_0}} + \int \mathrm{d}\mathbf{r}' \frac{\delta^2 F[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}')}\bigg|_{\mathrm{n=n_0}} n_1(\mathbf{r}') + \ldots . \Longrightarrow$$ **QHD equations**

The electronic polarization function $\Pi^{-1}_{\mathrm{QHD}}(k,\omega) = e\tilde{\varphi}_1/\tilde{n}_1$

$$\Pi^{-1}_{\mathrm{QHD}}(k,\omega) = \frac{m_e\omega^2}{n_0 k^2} - \mathfrak{F}\left[\frac{\delta^2 F[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t)}\bigg|_{\mathrm{n=n_0}}\right]$$

↓ ↑

The idea is $\Pi_{\mathrm{QHD}}(k,\omega) \equiv \Pi_{\mathrm{LR}}(k,\omega)$

?

$\Pi_{\mathrm{LR}}(k,\omega)$ is linear response theory result

(II) The equilibrium system is subject to an external perturbation

$$n(\mathbf{r},t) = n_0(\mathbf{r}) + n_1(\mathbf{r},t) \quad w(\mathbf{r},t) = w_1(\mathbf{r},t) \quad \varphi(\mathbf{r},t) = \varphi_0(\mathbf{r}) + \varphi_1(\mathbf{r},t)$$

$$\frac{\delta F[n]}{\delta n(\mathbf{r})} = \left.\frac{\delta F[n]}{\delta n(\mathbf{r})}\right|_{\mathrm{n=n_0}} + \int d\mathbf{r}' \left.\frac{\delta^2 F[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}')}\right|_{\mathrm{n=n_0}} n_1(\mathbf{r}') + \dots$$

→ **QHD equations**

The electronic polarization function $\Pi^{-1}_{\mathrm{QHD}}(k,\omega) = e\tilde{\varphi}_1/\tilde{n}_1$

$$\Pi^{-1}_{\mathrm{QHD}}(k,\omega) = \frac{m_e\omega^2}{n_0 k^2} - \mathfrak{F}\left[\left.\frac{\delta^2 F[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t)}\right|_{\mathrm{n=n_0}}\right]$$

↓ ↑ **?**

The idea is

$$\Pi_{\mathrm{QHD}}(k,\omega) \equiv \Pi_{\mathrm{LR}}(k,\omega)$$

$\Pi_{\mathrm{LR}}(k,\omega)$ is the linear response theory result

↓

$$-\mathfrak{F}\left[\left.\frac{\delta^2 F_{\mathrm{id}}}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t)}\right|_{\mathrm{n=n_0}}\right] = \frac{1}{\Pi_{\mathrm{RPA}}(k,\omega)} - \frac{1}{\Pi^0(\omega)}$$

$$\mathfrak{F}\left[\left.\frac{\delta^2 F_{\mathrm{xc}}[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t)}\right|_{\mathrm{n=n_0}}\right] = -\frac{4\pi e^2}{k^2} G(k,\omega)$$

Π_{RPA} corresponds to random phase approximation

$G(k,\omega)$ is the dynamical local field correction

Field theoretical approach

(I) For an equilibrium density profile (that is current free), the Euler-Lagrange equation underlying OF-DFT follows

$$\frac{\delta F[n_0(\mathbf{r})]}{\delta n_0(\mathbf{r})} + e\varphi_0(\mathbf{r}) = \mu_0$$

(II) The equilibrium system is subject to an external perturbation

$$n(\mathbf{r},t) = n_0(\mathbf{r}) + n_1(\mathbf{r},t) \quad w(\mathbf{r},t) = w_1(\mathbf{r},t) \quad \varphi(\mathbf{r},t) = \varphi_0(\mathbf{r}) + \varphi_1(\mathbf{r},t)$$

$$-\mathfrak{F}\left[\frac{\delta^2 F_{\mathrm{id}}}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t)}\bigg|_{\mathrm{n=n_0}}\right] = \frac{1}{\Pi_{\mathrm{RPA}}(k,\omega)} - \frac{1}{\Pi^0(\omega)}$$

$$\mathfrak{F}\left[\frac{\delta^2 F_{\mathrm{xc}}[n]}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t)}\bigg|_{\mathrm{n=n_0}}\right] = -\frac{4\pi e^2}{k^2}G(k,\omega)$$

$$\Pi^0(\omega) \equiv \lim_{k\to 0}\Pi_{\mathrm{RPA}}(k,\omega) = \frac{k^2}{\omega^2}\frac{n_0}{m_e}$$

Zh. Moldabekov et al., *Theoretical foundations of quantum hydrodynamics for plasmas*. POP **25**, 031903 (2018)

Field theoretical approach

For application *G* from other methods can be used

$$\mathfrak{F}\left[\frac{\delta^2 F_{\mathrm{xc}}}{\delta n(\mathbf{r})\delta n(\mathbf{r}')}\bigg|_{\mathrm{n=n_0}}\right] = -\tilde{u}(k)G(k,\omega)$$

For example:

(I) quantum Monte-Carlo simulations data based parametrization **[Dornheim et al 2019, Corradini 1998]**

(II) dynamical collision frequency **[Reinholz et al., 2000]**

(III) STLS approximation **[Singwi 1968, Tanaka 1986]**

...

Results for the Bohm potential: Gradient expansion

$$-\mathfrak{F}\left[\frac{\delta^2 F_{\rm id}}{\delta n(\mathbf{r},t)\delta n(\mathbf{r}',t)}\bigg|_{\rm n=n_0}\right] = \frac{1}{\Pi_{\rm RPA}(k,\omega)} - \frac{1}{\Pi^0(\omega)}$$

$$F_{\rm id}[n] = F_0[n(\mathbf{r},t)] + \int \mathbf{dr}\, a_2\,[n(\mathbf{r},t)]\,|\,\nabla\tilde{n}(\mathbf{r},t)\,|^2$$

The electronic pressure term in LDA

Gives the Bohm potential

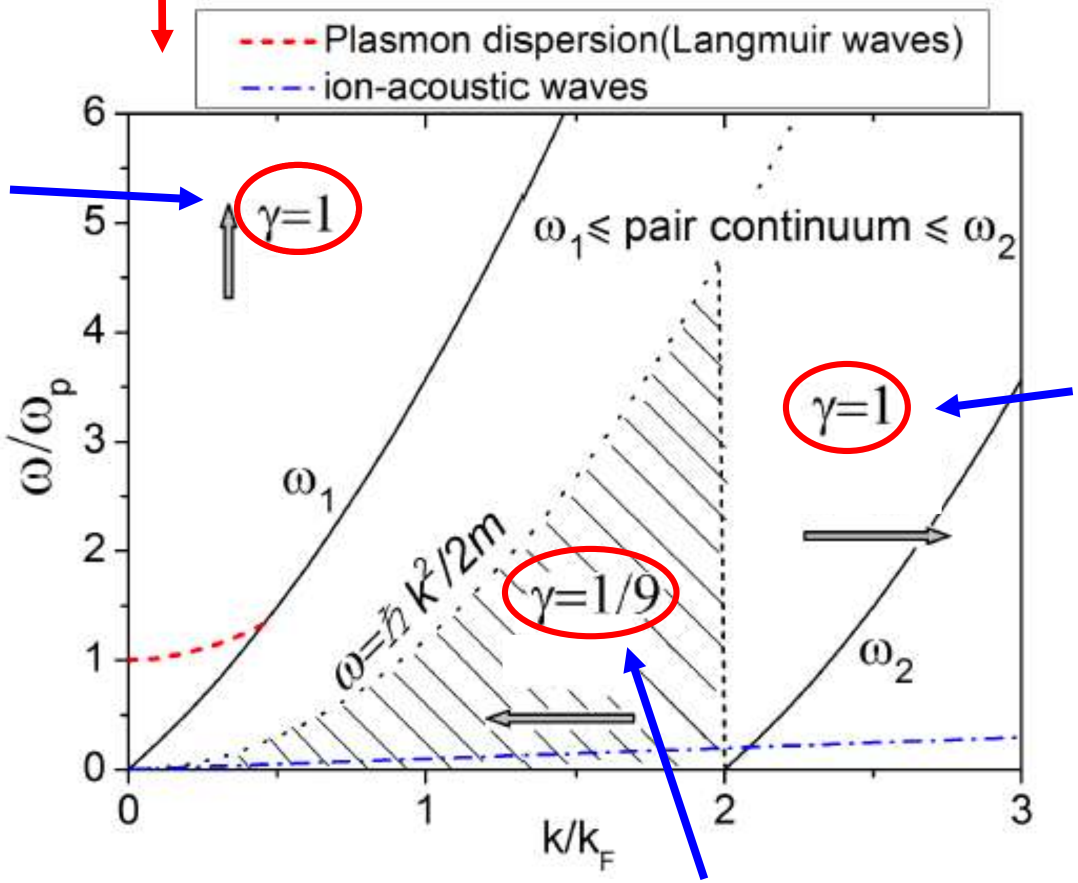
the Bohm potential

$$V_B = \frac{\delta}{\delta n}\int \mathbf{dr}\, a_2\,[n]\,|\,\nabla n(\mathbf{r})\,|^2 = \gamma\,\frac{\hbar^2}{8m}\left(\left|\frac{\nabla n}{n}\right|^2 - 2\frac{\nabla^2 n}{n}\right)$$

Zh. Moldabekov et al., *Theoretical foundations of quantum hydrodynamics for plasmas*. Physics of Plasmas **25**, 031903 (2018)

$$V_B = \gamma \frac{\hbar^2}{8m}\left(\left|\frac{\nabla n}{n}\right|^2 - 2\frac{\nabla^2 n}{n}\right)$$

High frequency limit [independent from temperature]



Single electron limit [independent from temperature]

High electron density or long wave length case $\theta \ll 1$
[in general is the function of temperature]

$$\gamma = -\frac{2}{9}\frac{I_{-3/2}(\eta)}{I^2_{-1/2}(\eta)}\theta^{-3/2}$$

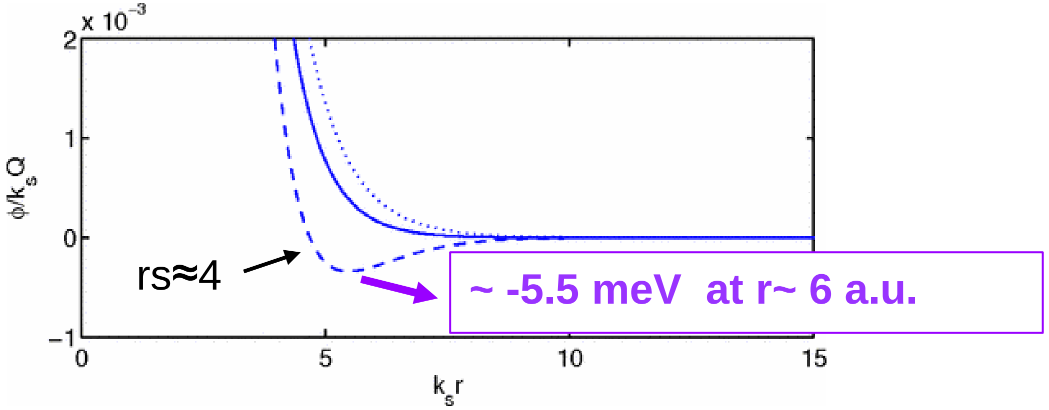
Zh. Moldabekov, M. Bonitz, and T. Ramazanov. *Theoretical foundations of quantum hydrodynamics for plasmas*. Physics of Plasmas **25**, 031903 (2018)

Field theoretical approach

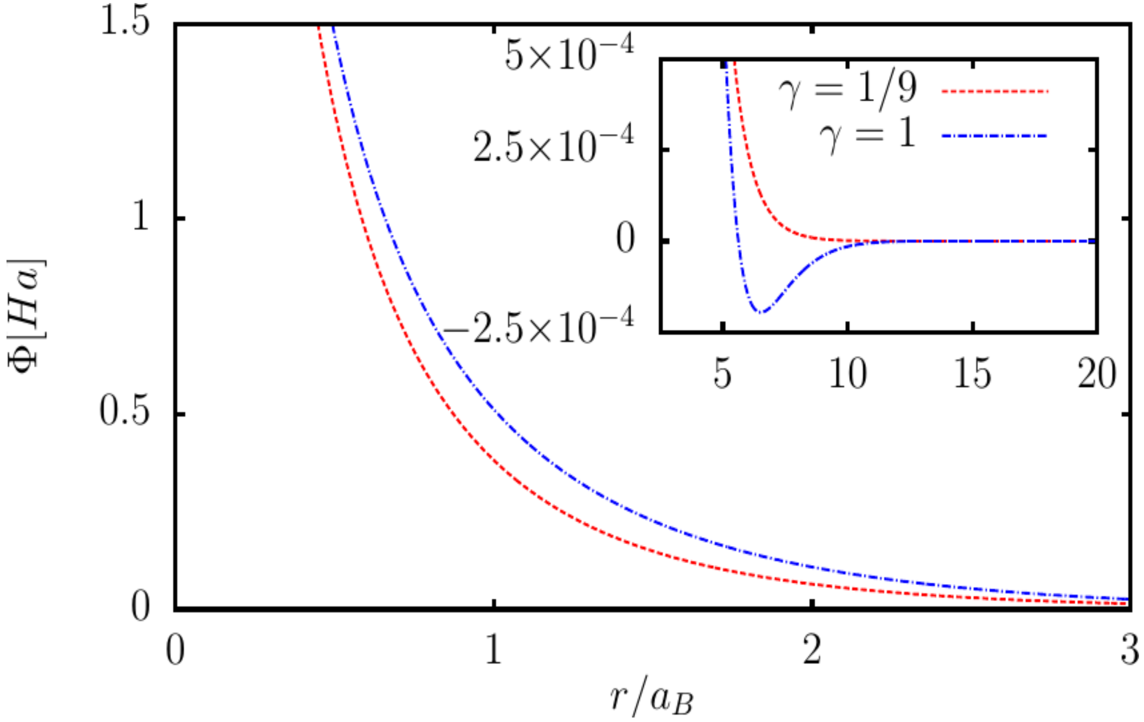
Example:

Incorrect prediction of novel mechanism for ion-ion attraction in fully ionized plasma

P. K. Shukla and B. Eliasson
Phys. Rev. Lett. 108, 165007 (2012)

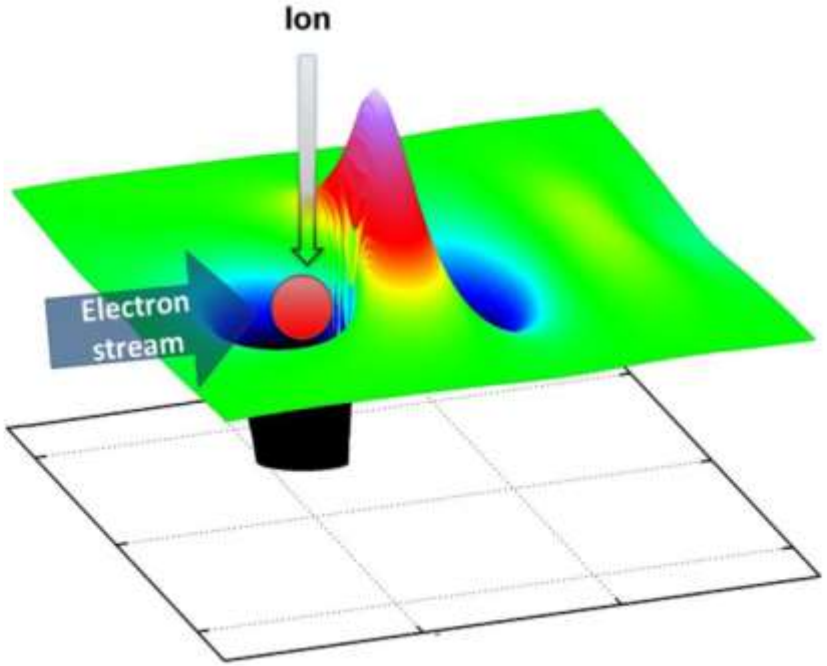


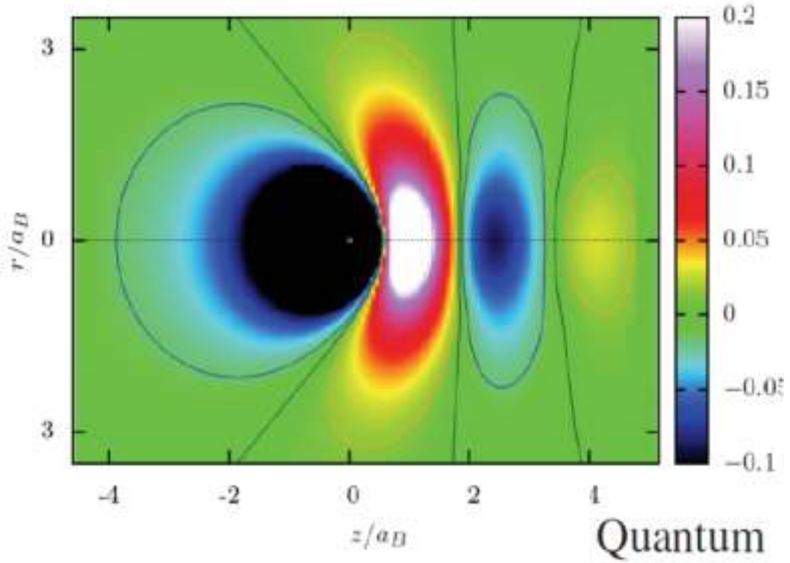
Incorrect prediction of novel mechanism
for ion-ion attraction is explained

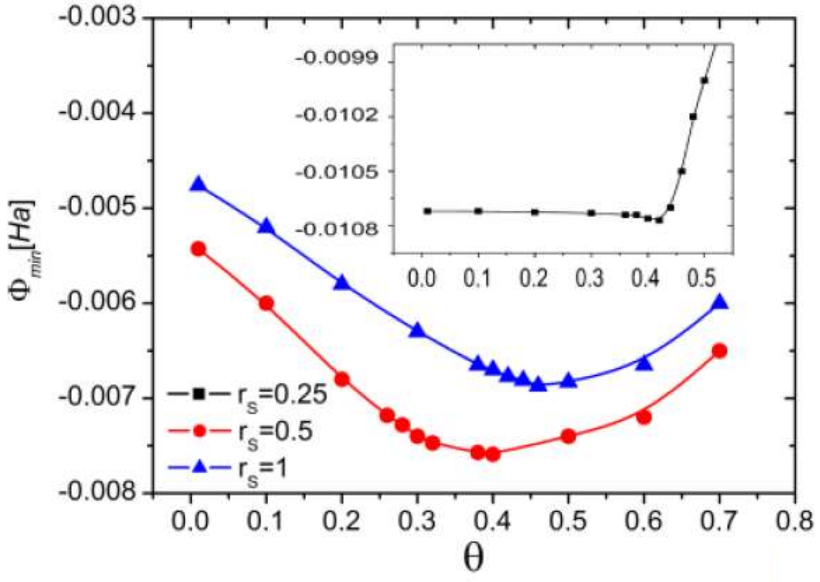


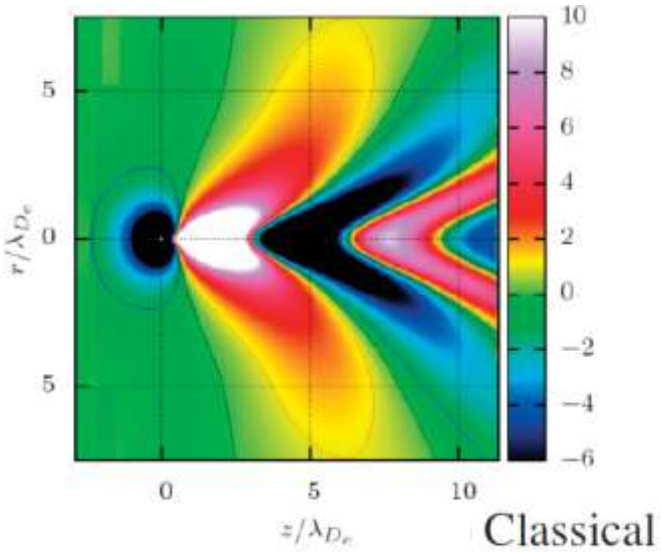
Zh. Moldabekov et al., *Theoretical foundations of quantum hydrodynamics for plasmas*. POP **25**, 031903 (2018)

The example of quantum non-locality effect









KSDFT and Bohm trajectories based approach

KSDFT and Bohm trajectories based approach

$$\phi_i(\mathbf{r},t) = A_i(\mathbf{r},t)e^{\frac{i}{\hbar}S_i(\mathbf{r},t)}$$

$$i = 1\ldots N \qquad n_i = A_i^2$$

$$\mathbf{p}_i = \nabla S_i$$

$$\frac{\partial n_i}{\partial t} + \nabla\cdot(\mathbf{v}_i n_i) = 0,$$

$$\frac{\partial \mathbf{p}_i}{\partial t} + (\mathbf{v}_i\cdot\nabla)\mathbf{p}_i = -\nabla(U_{\rm tot}[n] + V^{\rm xc}[n] + Q_i)$$

$$Q_i(\mathbf{r}) = -\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{n_i(\mathbf{r})}}{\sqrt{n_i(\mathbf{r})}},$$

M. Bonitz, Z.A. Moldabekov, T. Ramazanov, Phys. Plasmas **26**, 090601 (2019);

KSDFT and Bohm trajectories based approach

$$\overline{n}(\mathbf{r},t) = \frac{1}{N}\sum_{i=1}^{\infty} f_i^{\mathrm{eq}}\, n_i(\mathbf{r},t)\,,$$

$$\overline{\mathbf{p}}(\mathbf{r},t) = \frac{1}{N}\sum_{i=1}^{\infty} f_i^{\mathrm{eq}}\, \mathbf{p}_i(\mathbf{r},t)\,,$$

$$\overline{Q}(\mathbf{r},t) = -\frac{\hbar^2}{2mN}\sum_{i=1}^{\infty} f_i^{\mathrm{eq}}\, \frac{\nabla^2\sqrt{n_i(\mathbf{r})}}{\sqrt{n_i(\mathbf{r})}}$$

$$n_i = \overline{n} + \delta n_i$$

$$\mathbf{p}_i = \overline{\mathbf{p}} + \delta\mathbf{p}_i$$

$$A_i = \overline{A} + \delta A_i$$

$$\overline{a_i b_i} = \overline{a}\cdot\overline{b} + \overline{\delta a_i \cdot \delta b_i}$$

M. Bonitz, Z.A. Moldabekov, T. Ramazanov, Phys. Plasmas **26**, 090601 (2019);

KSDFT and Bohm trajectories based approach

$$\frac{\partial \bar{n}}{\partial t} + \frac{1}{m}\nabla(\bar{\mathbf{p}}\cdot\bar{n}) = -\frac{1}{m}\nabla\,\overline{\delta\mathbf{p}_i\delta n_i},$$

$$\frac{\partial \bar{\mathbf{p}}}{\partial t} + \frac{1}{m}\bar{\mathbf{p}}\cdot\mathrm{div}\bar{\mathbf{p}} = -\nabla\left(U^{\mathrm{H}}_{F0} + \bar{\mathrm{Q}}\right) - \frac{1}{m}\overline{\delta\mathbf{p}_i\mathrm{div}\delta\mathbf{p}_i}$$

$$\bar{\mathrm{Q}} = -\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\bar{n}}}{\sqrt{\bar{n}}} + Q^{\Delta},$$

$$Q^{\Delta} \approx \frac{\hbar^2}{2m\bar{n}}\overline{\delta A_i\cdot\nabla^2\delta A_i} + O\left(\left(\frac{\delta A_i}{\bar{A}}\right)^2\right).$$

$$\frac{1}{m}\overline{\delta p_{i\alpha}\partial_\beta\delta p_{i\beta}} = \frac{1}{2m}\partial_\alpha\overline{\delta p^2_{i\alpha}} + \frac{1}{m}\partial_\gamma\overline{\delta p_{i\alpha}\delta p_{i\gamma}}, \quad \gamma \neq \alpha,$$

$$= \frac{1}{3}\partial_\alpha\overline{E_{\mathrm{kin}}} + \frac{1}{\bar{n}}\partial_\gamma\bar{\sigma}_{\alpha\gamma},$$

$$\approx \frac{1}{5}\partial_\alpha\overline{E_{\mathrm{F}}}, \quad \text{ideal Fermi gas, } T = 0.$$

M. Bonitz, Z.A. Moldabekov, T. Ramazanov, Phys. Plasmas **26**, 090601 (2019);

Are there additional restrictions due to strong ionic coupling?

Now we consider two-component plasma with *Γ >1*

The coupling parameter of the ions

$$\Gamma = Q_i^2/(ak_BT_i)$$

Ion-ion interaction in the medium of quantum electrons

$$\Phi(\mathbf{r}_{j'},\mathbf{r}_j) = \frac{Z^2e^2}{|\mathbf{r}_{j'}-\mathbf{r}_j|} + \int \frac{\mathrm{d}^3k}{(2\pi)^3}\,|\tilde{\varphi}_{\mathrm{ei}}(\mathbf{k})|^2\,\chi_e(\mathbf{k})\;e^{i\mathbf{k}\cdot(\mathbf{r}_{j'}-\mathbf{r}_j)}$$

$$\chi_e^{-1}(\mathbf{k},\omega) = \chi_0^{-1}(\mathbf{k},\omega) + \frac{4\pi e^2}{k^2}\left[G(\mathbf{k},\omega)-1\right]$$

(I) (QMC) quantum Monte-Carlo simulations data based parameterization:

$$G(k) = Ck^2 + \frac{Bk^2}{\tilde{g}+k^2} + \tilde{\alpha}k^4\exp\left(-\tilde{\beta}k^2\right)$$

[Corradini et al, 1998]

(II) STLS approximation:

$$G^{\mathrm{STLS}}\left(\left[S^{\mathrm{STLS}}\right],\mathbf{k},\omega=0\right) = -\frac{1}{n}\int\frac{\mathrm{d}\mathbf{k}'}{(2\pi)^3}\frac{\mathbf{k}\cdot\mathbf{k}'}{k'^2}\left[S^{\mathrm{STLS}}(\mathbf{k}-\mathbf{k}')-1\right]$$

$$S^{\mathrm{STLS}}\left(\left[G^{\mathrm{STLS}}\right],\mathbf{k}\right) = -\frac{1}{\beta n}\sum_{l=-\infty}^{\infty}\frac{\chi_0(\mathbf{k},z_l)}{1+\frac{4\pi e^2}{k^2}\left[G^{\mathrm{STLS}}(\mathbf{k},0)-1\right]\chi_0(\mathbf{k},z_l)}$$

[Singwi et al., 1968, Tanaka 1986]

(III) RPA: $G = 0$ & $\chi_e^{-1}(\mathbf{k},\omega) = \chi_0^{-1}(\mathbf{k},\omega) - \frac{4\pi e^2}{k^2}$

(IV) (SM) Second order long wavelength app. to RPA $\chi_0^{-1}(k\to 0)\approx \tilde{a}_0 + \tilde{a}_2\cdot k^2$

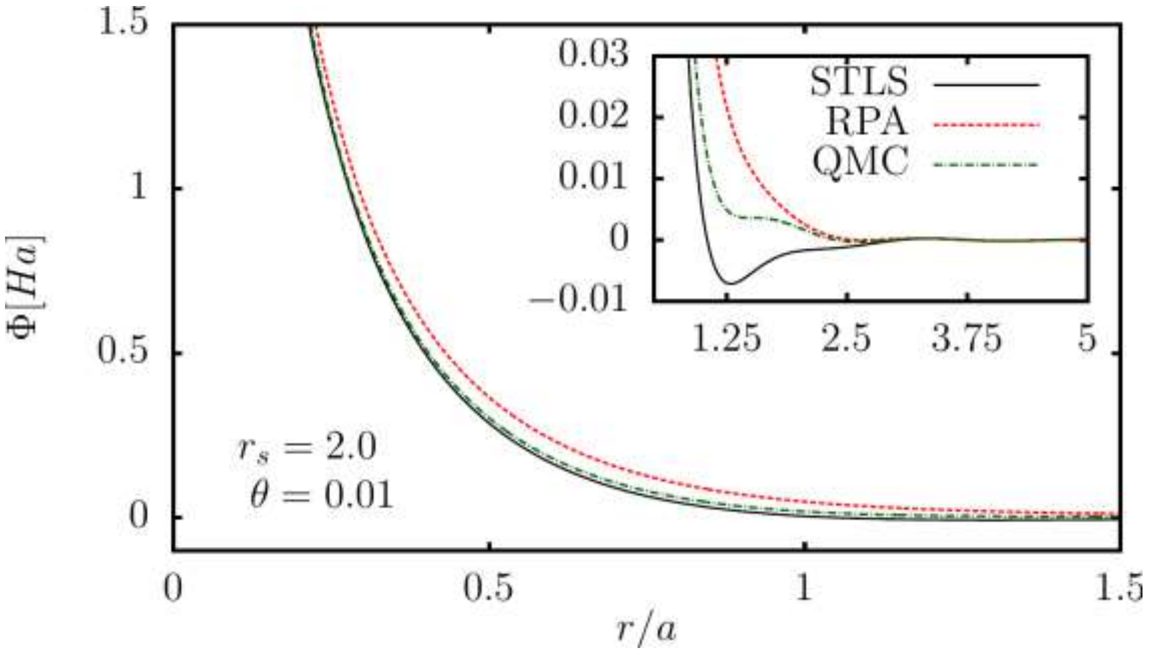
$$\phi(r;n,T) = \frac{Q^2}{2r}\left[(1+b)e^{-k_+r} + (1-b)e^{-k_-r}\right]$$

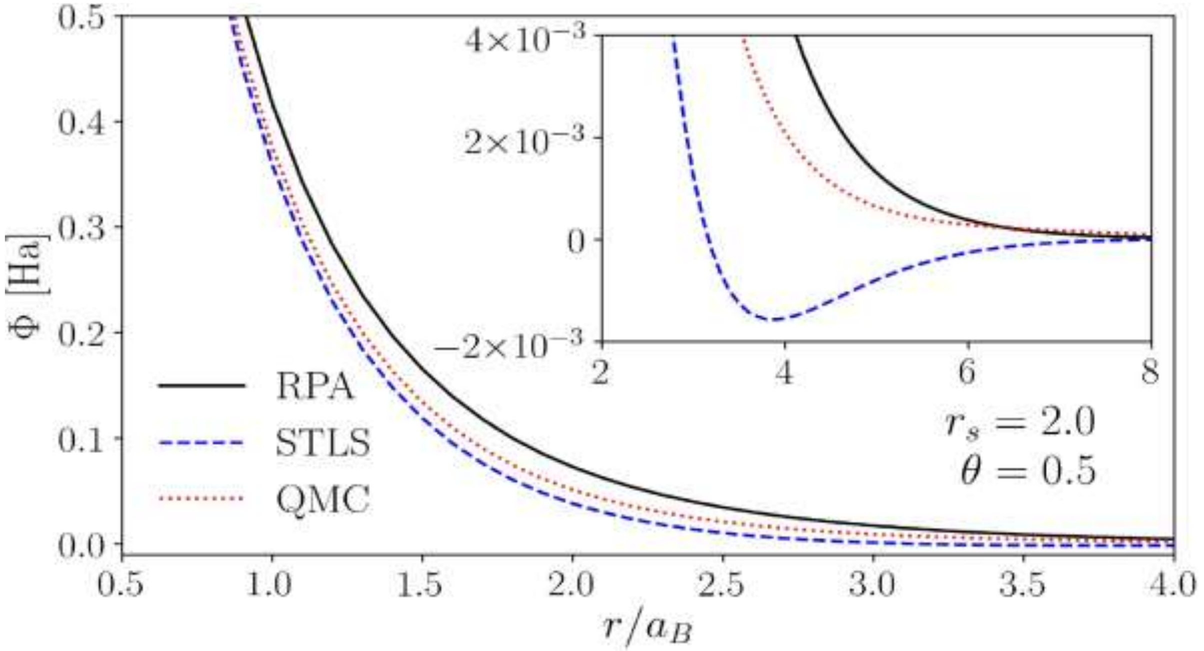
(V) (Yukawa) Second order long wavelength app. to RPA $\chi_0^{-1}(k\to 0)\approx \tilde{a}_0$

$$\Phi_Y(r;n,T) = \frac{Q^2}{r}e^{-k_sr}$$

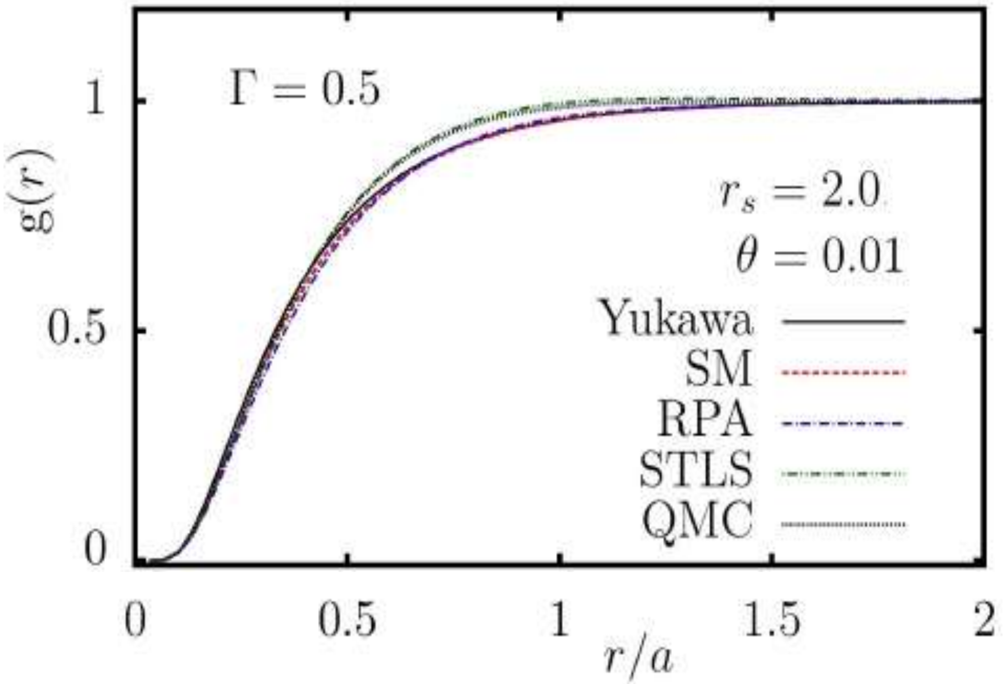
$r_s = 2.0$

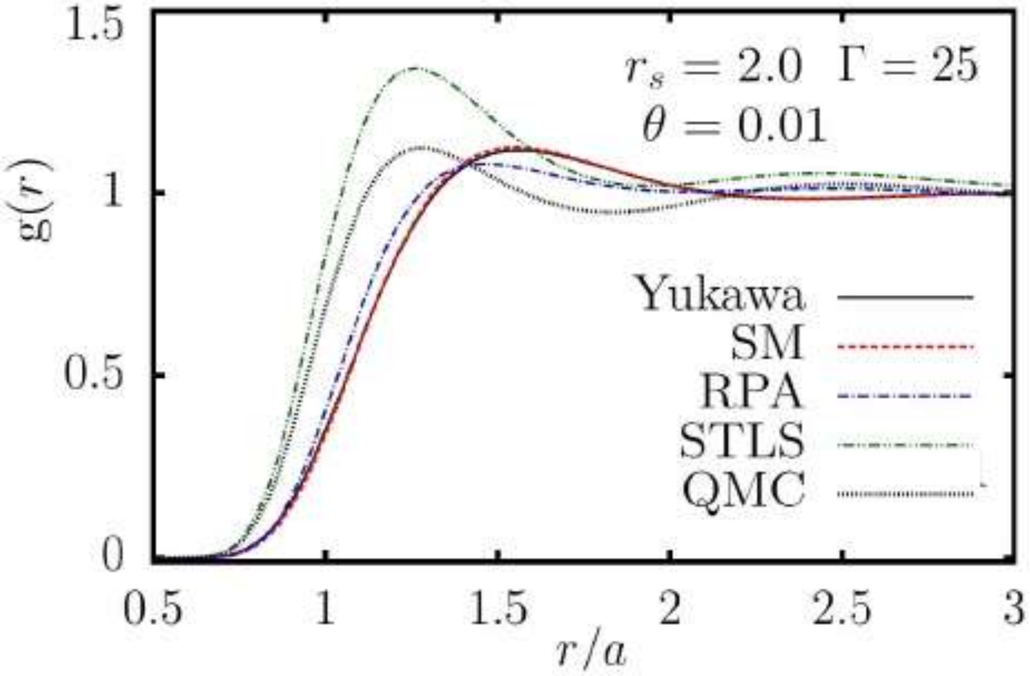
QMC data allows to check quality of the STLS based description





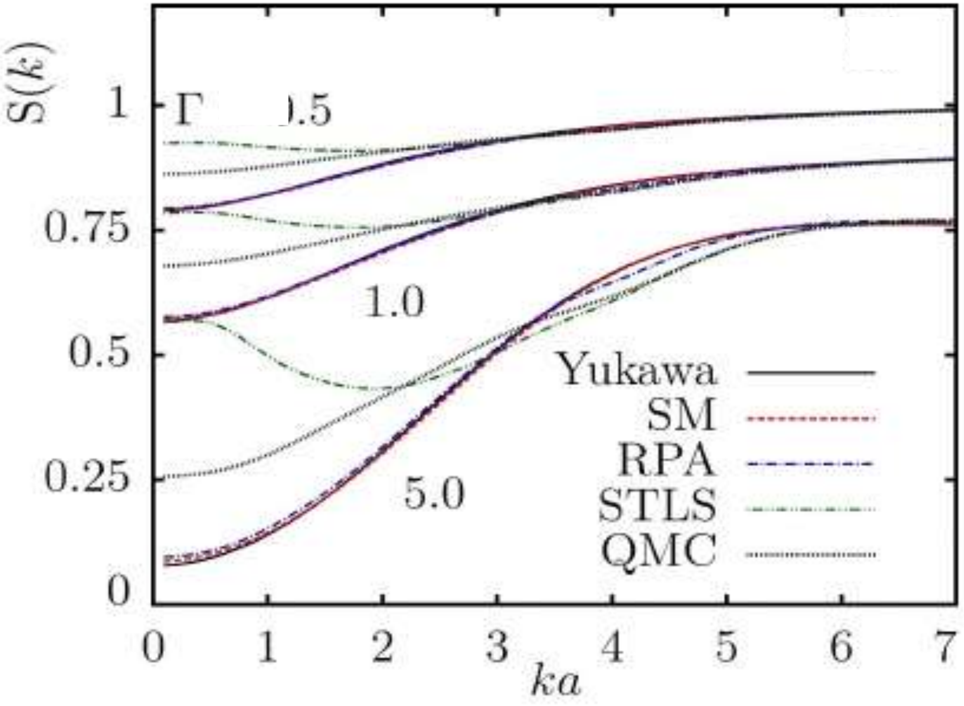
Radial pair distribution function

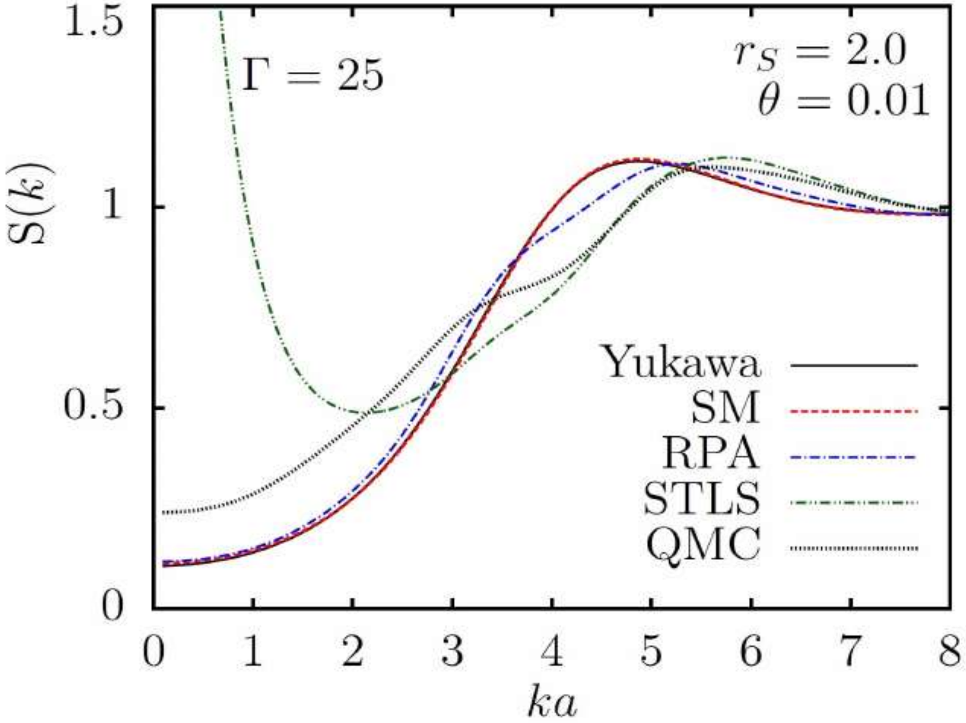




Zh. Moldabekov et al., *Structural characteristics of strongly coupled ions in dense quantum plasma,* Phys. Rev. **E** 98, 023207 (2018).

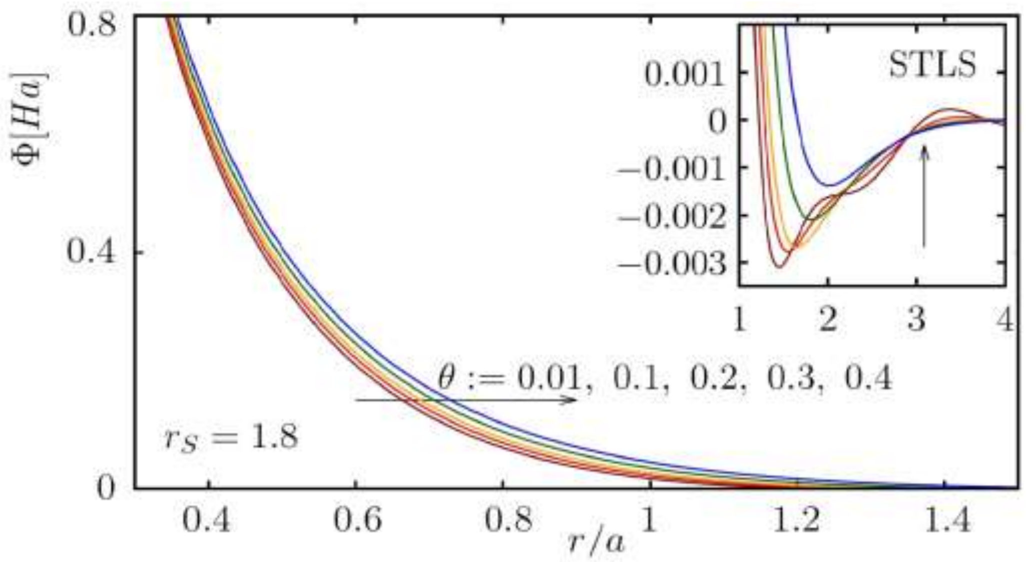
Static structure factor



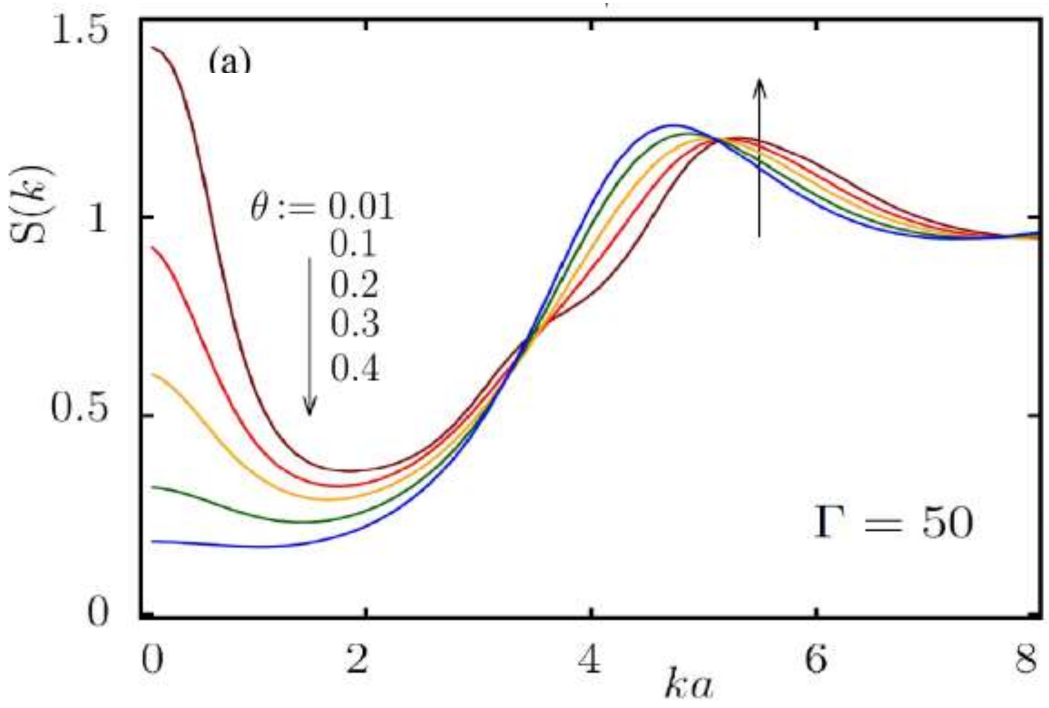


Zh. Moldabekov et al., *Structural characteristics of strongly coupled ions in dense quantum plasma,*
Phys. Rev. **E** 98, 023207 (2018).

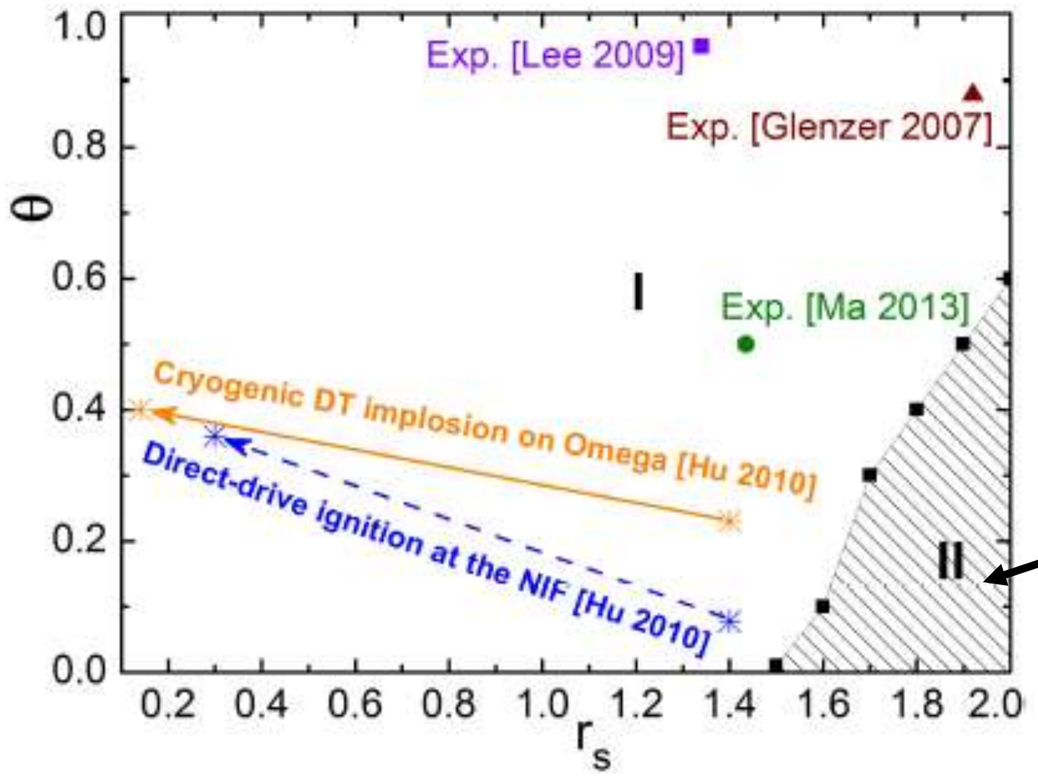
STLS potential



Static structure factor



The applicability limits of the STLS approximation for electron-ion plasmas with Γ > 1

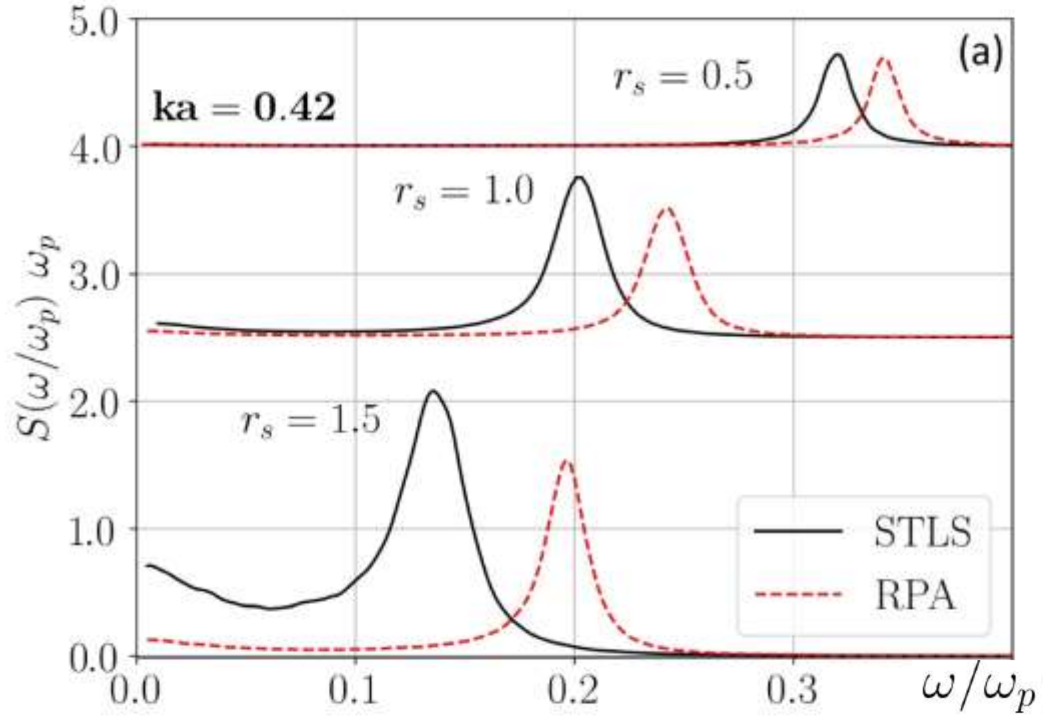


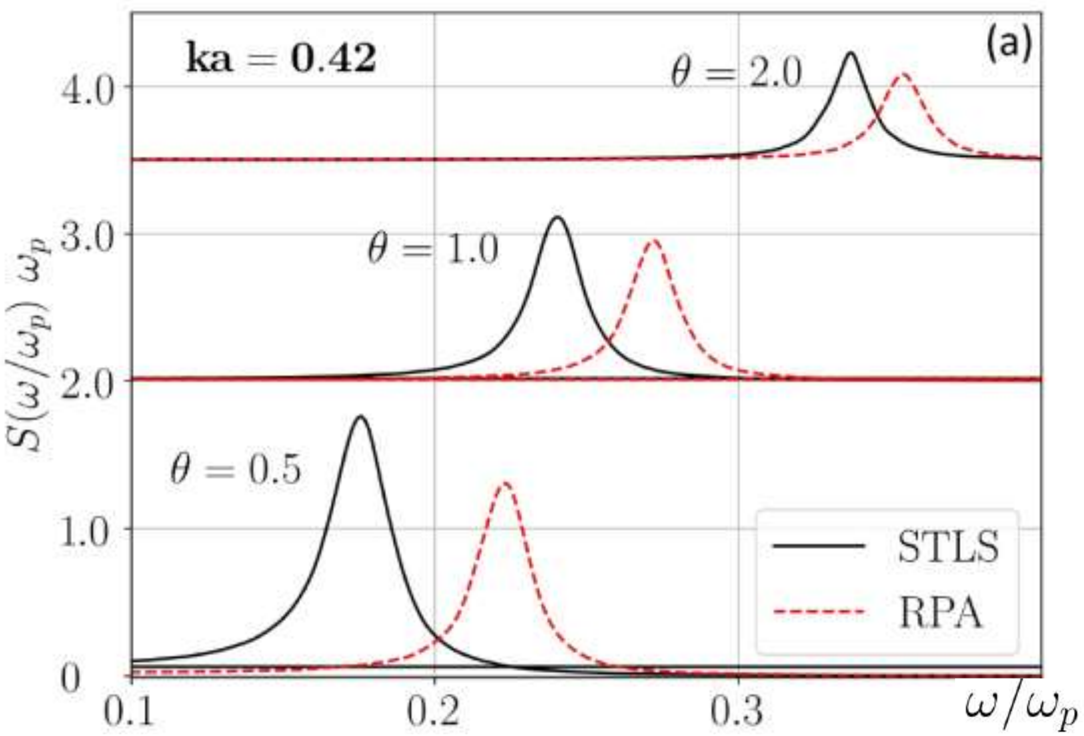
the STLS scheme cannot be used

Examples of the experimental plasma parameters with Γ> 1. The data for ICF experiments were extracted from Ref. [Hu 2010].

Zh. Moldabekov et al., *Structural characteristics of strongly coupled ions in dense quantum plasma,* Phys. Rev. **E** 98, 023207 (2018).

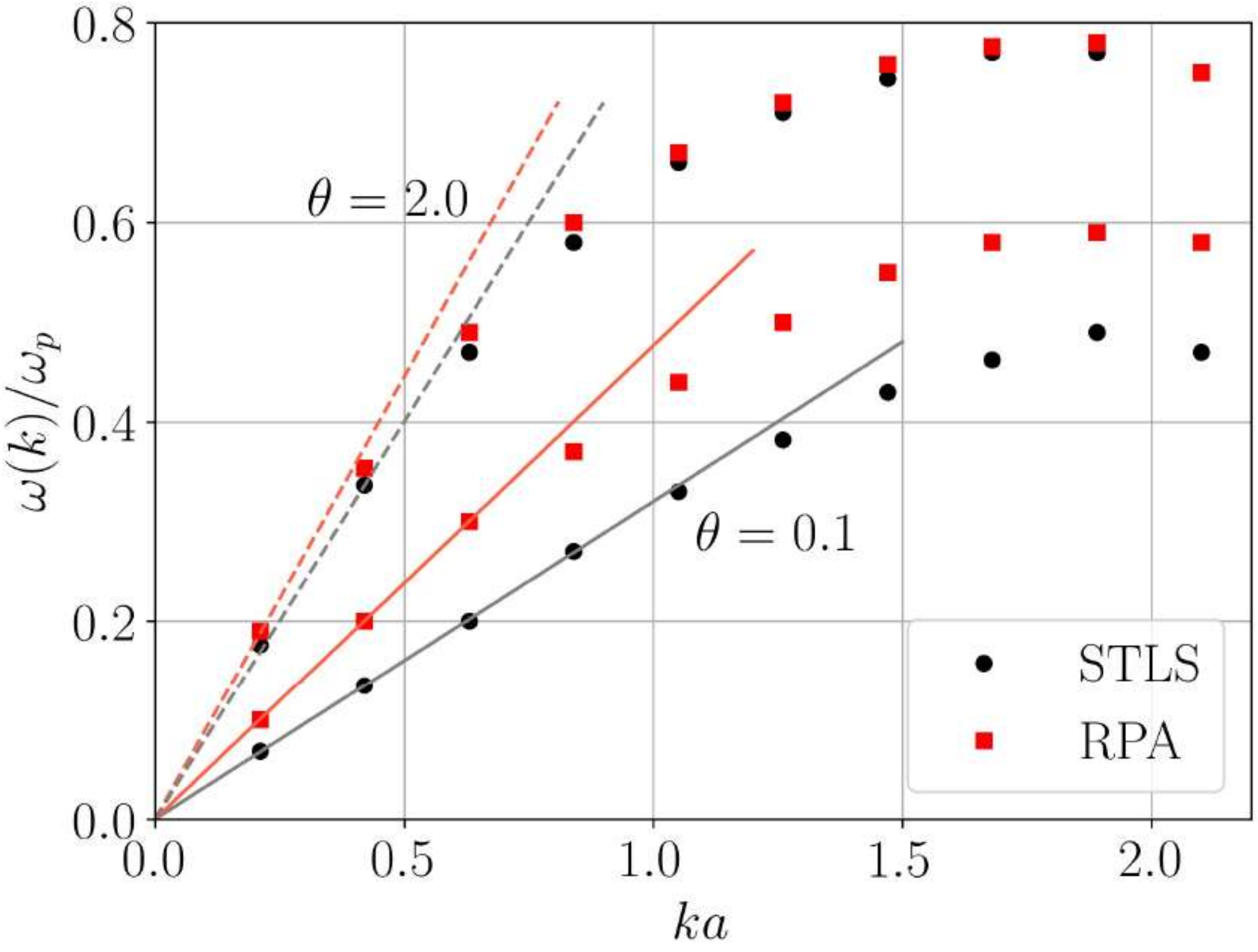
Results for the dynamical structure factor of ions



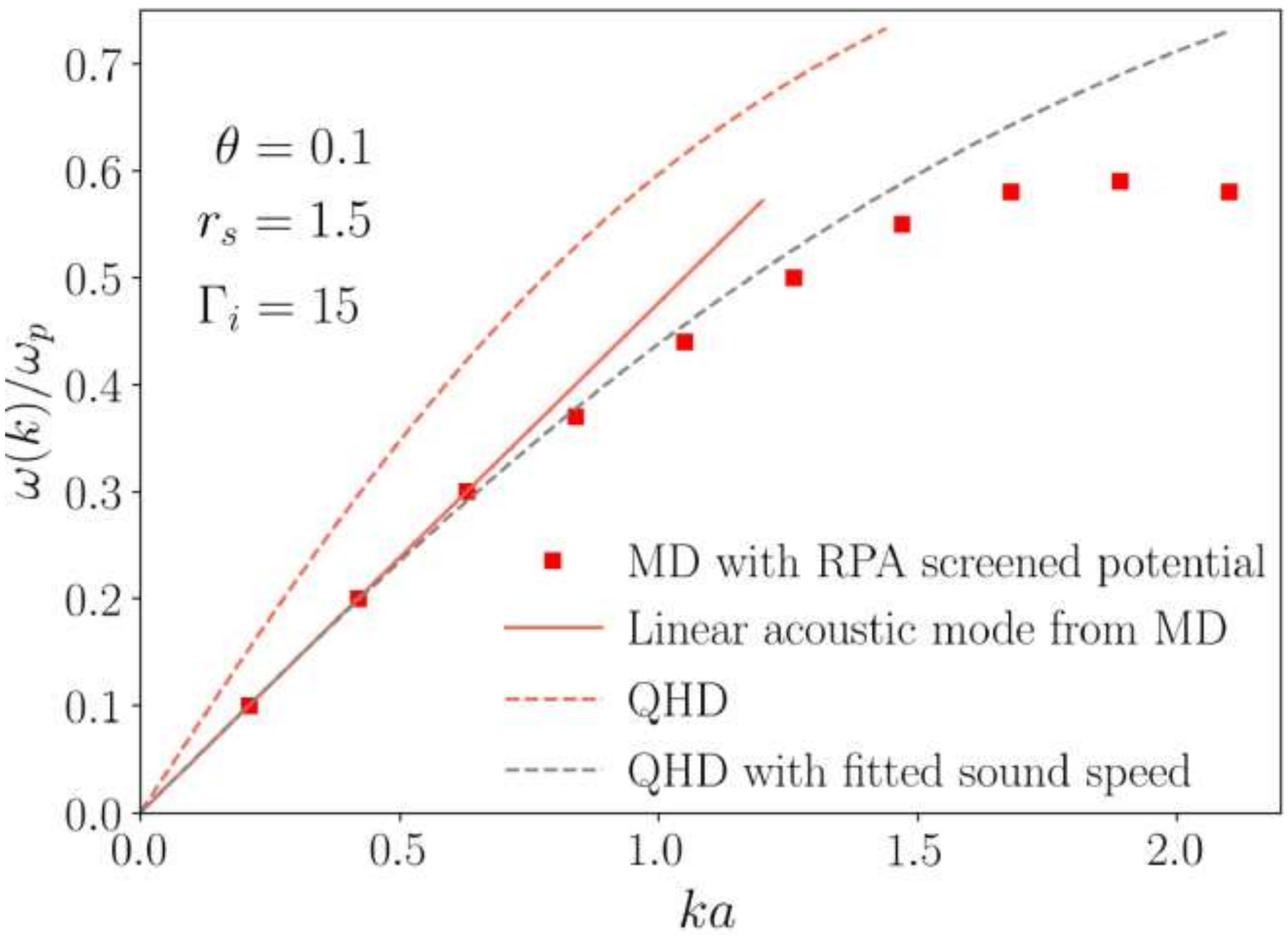


Zh. Moldabekov et al., Dynamical structure factor of strongly coupled ions in a dense quantum plasma,
Phys. Rev. E 99, 053203 (2019).

$r_s = 1.5$



Zh. Moldabekov et al., Phys. Rev. E 99, 053203 (2019).



$$\omega^2(k) = c_s^2 k^2 \times \frac{\omega_{pi}^2 \left[1 + A(\gamma, c_s)k^2\right]}{\omega_{pi}^2 + c_s^2 k^2 \left[1 + A(\gamma, c_s)k^2\right]} \qquad A(\gamma, c_s) = \gamma\hbar^2/(12 m_e m_i c_s^2)$$

F. Haas and S. Mahmood, PRE 92, 053112 (2015).

Zh. Moldabekov et al., PRE 99, 053203 (2019).

Possible applications of QHD:

- Study of the effect of quantum non-locality on instabilities and turbulence in quantum plasmas
- Laser-dense plasma interaction [a current density formulation of QHD is needed]
- MD-QHD scheme for a large scale simulation of ionic dynamics beyond Born–Oppenheimer approximation

How important are the effects beyond the Born–Oppenheimer approximation for dense plasmas ?

The **electronic friction** in the Langevin dynamics of ions is a correction to the Born-Oppenheimer approximation

Stopping power:

$$S(v) = \frac{2Z^2e^2}{\pi v^2} \int_0^\infty \frac{\mathrm{d}k}{k} \int_0^{kv} \mathrm{d}\omega \, \omega \, \mathrm{Im}\left[\frac{-1}{\epsilon(k,\omega)}\right]$$

→

Friction function Q :

$$S(v) = Z^2 e^2 Q(v) \cdot v$$

The density response function

$$\chi_e^{-1}(\mathbf{k},\omega) = \chi_0^{-1}(\mathbf{k},\omega) + \frac{4\pi e^2}{k^2}\left[G(\mathbf{k},\omega) - 1\right]$$

the dielectric function

$$\epsilon^{-1}(\mathbf{k},\omega) = 1 + \frac{4\pi e^2}{k^2}\chi_e(\mathbf{k},\omega)$$

RPA: $G = 0$ **&** $\chi_e^{-1}(\mathbf{k},\omega) = \chi_0^{-1}(\mathbf{k},\omega) - \frac{4\pi e^2}{k^2}$

STLS approximation:

$$f(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}';t) = f(\mathbf{r},\mathbf{p};t)f(\mathbf{r}',\mathbf{p}';t)g(|\mathbf{r}-\mathbf{r}'|)$$

$$G^{\mathrm{STLS}}\left(\left[S^{\mathrm{STLS}}\right],\mathbf{k},\omega=0\right) = -\frac{1}{n}\int\frac{\mathrm{d}\mathbf{k}'}{(2\pi)^3}\frac{\mathbf{k}\cdot\mathbf{k}'}{k'^2}\left[S^{\mathrm{STLS}}(\mathbf{k}-\mathbf{k}')-1\right]$$

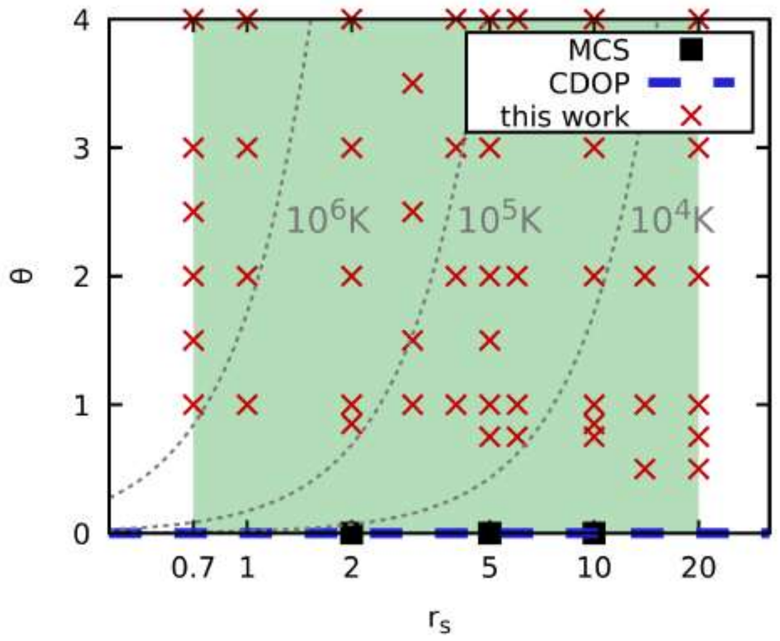
$$S^{\mathrm{STLS}}\left(\left[G^{\mathrm{STLS}}\right],\mathbf{k}\right) = -\frac{1}{\beta n}\sum_{l=-\infty}^{\infty}\frac{\chi_0(\mathbf{k},z_l)}{1+\frac{4\pi e^2}{k^2}\left[G^{\mathrm{STLS}}(\mathbf{k},0)-1\right]\chi_0(\mathbf{k},z_l)}$$

[Singwi et al., 1968, Tanaka 1986]

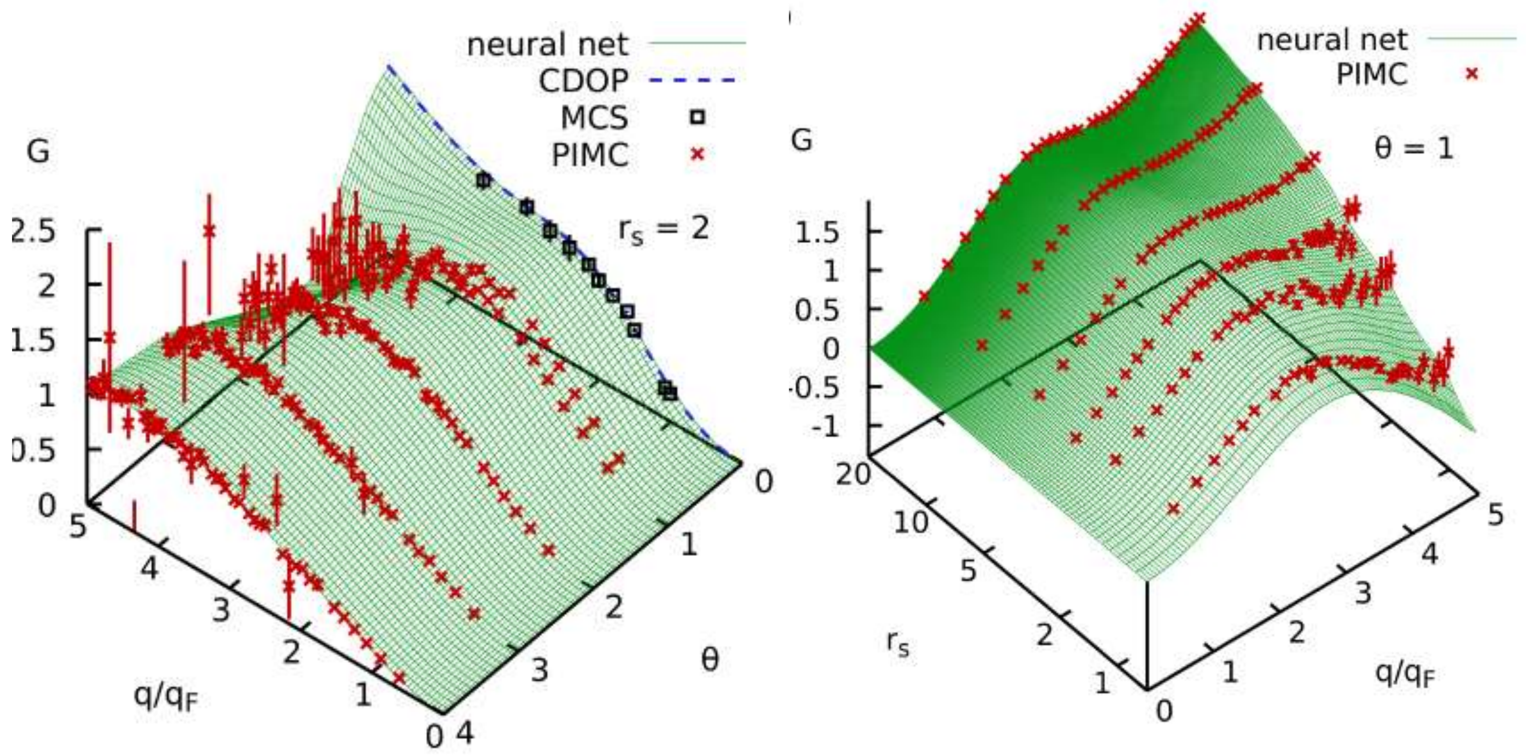
Mermin, i.e. relaxation time approximation

$$\epsilon_M(\mathbf{k},\omega) = 1 + \frac{(\omega+i\nu)[\epsilon_{\mathrm{RPA}}(\mathbf{k},\omega+i\nu)-1]}{\omega+i\nu[\epsilon_{\mathrm{RPA}}(\mathbf{k},\omega+i\nu)-1]/[\epsilon_{\mathrm{RPA}}(\mathbf{k},0)-1]}$$

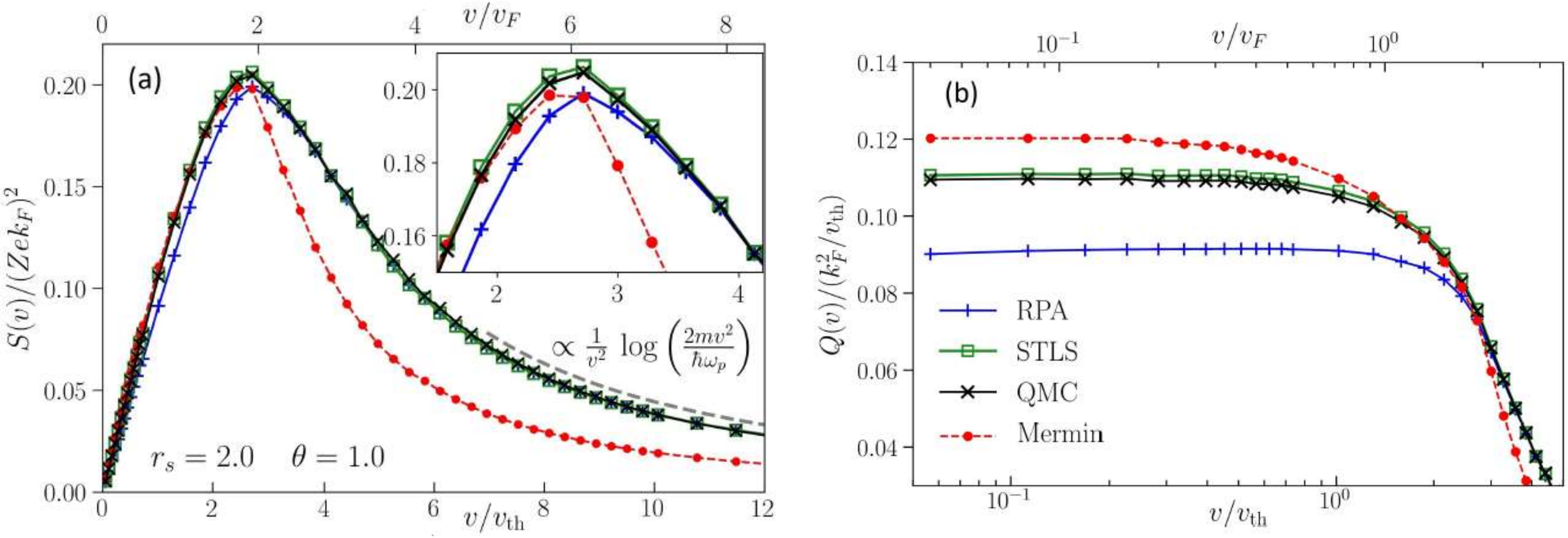
The static local field correction of the warm dense electron gas: An *ab initio* path integral Monte Carlo study and machine learning representation



$$G(q) = 1 - \frac{q^2}{4\pi}\left(\frac{1}{\chi_0(q)} - \frac{1}{\chi(q)}\right)$$



T. Dornheim, J. Vorberger, S. Groth, N. Hoffmann, Zh. A. Moldabekov, and M. Bonitz, J. Chem. Phys. **151**, 194104 (2019)



Zh. A. Moldabekov et al., Ion energy-loss characteristics and friction in a free-electron gas at warm dense matter and nonideal dense plasma conditions, Phys. Rev. E 101, 053203 (2020)

IMPLICATIONS FOR THE LANGEVIN DYNAMICS OF IONS

$$M\ddot{\mathbf{r}}_i = \sum_{j\neq i} \mathbf{F}_{ij} - \gamma M \dot{\mathbf{r}}_i + \mathbf{f}_i(t)$$

$$S = \delta E/\delta l = \gamma M |\dot{\mathbf{r}}|$$

$$\frac{\gamma}{\omega_{pi}} = 5\times 10^{-2}\,\Gamma^{1/2}\left(\frac{T_i}{T_e}\right)^{1/2}\frac{Z^{2/3}}{A^{1/2}}\,Q^*(\theta, r_s)$$

$$\gamma(\theta, r_s) = \frac{Z^2e^2}{M} Q(\theta, r_s, v)\Big|_{v/v_{\rm th}\ll 1}$$

$$Q^*(\theta, r_s) = Q/(k_F^2/v_{\rm th})$$

r_s \ θ	0.5	1.0	2.0
4.0	0.1540	0.178	0.1720
2.0	0.0989	0.110	0.1050
1.0	0.0636	0.070	0.0626

ICF

(i) with $T_e/T_i = 1$, $\Gamma = 6$, r_s find $\gamma/\omega_{pi} \simeq 0.012$.

WDM

(ii) with $T_e/T_i = \Gamma = 10$, $r_s = 2$ and $\theta = 1.0$ we find $\gamma/\omega_{pi} \simeq 0.01$

Zh. A. Moldabekov et al., Phys. Rev. E 101, 053203 (2020)

Thank you for your attention