Saint Petersburg Academic University

Ioffe Physical Technical Institute

Diffusion currents and diffusion coefficients in dense stellar matter

Beznogov M. V., Yakovlev D. G.

Physics of Neutron Stars 2014, Saint Petersburg,

July 31st, 2014

Outline

Diffusion currents and diffusion coefficients in dense stellar matter

- **Introduction**
- **Main part**
  - Part I: Coulomb separation of ions in dense stellar matter
  - Part II: Effective potential approach to calculation of inter-diffusion coefficients.
- **Discussion**
- **Conclusion**

Introduction

Why do we study diffusion?

Because many astrophysical objects (in particular, stars) contain mixtures of different ions.

Ion diffusion can be most important

For example, degenerate cores of white dwarfs (WDs):

- Low mass WDs: mixture of ^{4}He – ^{12}C
- Intermediate and massive WDs: mixture of ^{12}C – ^{16}O (as well as Ne and some other elements)

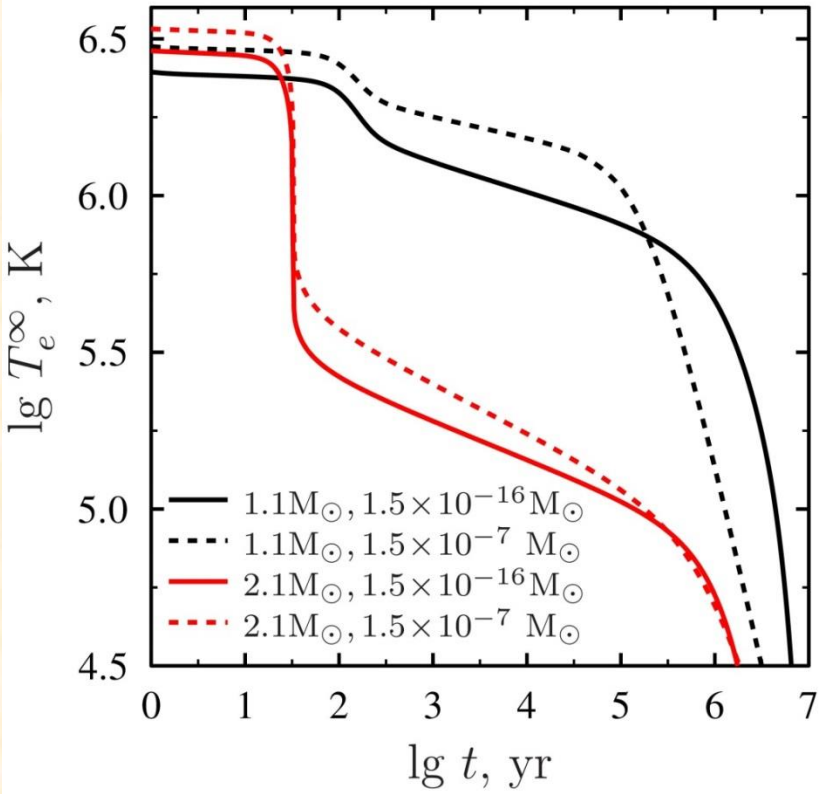
Neutron stars (NSs) – outer envelopes:

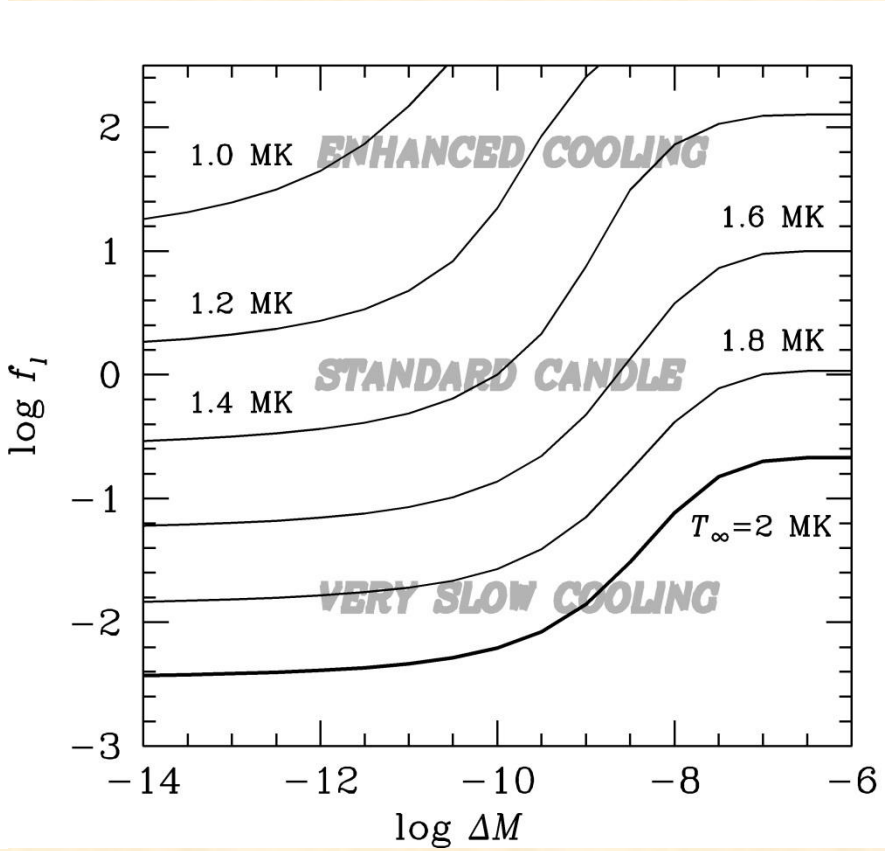
- Possible chemical species: ^{1}H, ^{4}He, ^{12}C, ^{56}Fe
- Diffusive nuclear burning of ^{1}H, ^{4}He

Diffusion – most important for thermal evolution of NSs

Crab pulsar

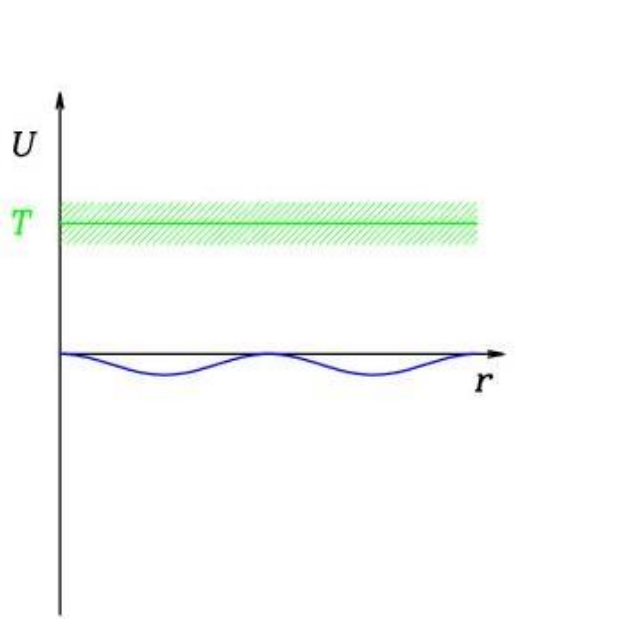
Weisskopf et al. (2011)

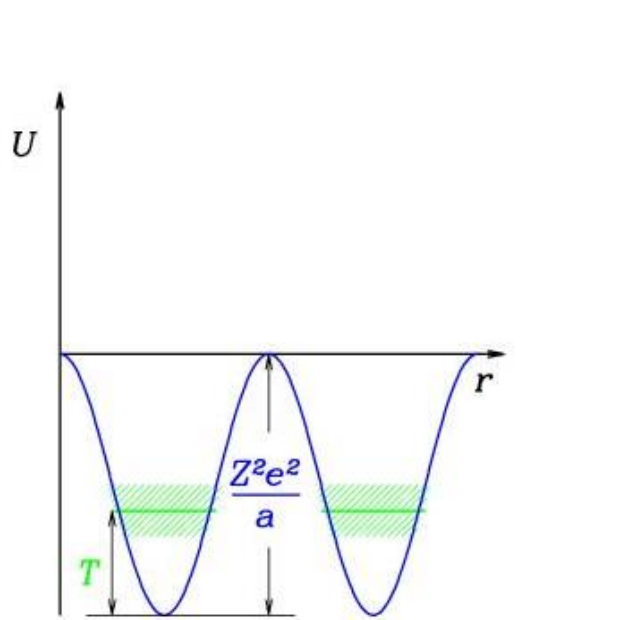




Weakly coupled (WC) plasma

Strongly coupled (SC) classical plasma

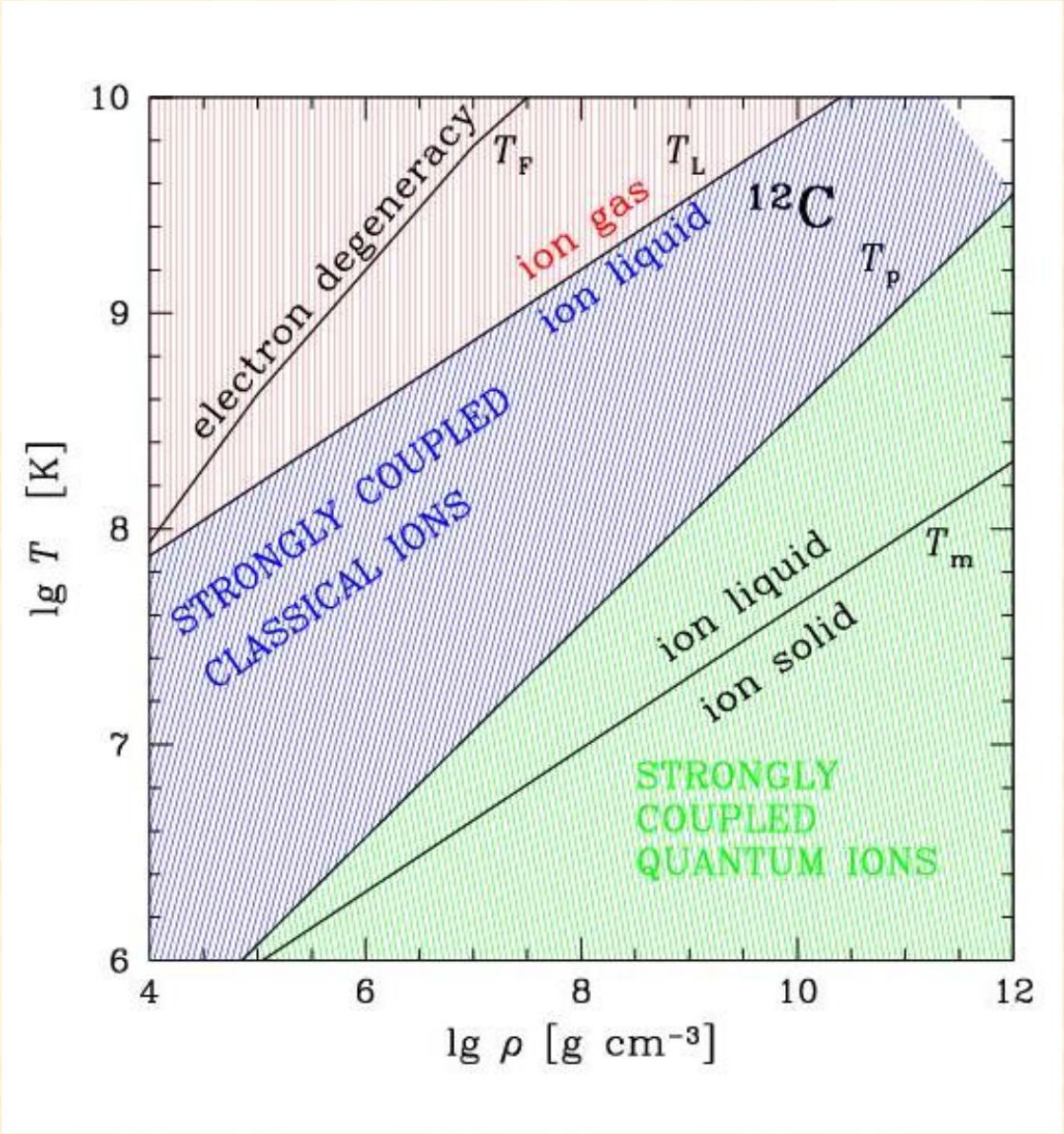




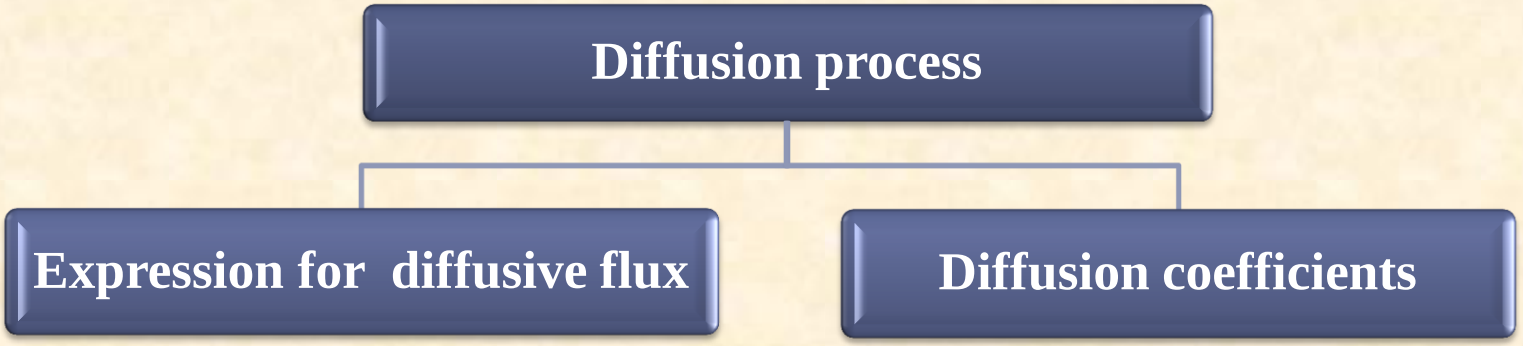
$\Gamma \ll 1$

$\Gamma \gg 1$

$$\Gamma = \frac{Z^{5/3}\bar{e}^2}{a_e k_B T}, a_e = \left(\frac{3}{4\pi n_e}\right)^{\frac{1}{3}}, n_e = Zn_i$$



SC plasma greatly affects microphysics of matter, particularly, diffusion of ions.



"Conventional" approach to diffusion in SC plasmas:

- Expressions for the diffusive currents are the same as in WC plasmas (classical Chapman-Enskog theory).
- Diffusion coefficients are computed using many techniques:
  - molecular dynamics (MD) simulations (both Kubo-Green relations and spatial diffusion formulae)
  - classical Chapman-Enskog method with screened Coulomb potential
  - Stokes-Einstein relation between diffusion and viscosity
  - kinetic theory calculations based on Kubo-Green relations
  - effective potential method
  - other methods and their combinations

Important: proper treatment of Coulomb interactions

Part I: Coulomb separation

Consider isothermal (T = const) multicomponent plasma, which consist of several fully ionized ion species (j = 1, 2,…) and neutralizing electron (e) background. *All following calculations assume* T = const.

Assume that matter is slightly off thermodynamic equilibrium due to presence of external forces and density gradients (no deviations from thermal equilibrium as T = const) Introduce generalized thermodynamic forces

$$\vec{\tilde{F}}_\alpha = \vec{F}_\alpha - \nabla\mu_\alpha = e_\alpha \vec{E} + m_\alpha \vec{g} - \nabla\mu_\alpha, \alpha = e, j$$

and characterize deviations from partial hydrostatic equilibrium of particles α by vector

$$\vec{d}_\alpha = \frac{\rho_\alpha}{\rho}\sum_\beta n_\beta \vec{\tilde{F}}_\beta - n_\alpha \vec{\tilde{F}}_\alpha, \text{ clearly } \sum_\alpha \vec{d}_\alpha = 0$$

Phenomenological diffusive current density:

$$\vec{J}_\alpha = \Phi \sum_{\beta\neq\alpha} m_\alpha m_\beta D_{\alpha\beta} \vec{d}_\beta, \sum_\alpha \vec{J}_\alpha = 0$$

Electrons are assumed to be in a state of mechanical (quasi)equilibrium, adjusting almost instantly to any changes in the state of the ion subsystem. This allows us to factor electrons out in the problem of ion transport.

Thus, selecting appropriate normalization function, we derive for a two component plasma (TCP aka BIM)

$$\vec{J}_2 = -\vec{J}_1 = \frac{n m_1 m_2}{\rho k_B T} D \vec{d}_1, \vec{d}_1 = -\vec{d}_2, D_{12} = D_{21} \equiv D$$

Writing explicitly expression for *d*, we obtain:

$$\vec{d}_1 = \frac{n_1 n_2}{n_e}\left(m_u Z_1 Z_2 \left(\frac{A_2}{Z_2} - \frac{A_1}{Z_1} \right) \frac{\nabla P}{\rho} + Z_2 \nabla \mu_1 - Z_1 \nabla \mu_2 \right)$$

Chemical potential of ions is separated into two terms

$$\mu_j = \mu_j^{id} + \mu_j^{C}$$

After simple algebra:

$$\vec{d}_c = 0.3\frac{\rho n_1 n_2}{n_e}\frac{Z_1 Z_2 \overline{e}^2 \vec{g}}{\gamma a_e P}\left(Z_2^{2/3} - Z_1^{2/3}\right)$$

Then the diffusive flux is:

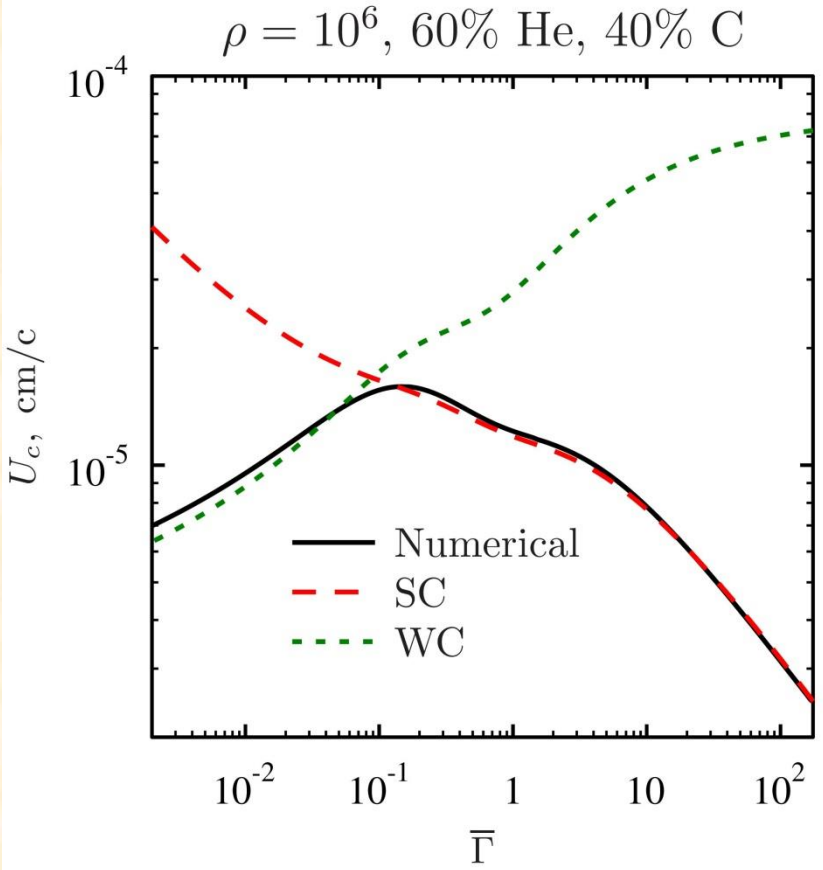
$$\vec{J}_2 = D\frac{m_1 m_2 n}{\rho n_e}\left(Z_2 n_2 \nabla n_1 - Z_1 n_1 \nabla n_2\right) + m_2 n_2\left(\vec{u}_a + \vec{u}_c\right),$$

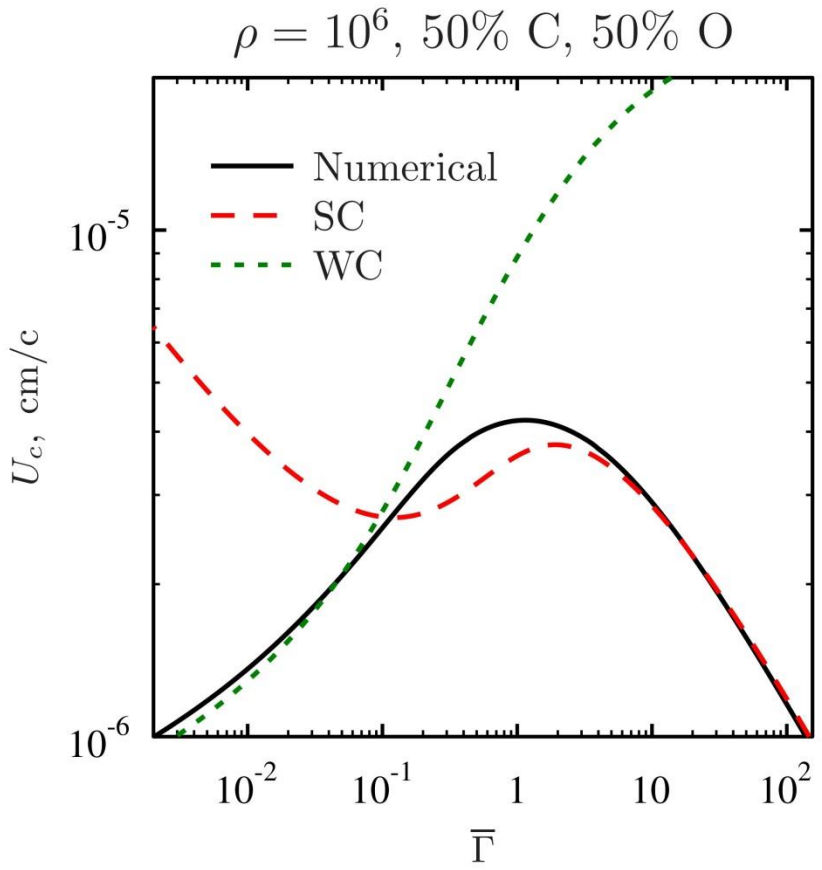
$$\vec{u}_a = \frac{\rho_1 n D}{\rho n_e k_B T} Z_1 Z_2 m_u \vec{g}\left(\frac{A_2}{Z_2} - \frac{A_1}{Z_1}\right) \mapsto \text{ drift velocity of gravitational separation}$$

$$\vec{u}_c = \frac{\rho_1 n D}{n_e k_B T} Z_1 Z_2 \vec{g}\frac{0.3\overline{e}^2}{\gamma a_e P}\left(Z_2^{2/3} - Z_1^{2/3}\right) \mapsto \text{drift velocity of Coulomb separation}$$

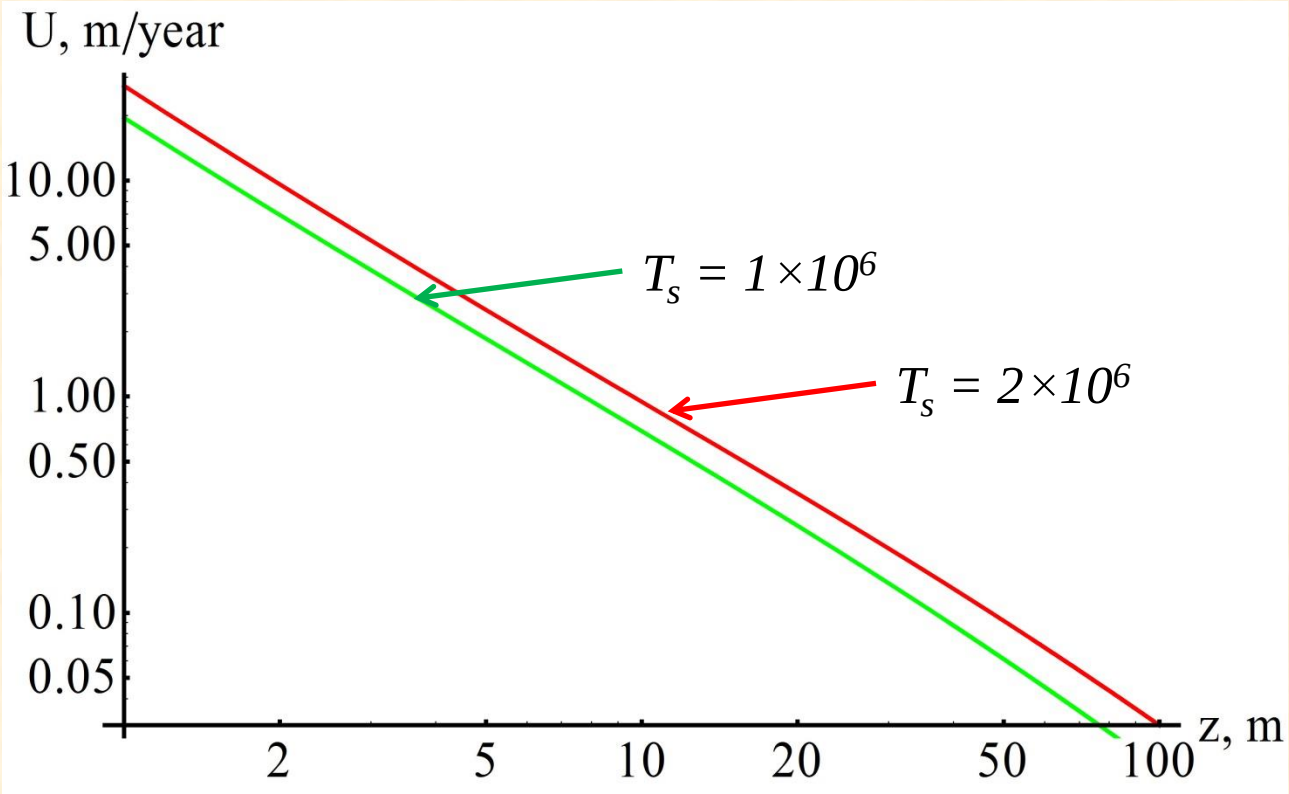
P. Chang, L. Bildsten, and P. Arras, Astrophys. J. **723**, 719 (2010). The authors considered the impact of strong Coulomb interactions on equilibrium plasma. We extended their approach to kinetics (diffusion).

Comparison of Coulomb separation velocity for WC and SC BIMs





Coulomb separation velocity for NS outer envelope



Part II: Diffusion coefficients

"Zoo" of diffusion coefficients

- D_{ij} – inter-diffusion coefficient, $i, j = 1, 2, \ldots$ – ion species
- D_{ii} – self-diffusion coefficient of the i^{th} component in a multicomponent plasma
- D_1 – self-diffusion coefficient in one component plasma (OCP)
- Ambipolar diffusion coefficients, diffusion in magnetic field coefficients, etc.

Consider BIM with rigid electron background.

BIM is characterized by ion mass (A_j) and charge (Z_j) numbers and two dimensionless parameters:

$$x_1 = \frac{n_1}{n}, \Gamma_0 = \frac{e^2}{a k_B T}, \text{ where } n = n_1 + n_2, a = \left(\frac{3}{4\pi n}\right)^{1/3}$$

In the following: length is measured in units of ion-sphere radius a and potentials in units of $k_B T/e$.

Introduce averaging of arbitrary quantity f_j in BIM:

$$\overline{f} = x_1 f_1 + x_2 f_2$$

Define mean plasma coupling as:

$$\overline{\Gamma} = \Gamma_0 \overline{Z^{5/3}}\,\overline{Z}^{1/3}$$

Let $g_{ij}(r)$, $h_{ij}(r)$, $c_{ij}(r)$ be radial distribution functions (RDFs), total and direct correlation functions, respectively.

Basic idea of the effective potential approach consists in the following relation between RDF and effective potential ("mean force potential"):

$$g_{ij}(r) = \exp\left(-\Phi_{ij}(r)\right)$$

For calculation of diffusion coefficients this idea was put forward by S. D. Baalrud and J. Daligault (Phys. Rev. Lett. **110**, 235001, 2013)

Hyper-netted chain method of RDFs calculation

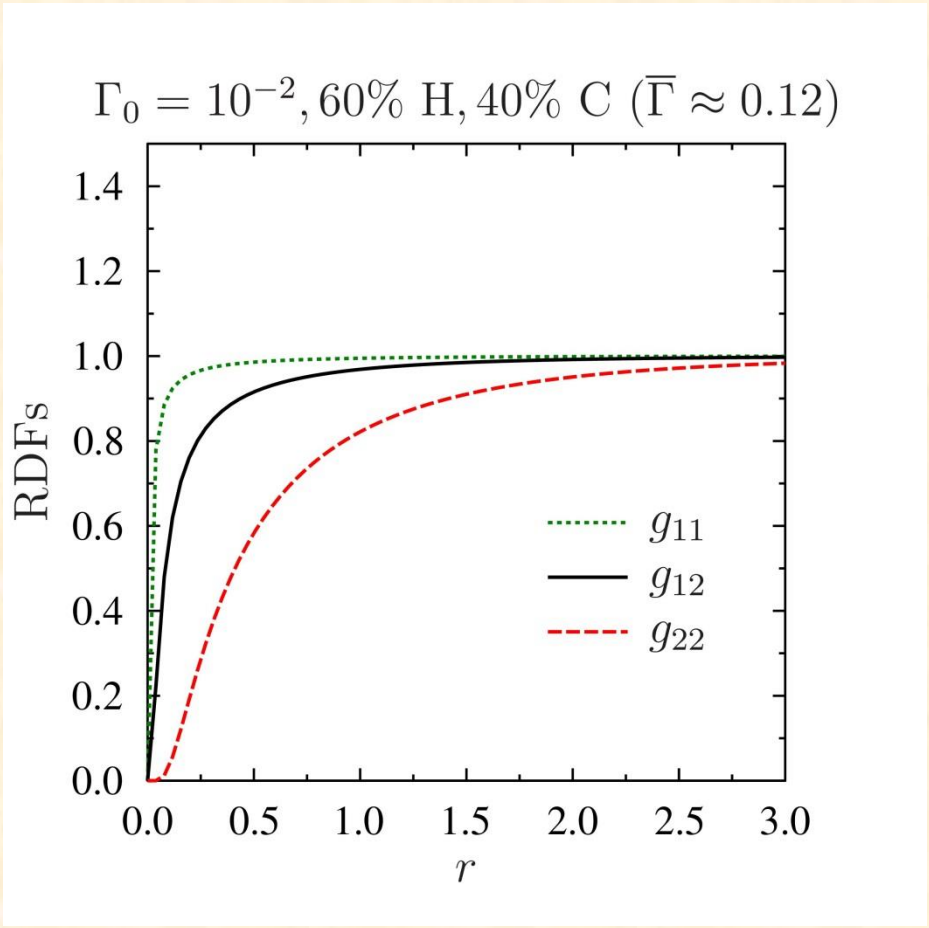
Ornstein-Zernike equations and HNC closure relations for BIM constitute nonlinear system of 6 coupled equations:

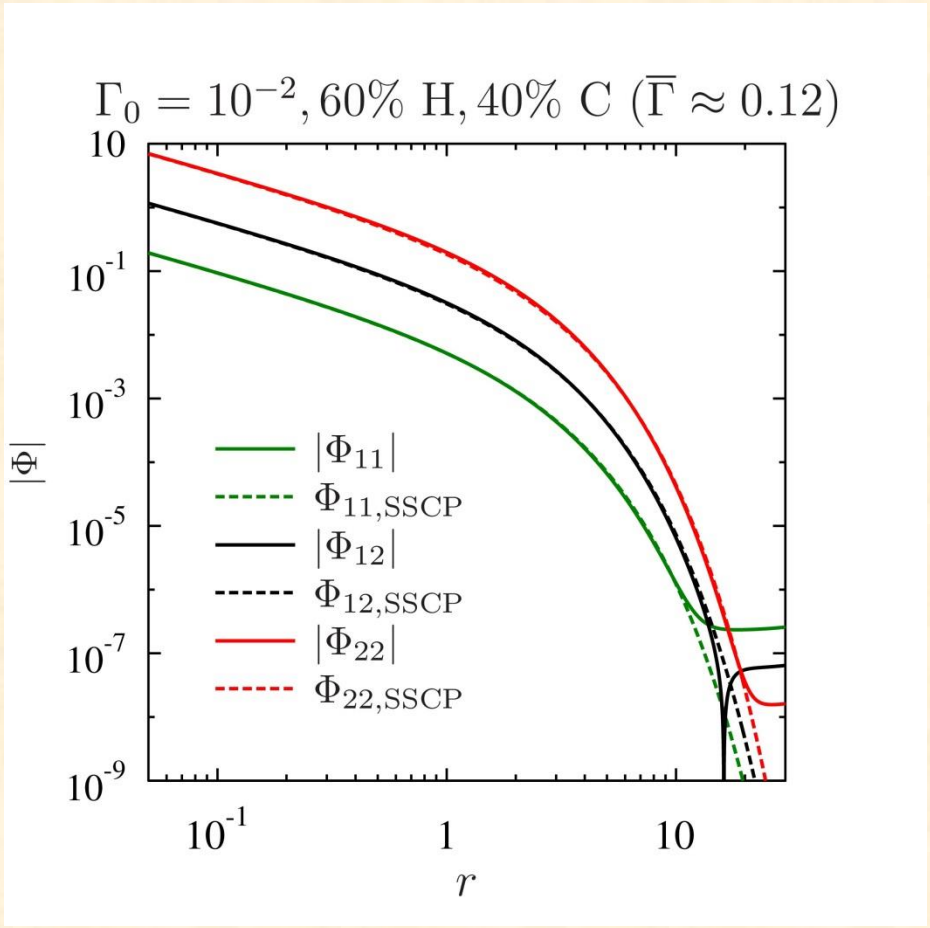
$$\hat{h}_{ij}(k) = \hat{c}_{ij}(k) + \frac{3}{4\pi}\sum_{q=1}^{2} x_q \hat{h}_{iq}(k)\hat{c}_{qj}(k)$$

$$g_{ij}(r) = h_{ij}(r) + 1 = \exp\left(h_{ij}(r) - c_{ij}(r) - \varphi_{ij}(r)\right), \text{ where } \varphi_{ij}(r) = \frac{Z_i Z_j \Gamma_0}{r}$$

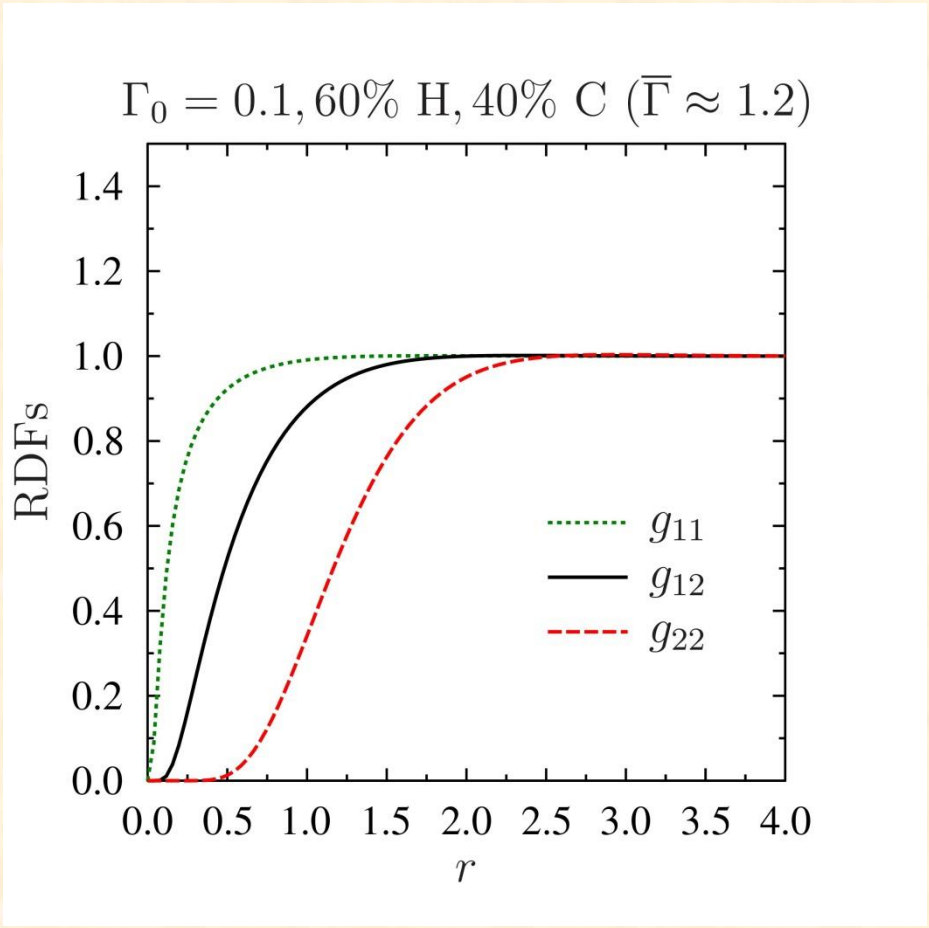
We solve this system by generalizing a technique proposed by Ng (J. Chem. Phys., **61**, 2680, 1974) to BIM.

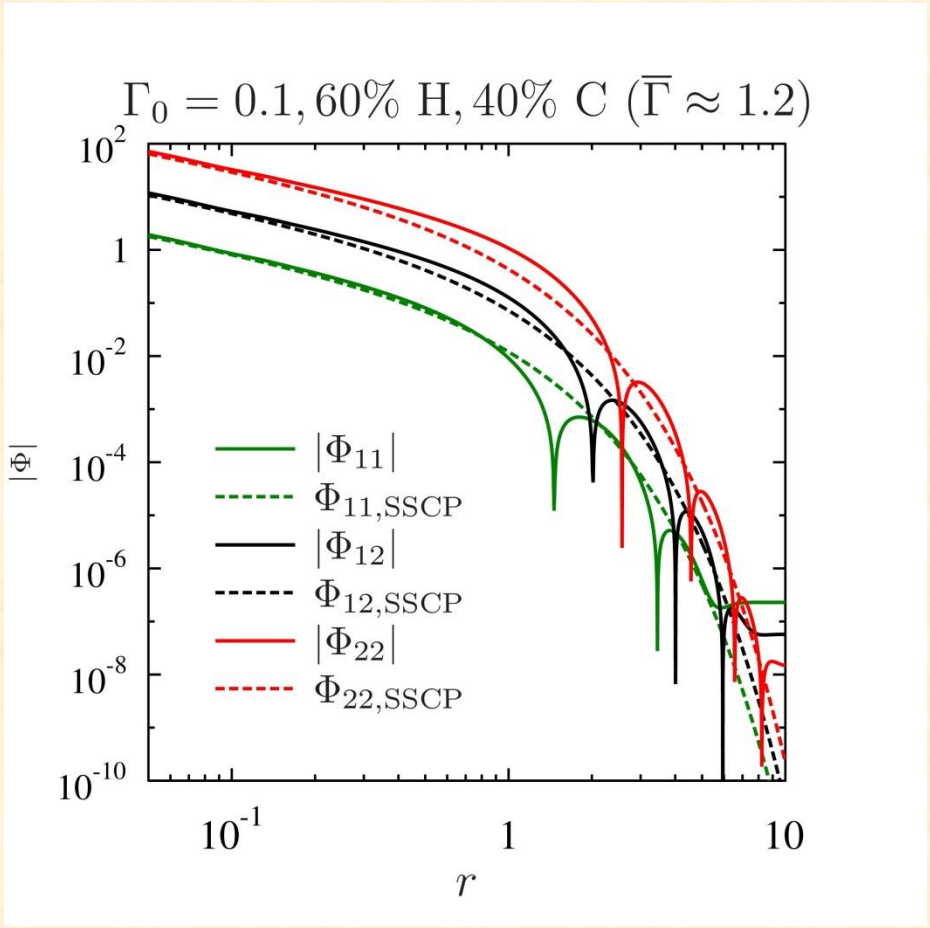
$$\Phi_{ij,\mathrm{SSCP}}(r) = \frac{Z_i Z_j \Gamma_0}{r} \exp\left(-\frac{r}{r_D}\right), \quad \frac{1}{r_D} = \sqrt{3\Gamma_0 \overline{Z^2}}, \quad r_D - \text{ Debye screening length}$$

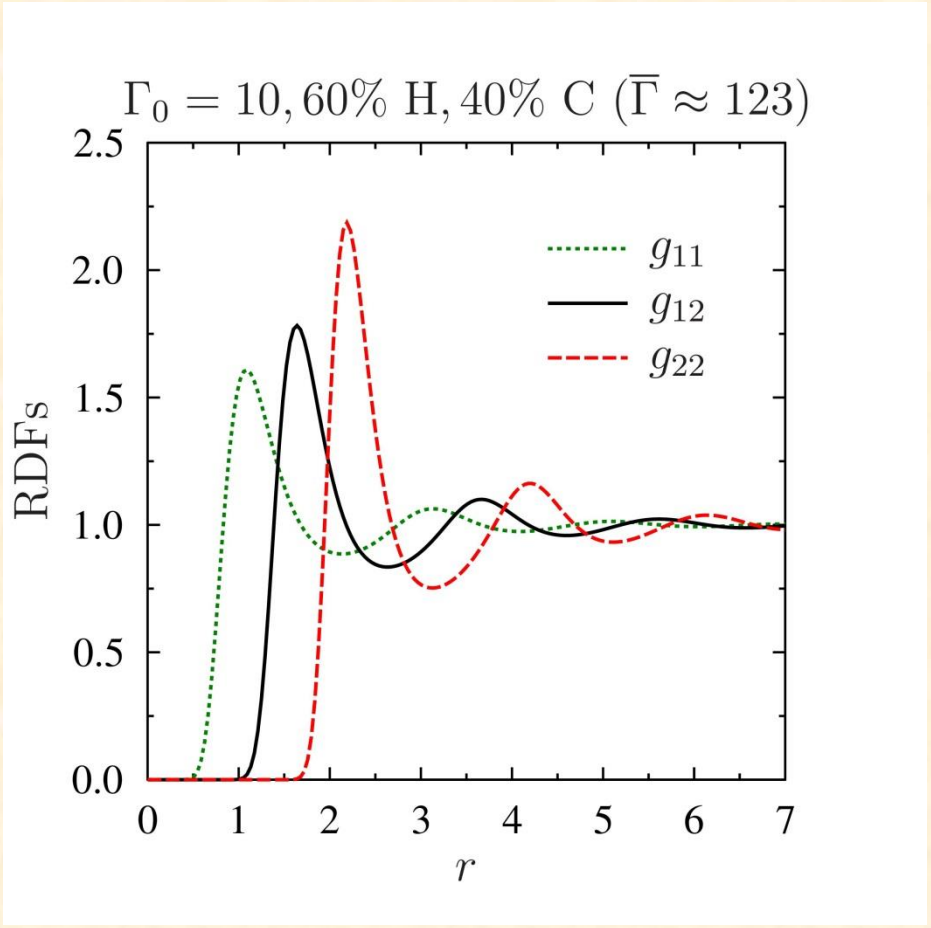


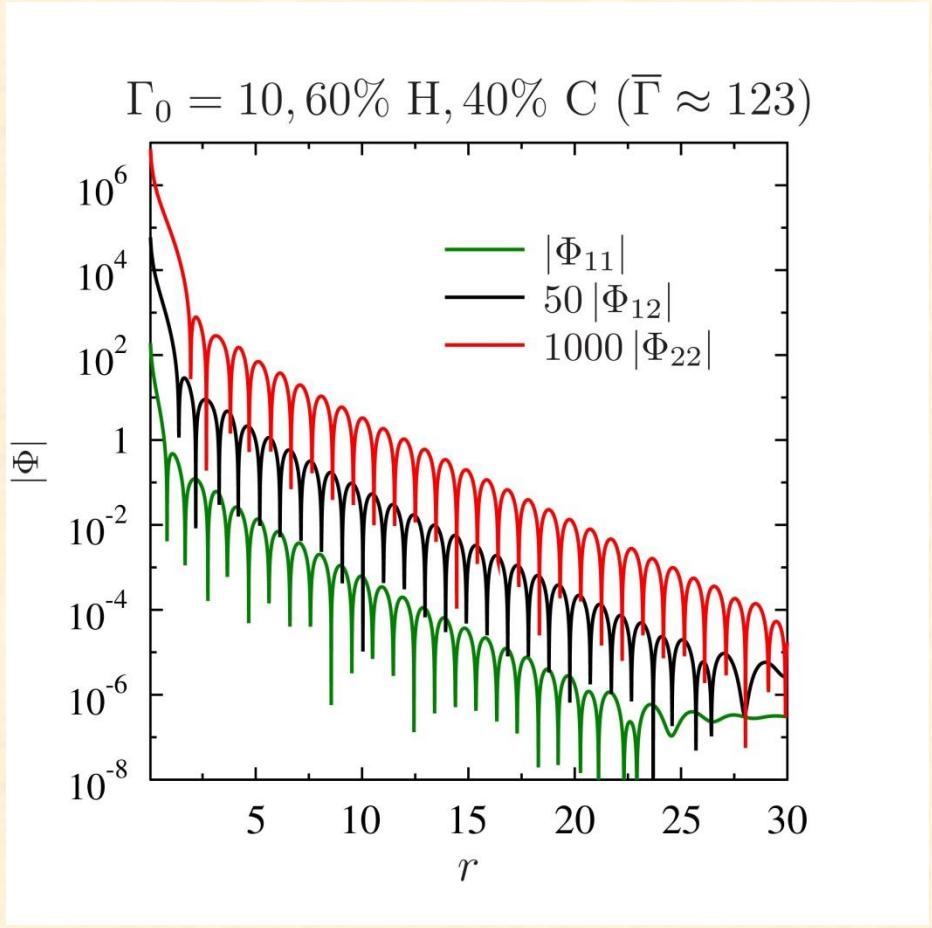


$$\Phi_{ij,\mathrm{SSCP}}(r) = \frac{Z_i Z_j \Gamma_0}{r} \exp\left(-\frac{r}{r_D}\right), \quad \frac{1}{r_D} = \sqrt{3\Gamma_0 \overline{Z^2}}, \quad r_D - \text{ Debye screening length}$$






$\Gamma_0 = 10, 60\%$ H, 40% C ($\overline{\Gamma} \approx 123$)
RDFs
r
g_{11}
g_{12}
g_{22}
0.0
0.5
1.0
1.5
2.0
2.5
0
1
2
3
4
5
6
7


$\Gamma_0 = 10, 60\%$ H, 40% C ($\overline{\Gamma} \approx 123$)
$|\Phi|$
r
$|\Phi_{11}|$
$50\,|\Phi_{12}|$
$1000\,|\Phi_{22}|$
10^{6}
10^{4}
10^{2}
1
10^{-2}
10^{-4}
10^{-6}
10^{-8}
5
10
15
20
25
30

Chapman-Enskog classical expression for the principal-order approximation to diffusion coefficient (*here in dimensional SGS units*)

$$D_{12} = \frac{3}{16}\frac{k_B T}{\mu n}\frac{1}{\tilde{\Omega}_{12}^{(1,1)}}$$

Introduce "hydrodynamic" plasma frequency:

$$\omega_p = \sqrt{\frac{4\pi n \overline{Z}^2 e^2}{\overline{A} m_0}}$$

and derive the diffusion coefficient in the units of $\omega_p a^2$:

$$D_{12}^* = \frac{D_{12}}{\omega_p a^2} = \frac{\pi^{3/2}}{2\sqrt{6}}\frac{1}{\sqrt{\Gamma_0}}\sqrt{\frac{\overline{A}\left(A_1 + A_2\right)}{\overline{Z}^2 A_1 A_2}}\frac{1}{\Omega_{12}^{(1,1)}}$$

Dimensionless collision integrals are:

$$\Omega_{12}^{(\xi,\zeta)} = \int_0^\infty \exp\left(-y^2\right) y^{2\zeta+3} Q_{12}^{(\xi)}(y)\, dy,$$

$$Q_{12}^{(\xi)}(u) = 2\pi \int_0^\infty \left(1 - \cos^\xi\left(\chi_{12}(b,u)\right)\right) b\, db,$$

$$\chi_{12}(b,u) = \left| \pi - 2b \int_{r_{12}^{\min}}^\infty \frac{dr}{r^2 \sqrt{1 - \frac{b^2}{r^2} - \frac{\phi_{12}}{u^2}}} \right|$$

$r_{12}^{\min}$ = classical distance of closest approach, u = relative velocity at infinity, b = impact parameter, χ = scattering angle, ϕ_{12} = interaction potential between particles 1 and 2.

In WC plasma we express diffusion coefficients analytically in terms of Coulomb logarithm:

$$D_{12}^{*(\mathrm{WC})} = \sqrt{\frac{\pi}{6}}\frac{1}{\Gamma_0^{5/2}}\sqrt{\frac{\overline{A}\left(A_1+A_2\right)}{\overline{Z}^2 A_1 A_2}}\frac{1}{Z_1^2 Z_2^2 \Lambda^{(\mathrm{WC})}},$$

$$\Lambda^{(\mathrm{WC})} = \ln\left(\frac{1}{\sqrt{3}\Gamma_0^{3/2} Z_1 Z_2 \sqrt{\overline{Z^2}}}\right), \Lambda^{(\mathrm{WC})} \gg 1$$

$\Lambda^{(\mathrm{WC})}$ has a simple physical meaning:

$$\Lambda^{(\mathrm{WC})} = \ln\left(\frac{\rho_{\max}}{\rho_{\min}}\right), \rho_{\max} = r_D = \sqrt{\frac{k_B T}{4\pi e^2\left(Z_1^2 n_1 + Z_2^2 n_2\right)}} \gg \rho_{\min} = \frac{Z_1 Z_2 e^2}{k_B T}$$

Our idea is to retain the same expression as for WC plasma, but suitable for arbitrary coupling strength. To achieve this, we replace $\Lambda^{(WC)}$ with Λ_{eff}.

$$D_{12}^{*(WC)} = \sqrt{\frac{\pi}{6}} \frac{1}{\Gamma_0^{5/2}} \sqrt{\frac{\overline{A}\left(A_1 + A_2\right)}{\overline{Z}^2 A_1 A_2}} \frac{1}{Z_1^2 Z_2^2 \Lambda^{(WC)}} \rightarrow$$

$$\rightarrow D_{12}^{*} = \sqrt{\frac{\pi}{6}} \frac{1}{\Gamma_0^{5/2}} \sqrt{\frac{\overline{A}\left(A_1 + A_2\right)}{\overline{Z}^2 A_1 A_2}} \frac{1}{Z_1^2 Z_2^2 \Lambda_{eff}}$$

Effective Coulomb logarithm is defined as:

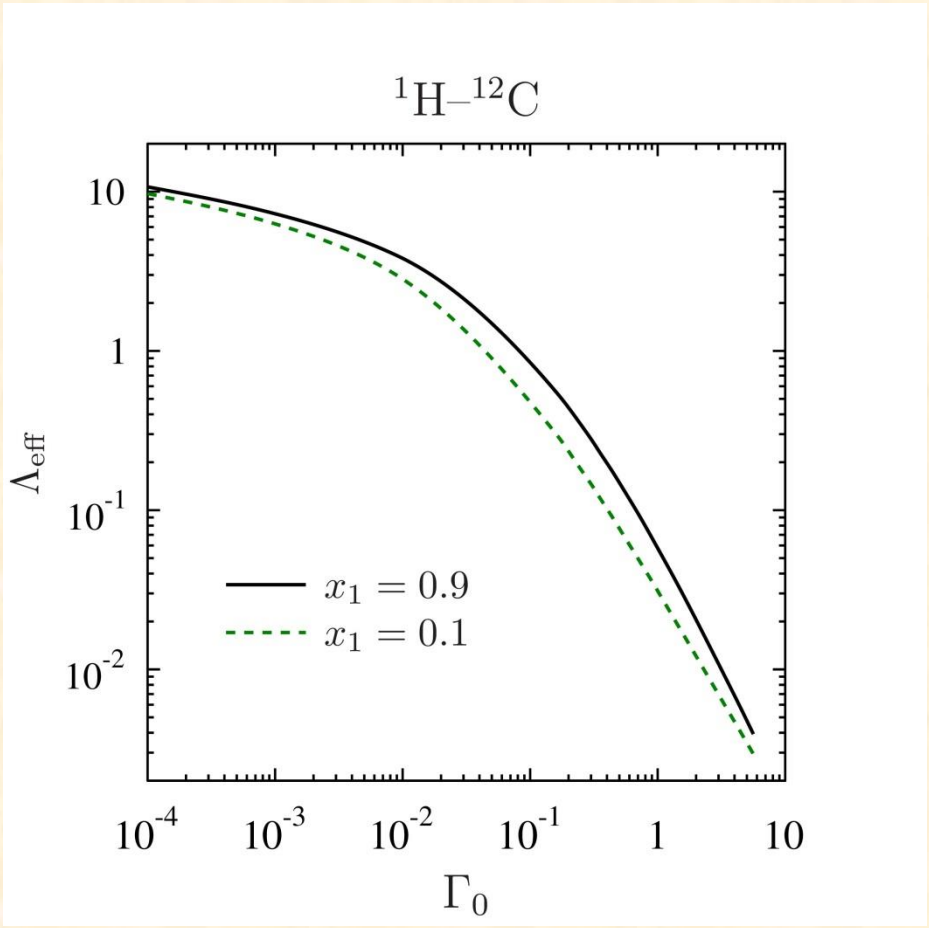
$$\Lambda_{eff} = \sqrt{\frac{\pi}{6}} \frac{1}{D_{12}^{*} Z_1^2 Z_2^2 \Gamma_0^{5/2}} \sqrt{\frac{\overline{A}\left(A_1 + A_2\right)}{\overline{Z}^2 A_1 A_2}}$$

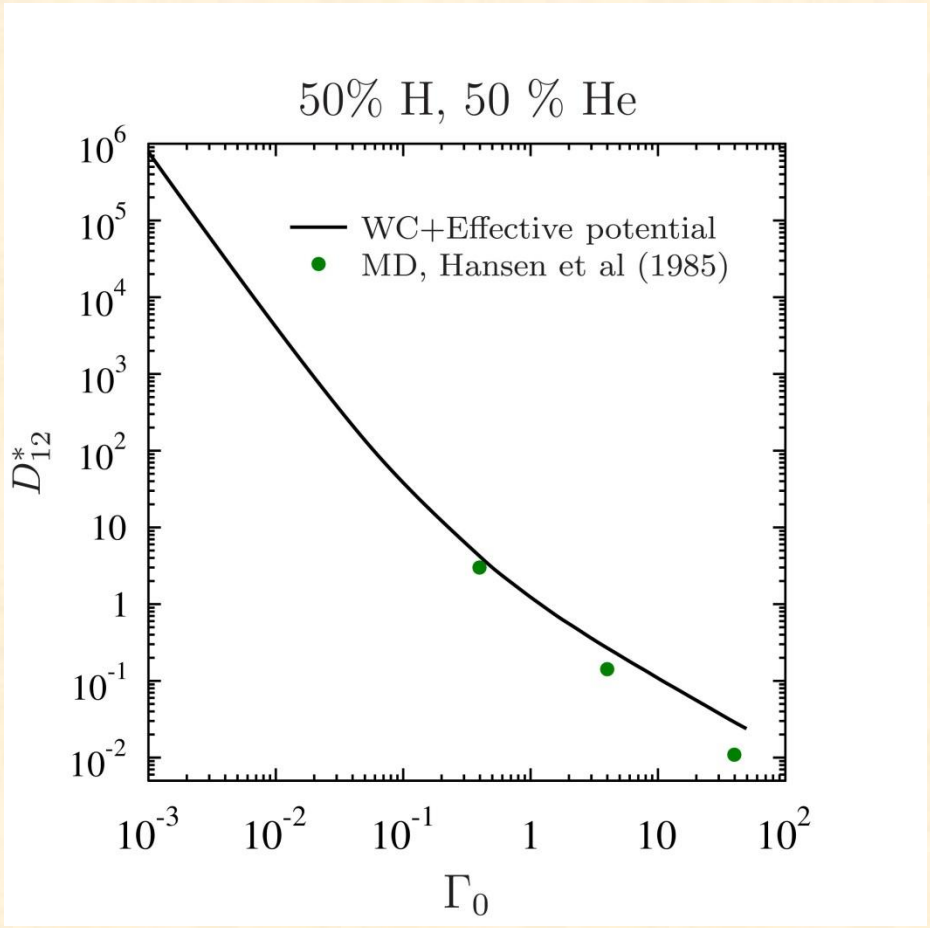
Analytic fit for Λ_{eff}

$$\Lambda_{eff}\left(\Gamma_0, x_1\right) = \ln\left(1 + \frac{p_1 x_1^2 + p_2 x_2^2 + p_3}{\Gamma_0^{p_4 x_1 + p_5}}\right)$$

Mixture	p_1	p_2	p_3	p_4	p_5	$\delta_{rms,}$ %	$\delta_{max,}$ %	$(x_1,\Gamma_0)_{max}$
^{1}H - ^{4}He	**$7.43*10^{-2}$**	**$-1.13*10^{-2}$**	**$1.72*10^{-1}$**	**$8.57*10^{-2}$**	**1.45**	**3.1**	**10**	**(0.7,0.4)**
^{1}H - ^{12}C	**$3.80*10^{-2}$**	**$6.57*10^{-3}$**	**$2.52*10^{-2}$**	**$1.39*10^{-1}$**	**1.34**	**5.6**	**18**	**(0.99,0.729)**
^{4}He - ^{12}C	**$7.01*10^{-3}$**	**$9.08*10^{-4}$**	**$1.09*10^{-2}$**	**$1.17*10^{-1}$**	**1.41**	**4.0**	**13**	**(0.9,5.785)**
^{12}C - ^{16}O	**$9.95*10^{-5}$**	**$-6.35*10^{-6}$**	**$1.61*10^{-3}$**	**$3.96*10^{-2}$**	**1.48**	**2.6**	**10**	**(0.9,0.015)**
^{16}O -^{79}Se	**$7.22*10^{-5}$**	**$5.00*10^{-5}$**	**$1.14*10^{-4}$**	**$1.33*10^{-1}$**	**1.38**	**4.1**	**16**	**(0.9,0.187)**

Λ_{eff} (left) and comparison with results of Hansen et al, Physica A **132**,472 (1985) (right)





Discussion

Well-known rule for approximate calculation of inter-diffusion coefficient via self-diffusion coefficients (Hansen et al, Physica A **132**,472,1985):

$$D_{12} \approx x_2 D_{11} + x_1 D_{22}$$

We established a similar rule:

$$D_{12}(n,T) \approx D_{12}^{\mathrm{S}}(n,\mathrm{T}) = x_2 D_1(\tilde{n}_1,T) + x_1 D_2(\tilde{n}_2,T), \text{ where } \tilde{n}_j = \frac{\overline{Z^2}}{Z_j^2} n$$

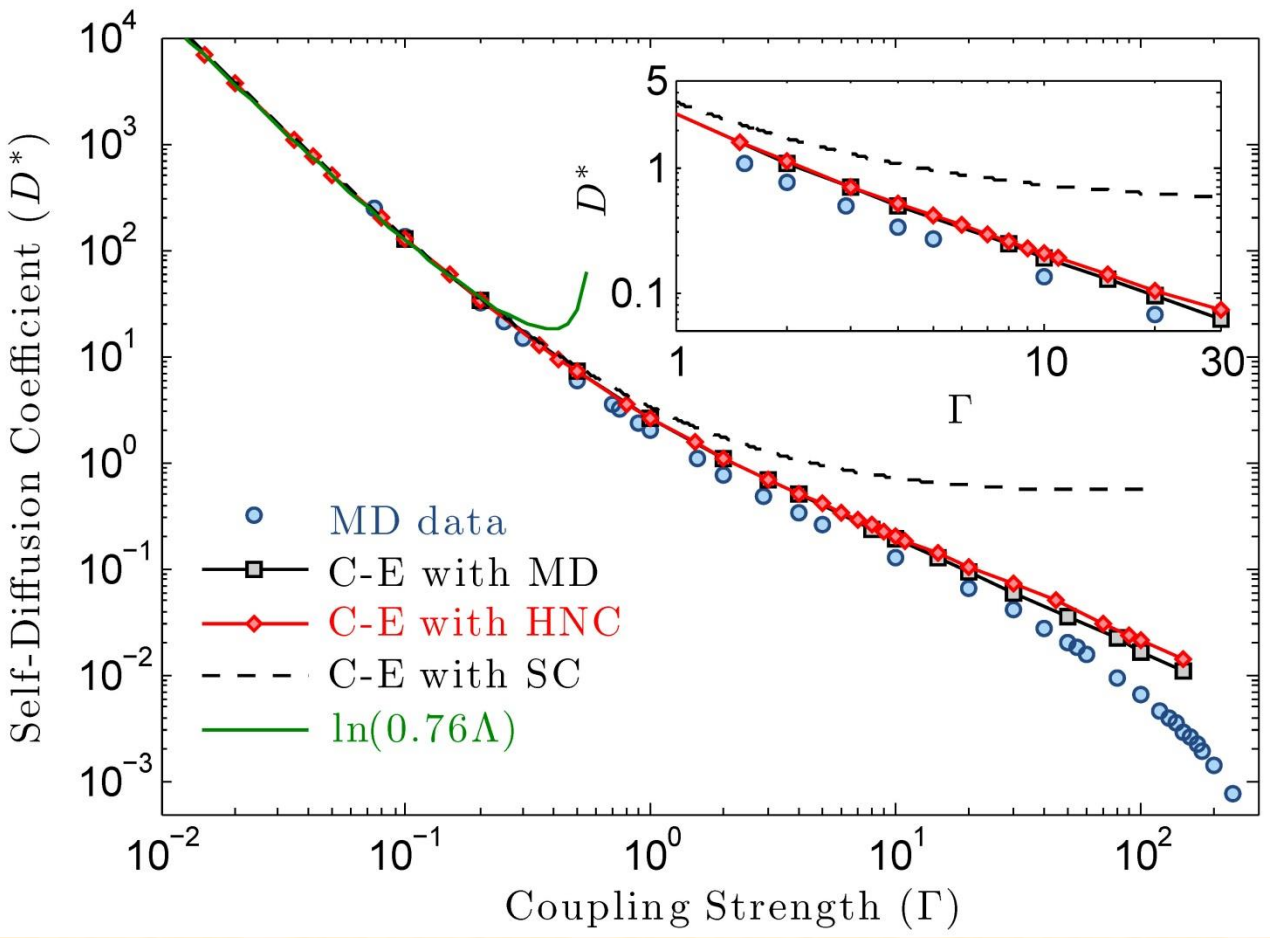
Such choice of $\tilde{n}_j$ ensures that "equivalent" OCPs have the same Debye screening length as the source BIM.

This rule works not only for WC plasma, but for SC plasma as well.

Discussion

^{1}H - ^{4}He					^{1}H - ^{12}C			
x_1	Γ_0	D_{12}^{*}	D_{12}^{*S}	D_{12}^{*MD}	x_1	Γ_0	D_{12}^{*}	D_{12}^{*S}
0.5	**0.397**	**4.20**	**3.73**	**3.00**	**0.2**	**5.75**	**0.0572**	**0.0322**
0.5	**3.992**	**0.268**	**0.230**	**0.142**	**0.5**	**5.75**	**0.0635**	**0.0354**
0.5	**39.738**	**0.0290**	**0.0242**	**0.0109**	**0.8**	**5.75**	**0.0688**	**0.0445**
0.75	**40.831**	**0.0279**	**0.0235**	**0.0122**				
0.25	**40.610**	**0.0277**	**0.0237**	**0.0076**				

Corrections to HNC calculation scheme



The graph is taken from

S. D. Baalrud and J. Daligault, PRL **110**, 235001 (2013).

Conclusions

Coulomb separation velocity in NSs' outer envelopes can reach up to one meter per year and more.

Full separation of helium from carbon in NS's outer envelope should occur on the timescale of several hundred years

Diffusion in NS's "heating blanket" greatly affects its chemical composition and, hence, heat conductivity. Thus, diffusion can greatly change NS cooling process.

As NS's outer envelope is not isothermal, precise calculations should take into account temperature variations. Therefore, one needs thermal diffusion coefficients in SC plasma.

They will also allow us to study how Coulomb interaction affects diffusive nuclear burning.

Conclusion

- For the first time effective potential method was applied to calculation of inter-diffusion coefficients in binary ionic mixtures.
- Despite some drawbacks (like systematical deviation from MD results) this method allows to make computations with reasonable accuracy and is suitable for further use.
- The method is applicable to any BIM in both WC and SC plasmas (in gaseous or liquid, but not solid state).
- We performed calculations for several ionic mixtures and presented the results in convenient and easy to use form of analytical fits to effective Coulomb logarithm.

We are planning to extend these results to non-isothermal systems and properly take into account thermodiffusion (contribution to the diffusive flux and thermodiffusion coefficient).

Thank you for your attention!