Thermodynamic functions of dense plasmas:
analytical approximations for astrophysical applications

Alexander Y. Potekhin[1] and **Gilles Chabrier**[2]

in collaboration with

A. I. Chugunov,[1] **H. E. DeWitt,**[3] **F. J. Rogers**[3]

[1] Ioffe Physical-Technical Institute, Saint-Petersburg 194021, Russia
[2] Ecole Normale Supérieure de Lyon, CRAL (UMR CNRS No.5574), 69364 Lyon, France
[3] Lawrence Livermore National Laboratory, Livermore, California 94550, USA

Basic parameters and notations

Electron number density n_e, temperature T (+ magnetic field B).

Ion number density n_i; $n_e = \langle Z \rangle n_\mathrm{i}$ $\quad n_\mathrm{i} = \sum_j n_j$ $\quad \langle f \rangle = \sum_j x_j f_j$ $\quad x_j \equiv \frac{n_j}{n_\mathrm{i}}$

Density parameter $r_s = a_e / a_0 = 1.172\, n_{24}^{-1/3} = (\rho_0/\rho)^{1/3}$ where $\rho_0 = \rho/(1\text{ g cm}^{-3})$

$$a_e = \left(\frac{4}{3}\pi n_e\right)^{-1/3} \qquad a_0 = \frac{\hbar^2}{m_e e^2} \qquad n_{24} \equiv \frac{n_e}{10^{24}\text{ cm}^{-3}}$$

Mass density $\rho = \frac{n_{24}}{1.66}\frac{A'}{\langle Z \rangle}$ $\quad A' \equiv \langle A \rangle + A''$ $\quad \rho_0 = 2.675\,\frac{A'}{\langle Z \rangle}\text{ g cm}^{-3}$

$$R_S = a_\mathrm{i}\frac{m_\mathrm{i}(Ze)^2}{\hbar^2} = 1822.9\, r_s\, A Z^{7/3} \qquad a_\mathrm{i} \equiv \left(\frac{4}{3}\pi n_\mathrm{i}\right)^{-1/3} = a_e Z^{1/3}$$

Fermi momentum $p_F = \hbar\,(3\pi^2 n_e)^{1/3}$

Relativity: $x_\mathrm{r} = \frac{p_F}{m_e c} = 1.00884 \left(\frac{\rho_6 \langle Z \rangle}{A'}\right)^{1/3} = 0.014005\, r_s^{-1}$

$$\gamma_\mathrm{r} \equiv \sqrt{1 + x_\mathrm{r}^2}$$

Basic parameters (continued)

(Kinetic) Fermi energy $\epsilon_{\mathrm{F}} = c\sqrt{(m_e c)^2 + p_F^2} - m_e c^2 = m_e c^2\,(\gamma_{\mathrm{r}} - 1)$

Fermi temperature $T_{\mathrm{F}} \equiv \frac{\epsilon_{\mathrm{F}}}{k_{\mathrm{B}}} = T_{\mathrm{r}}\,(\gamma_{\mathrm{r}} - 1) \approx \begin{cases} 1.163 \times 10^6\, r_s^{-2}\ \mathrm{K} & (x_{\mathrm{r}} \ll 1) \\ T_{\mathrm{r}} x_{\mathrm{r}} & (x_{\mathrm{r}} \gg 1) \end{cases}$

Relativistic unit of T: $T_{\mathrm{r}} \equiv \frac{m_e c^2}{k_{\mathrm{B}}} = 5.93 \times 10^9\ \mathrm{K}$ $\quad \tau \equiv T/T_{\mathrm{r}}$ $\quad$ (non)degeneracy: $\theta \equiv T/T_{\mathrm{F}}$

Coupling parameters: $\Gamma_j = \frac{(Z_j e)^2}{a_j k_{\mathrm{B}} T} = \Gamma_e Z_j^{5/3}$ $\quad \Gamma_e \equiv \frac{e^2}{a_e k_{\mathrm{B}} T} \approx \frac{22.75}{T_6}\left(\rho_6 \frac{\langle Z \rangle}{A'}\right)^{1/3}$

$a_j = a_e Z_j^{1/3}$ $\quad \Gamma = \Gamma_e \langle Z^{5/3} \rangle$

Thermal de Broglie wavelengths: $\lambda_j = \left(\frac{2\pi\hbar^2}{m_j k_{\mathrm{B}} T}\right)^{1/2}$ $\quad \lambda_e = \left(\frac{2\pi\hbar^2}{m_e k_{\mathrm{B}} T}\right)^{1/2}$

Ion plasma frequency and ion plasma temperature:

$$\omega_{\mathrm{p}} = \left(4\pi e^2 n_{\mathrm{i}} \left\langle Z^2/m_{\mathrm{i}} \right\rangle\right)^{1/2} \qquad T_{\mathrm{p}} \equiv \frac{\hbar\omega_{\mathrm{p}}}{k_{\mathrm{B}}} \approx 7.832 \times 10^6 \left(\frac{\rho_6}{A'}\left\langle \frac{Z^2}{A} \right\rangle\right)^{1/2}\ \mathrm{K}$$

Ionic quantum parameter: $\eta = \frac{T_{\mathrm{p}}}{T}$ $\quad$ OCP: $\eta \approx 7.832 \frac{Z\sqrt{\rho_6}}{T_6 A}$

Free energy decomposition

$$F = F_{\rm id}^{\rm i} + F_{\rm id}^{(e)} + F_{ee} + F_{\rm ii} + F_{\rm ie}.$$

$$P = -(\partial F/\partial V)_T \qquad S = -(\partial F/\partial T)_V \qquad U = F + TS$$

$$C_V = (\partial S/\partial \ln T)_V \qquad \chi_T = (\partial \ln P/\partial \ln T)_V \qquad \chi_\rho = -(\partial \ln P/\partial \ln V)_T$$

Ideal ion gas

$$F_{\rm id}^{(j)} = N_j k_{\rm B} T \left[\ln(n_j \lambda_j^3/g_j) - 1\right] \qquad F_{\rm id}^{\rm i} = \sum_j F_{\rm id}^{(j)} \qquad S_{\rm mix} = -k_{\rm B} \sum_j N_j \ln x_j$$

OCP: $$F_{\rm id}^{\rm i} = N_{\rm i} k_{\rm B} T \left[\ln(n_{\rm i} \lambda_{\rm i}^3/g_{\rm i}) - 1\right] \qquad \frac{F_{\rm id}^{\rm i}}{N_{\rm i} k_{\rm B} T} = 3\ln\eta - \frac{3}{2}\ln\Gamma - \frac{1}{2}\ln\frac{6}{\pi} - \ln g_{\rm i} - 1$$

Ideal Fermi gas

$$F_{\rm id}^{(e)} = \mu_e N_e - P_{\rm id}^{(e)} V$$

$$P_{\rm id}^{(e)} = \frac{8}{3\sqrt{\pi}} \frac{k_{\rm B} T}{\lambda_e^3} \left[I_{3/2}(\chi_e, \tau) + \frac{\tau}{2} I_{5/2}(\chi_e, \tau)\right] \qquad n_e = \frac{4}{\sqrt{\pi}\,\lambda_e^3} \left[I_{1/2}(\chi_e, \tau) + \tau I_{3/2}(\chi_e, \tau)\right]$$

$$I_\nu(\chi_e, \tau) \equiv \int_0^\infty \frac{x^\nu\,(1 + \tau x/2)^{1/2}}{\exp(x - \chi_e) + 1}\,{\rm d}x \qquad \chi_e = \frac{\mu_e}{k_{\rm B} T}$$

S. I. Blinnikov, N. V. Dunina-Barkovskaya, D. K. Nadyozhin, *Astrophys. J. Suppl. Ser.*, **106**, 171 (1996); erratum: *ibid.*, **118**, 603 (1998);

G. Chabrier, A. Y. Potekhin, *Phys. Rev. E*, **58**, 4941 (1998).

Ideal Fermi gas

(continued: low temperatures, high densities)

$$I_\nu(\chi,\tau) = I_\nu^{\rm nr}(\chi) + \sum_{m=0}^{\infty} (-1)^m \frac{(2m-1)!!\,\tau^{m+1}}{4^{m+1} m!} I_{\nu+m+1}^{\rm nr}(\chi)$$

$$I_\nu^{\rm nr}(\chi) = \int_0^\infty \frac{x^\nu \, {\rm d}x}{e^{x-\chi}+1} = \frac{\chi^{\nu+1}}{\nu+1} + \frac{\pi^2}{6}\nu\,\chi^{\nu-1} + \frac{7\pi^4}{360}\nu(\nu-1)(\nu-2)\,\chi^{\nu-3} + O(\chi^{\nu-5})$$

$$\frac{F_{\rm id}^{(e)}}{V} \approx \frac{P_{\rm r}}{8\pi^2}\left[x_{\rm r}\,(1+2x_{\rm r}^2)\,\gamma_{\rm r} - \ln(x_{\rm r}+\gamma_{\rm r})\right] - P_{\rm r}\,\frac{x_{\rm r}\gamma_{\rm r}\tau^2}{6}$$

$$P_{\rm r} \equiv m_e c^2\,(m_e c/\hbar)^3 = 1.4218\times 10^{25}\ {\rm dyn\ cm}^{-2}$$

$$x_{\rm r} < 10^{-5}: \qquad F_{\rm id}^{(e)}/V \approx P_{\rm r} x_{\rm r}^5/(10\pi^2) - P_{\rm r}\,x_{\rm r}\gamma_{\rm r}\tau^2/6$$

Alternative – numerical calculation, composition of tables, and interpolation

F. X. Timmes, D. Arnett, *Astrophys. J. Suppl. Ser.*, **125**, 277 (1999);
F. X. Timmes, F. D. Swesty, *Astrophys. J. Suppl. Ser.*, **126**, 501 (2000).

Electron exchange and correlation

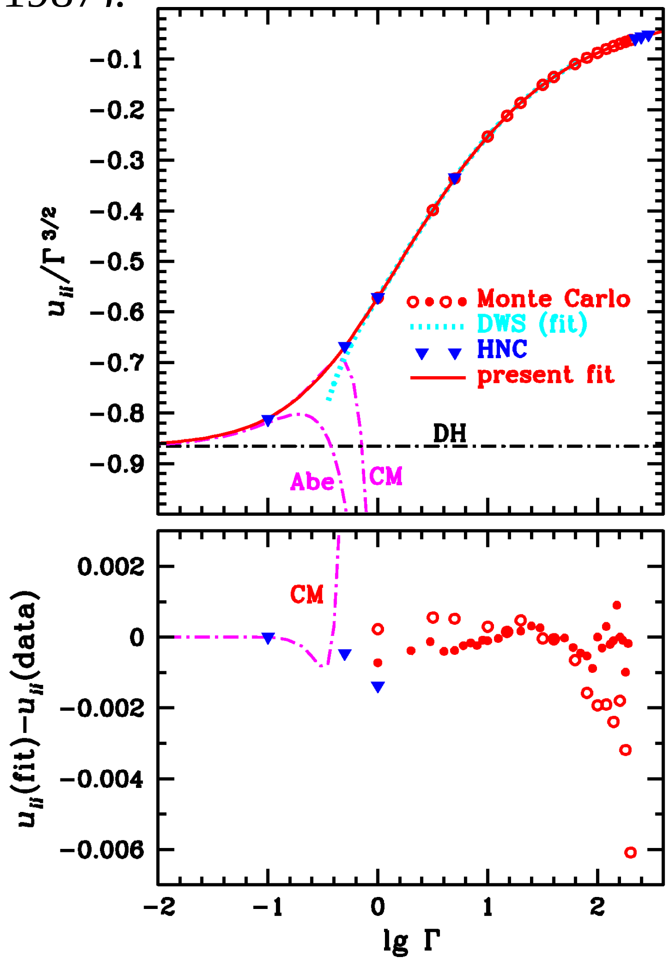
S. Tanaka, S. Mitake, S. Ichimaru, *Phys. Rev. A*, **32**, 1896 (1985);
S. Ichimaru, H. Iyetomi, S. Tanaka, *Phys. Rep.*, **149**, 91 (1987).

Classical ion liquid

The best numerical Monte Carlo results at $1 < \Gamma < 190$:
J. M. Caillol, *J. Chem. Phys.*, **111**, 6538 (1999).

Debye – Hückel formula + corrections up to $O(\Gamma^{9/2} \ln \Gamma)$:
E.G.D. Cohen & T.J. Murphy, *Phys. Fluids*, **12**, 1404 (1969).

Fit formula reproducing Caillol's results at $1 < \Gamma < 190$ with a fractional error $\approx 1/10^6$, and also reproducing the Cohen – Murphy formula at $\Gamma<0,3$
A. Y. Potekhin, G. Chabrier, *Phys. Rev. E*, **62**, 8554 (2000)



Quantum corrections

J. P. Hansen, *Phys. Rev. A*, **8**, 3096 (1973): $$\frac{F_{\rm WK}}{N_{\rm i} k_{\rm B} T} = \frac{\eta^2}{24}$$

Next order corrections – J. P. Hansen, P. Vieillefosse, *Phys. Lett. A*, **53**, 187 (1975).

Numerical results beyond perturbation theory are wanted for quantum liquid

Coulomb (Wigner) crystal

Harmonic approximation:

$$F_{\rm lat} = U_{\rm M} + U_{\rm q} + 3N_{\rm i}k_{\rm B}T\,\langle \ln[1-\exp(-\hbar\omega_{\boldsymbol{k}s}/k_{\rm B}T)]\rangle_{\rm ph}$$

$$U_{\rm M} = N_{\rm i}C_{\rm M}(Ze)^2/a_{\rm i} \qquad U_{\rm q} = \tfrac{3}{2}N_{\rm i}\hbar\omega_{\rm p}u_1 \qquad u_1 = \langle\omega_{\boldsymbol{k}s}\rangle_{\rm ph}$$

With anharmonic corrections, $\dfrac{F_{\rm lat}}{N_{\rm i}k_BT} = C_{\rm M}\Gamma + 1.5u_1\eta + f_{\rm th} + f_{\rm ah}$

$C_{\rm M}$, u_1, $f_{\rm th}$: analytic formulae [D. A. Baiko, A. Y. Potekhin, D. G. Yakovlev, 2001, *Phys. Rev. E*, **64**, 057402]

Classical anharmonic corrections

R. T. Farouki, S. Hamaguchi, 1993, *Phys. Rev. E*, **47**, 4330: $f_{\rm ah}^{(0)}(\Gamma) = -\sum_{k=1}^{3}\dfrac{a_k}{k\Gamma^k}$

Quantum anharmonic corrections

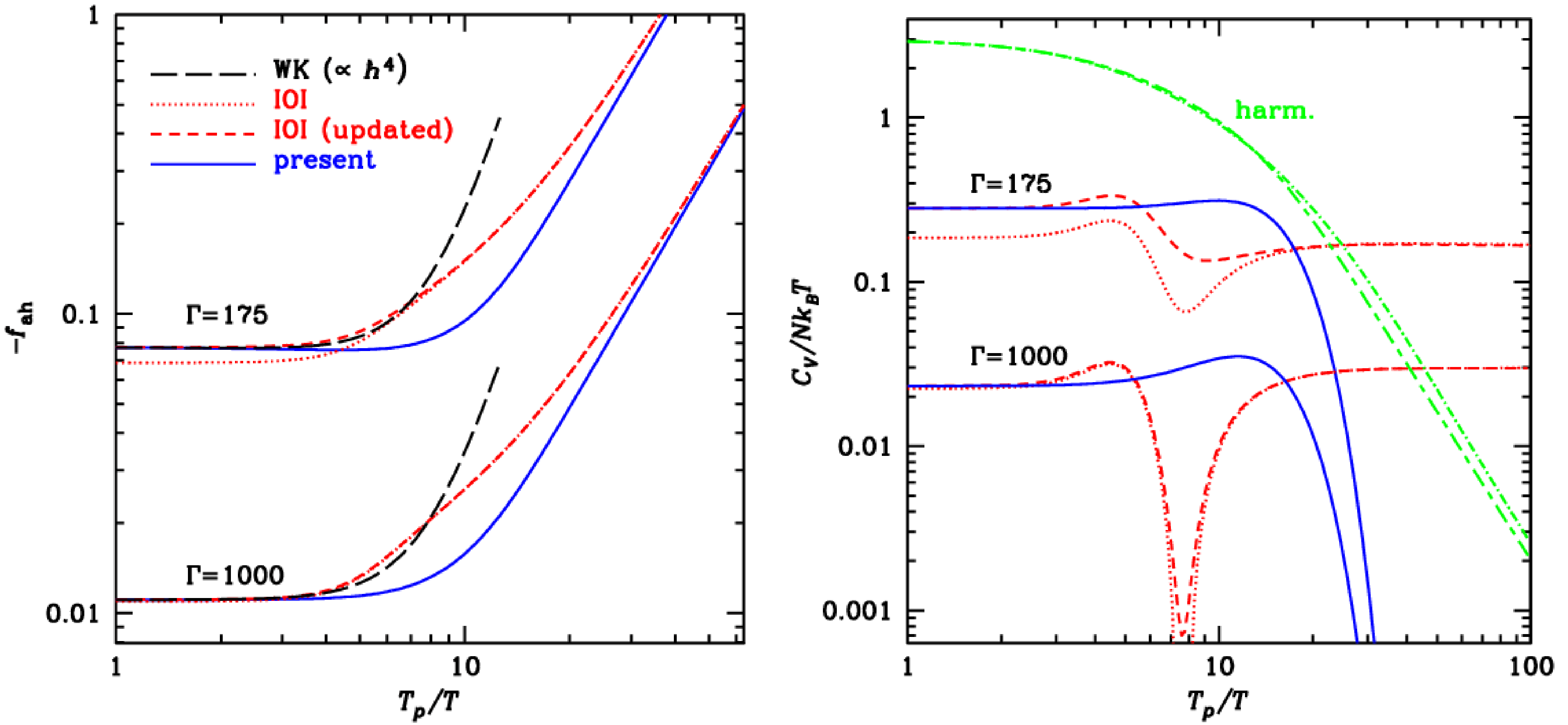
high-T perturbation [J. P. Hansen, P. Vieillefosse, *Phys. Lett. A*, **53**, 187(1975)]

$$f_{\rm ah}^{(4)}(\Gamma,\eta) = f_{\rm ah}^{(0)}(\Gamma) - (0.0018046/\Gamma + 0.085072/\Gamma^2)\,\eta^4$$

T=0 [e.g., W. J. Carr, Jr., et al., *Phys. Rev.*, **124**, 747 (1961)] $u_{{\rm ah},T\to 0} = -\dfrac{b_1\eta^2}{\Gamma}$ $\qquad b_1 \approx 0{,}12$

Interpolation: $f_{\rm ah} = f_{\rm ah}^{(0)}(\Gamma)\,e^{-c_1\eta^2} - \dfrac{b_1\eta^2}{\Gamma}$ $\qquad c_1 = b_1/a_1 \approx 0.0112$

Anharmonic corrections



WK (Wigner – Kirkwood): J. P. Hansen & P. Vieillefosse, *Phys. Lett. A*, **53**, 187 (1975) – perturbation.
IOI: H. Iyetomi, S. Ogata, S. Ichimaru, *Phys. Rev. B*, **47**, 11703 (1993) – simulations and analytic model.
"present" – interpolation

Reliable and usable numerical results beyond perturbation theory and beyond the harmonic model are wanted for quantum crystal

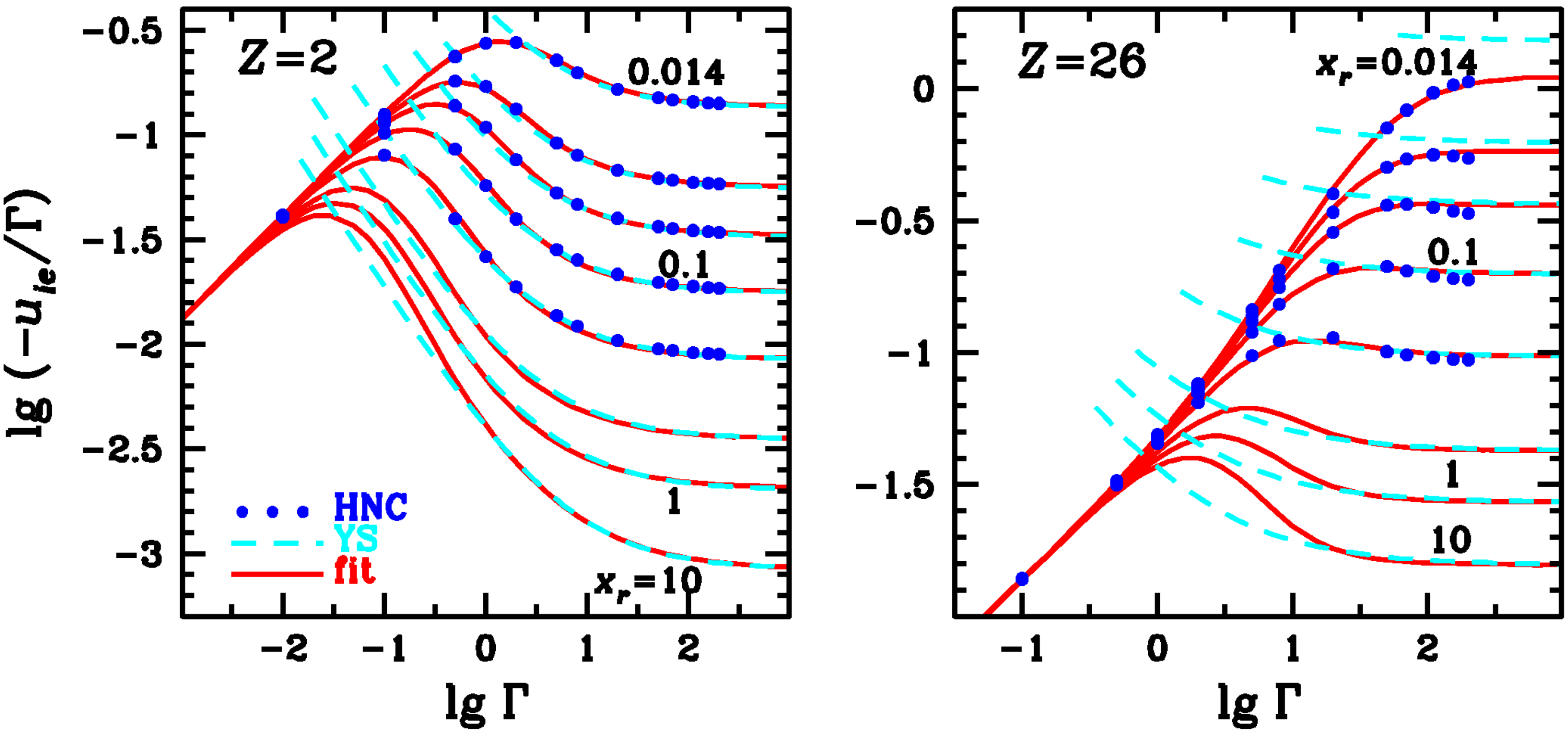
Electron-ion interaction

Electron polarization in Coulomb liquid

Potekhin & Chabrier, *Phys. Rev. E*, **62**, 8554 (2000): HNC calculations + fit

$$f_{\mathrm{ie}} \equiv \frac{F_{\mathrm{ie}}}{N_{\mathrm{i}} k_{\mathrm{B}} T} = -\Gamma_e \frac{c_{\mathrm{DH}}\sqrt{\Gamma_e} + c_{\mathrm{TF}} a \Gamma_e^{\nu} g_1(r_s, \Gamma_e) g_3(x_{\mathrm{r}})}{1 + \left[b\sqrt{\Gamma_e} + a g_2(r_s, \Gamma_e)\Gamma_e^{\nu}/r_s\right]\gamma_{\mathrm{r}}^{-1}}$$

$$c_{\mathrm{DH}} = (Z/\sqrt{3})\left[(1+Z)^{3/2} - 1 - Z^{3/2}\right]$$



Electron-ion interaction

Electron polarization in Coulomb crystal

For Yukawa potential model – S. Hamaguchi, R. T. Farouki, D. H. E. Dubin, *Phys. Rev. E.*, **56**, 4671 (1997).
In the harmonic approximation – D. A. Baiko, *Phys. Rev. E.*, **66**, 056405 (2002).
Semiclassical perturbation theory – Potekhin & Chabrier, *Phys. Rev. E*, **62**, 8554 (2000)
+ update:

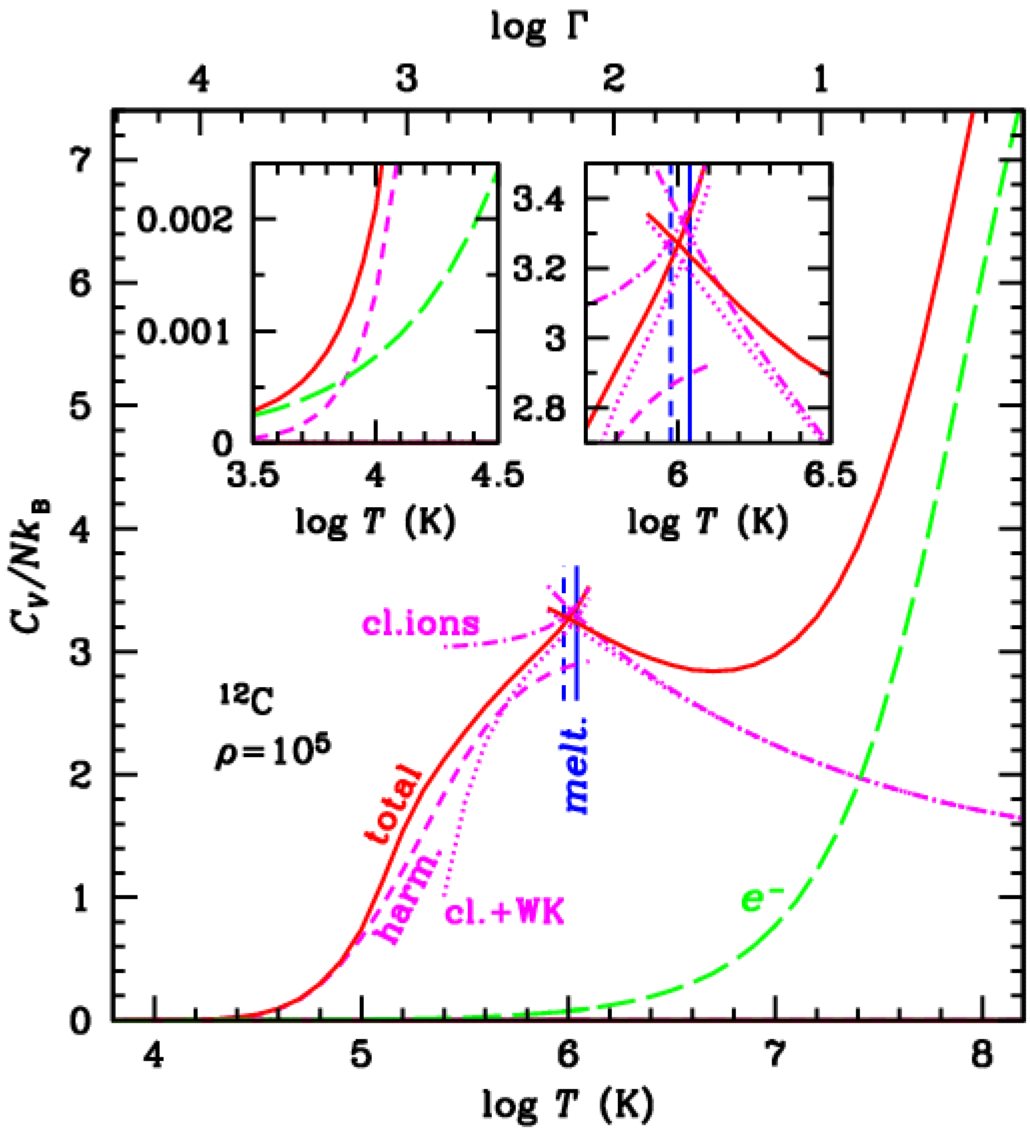
$$f_{\mathrm{ie}} = -f_\infty(x_\mathrm{r})\,\Gamma\left[1 + A(x_\mathrm{r})\left(Q(\eta)/\Gamma\right)^s\right]$$

New formula for quantum suppression factor:

$$Q(\eta) = \left(\frac{\ln\left(1 + e^{(q\eta)^2}\right)}{\ln\left(e - (e-2)e^{-(q\eta)^2}\right)}\right)^{1/2}$$

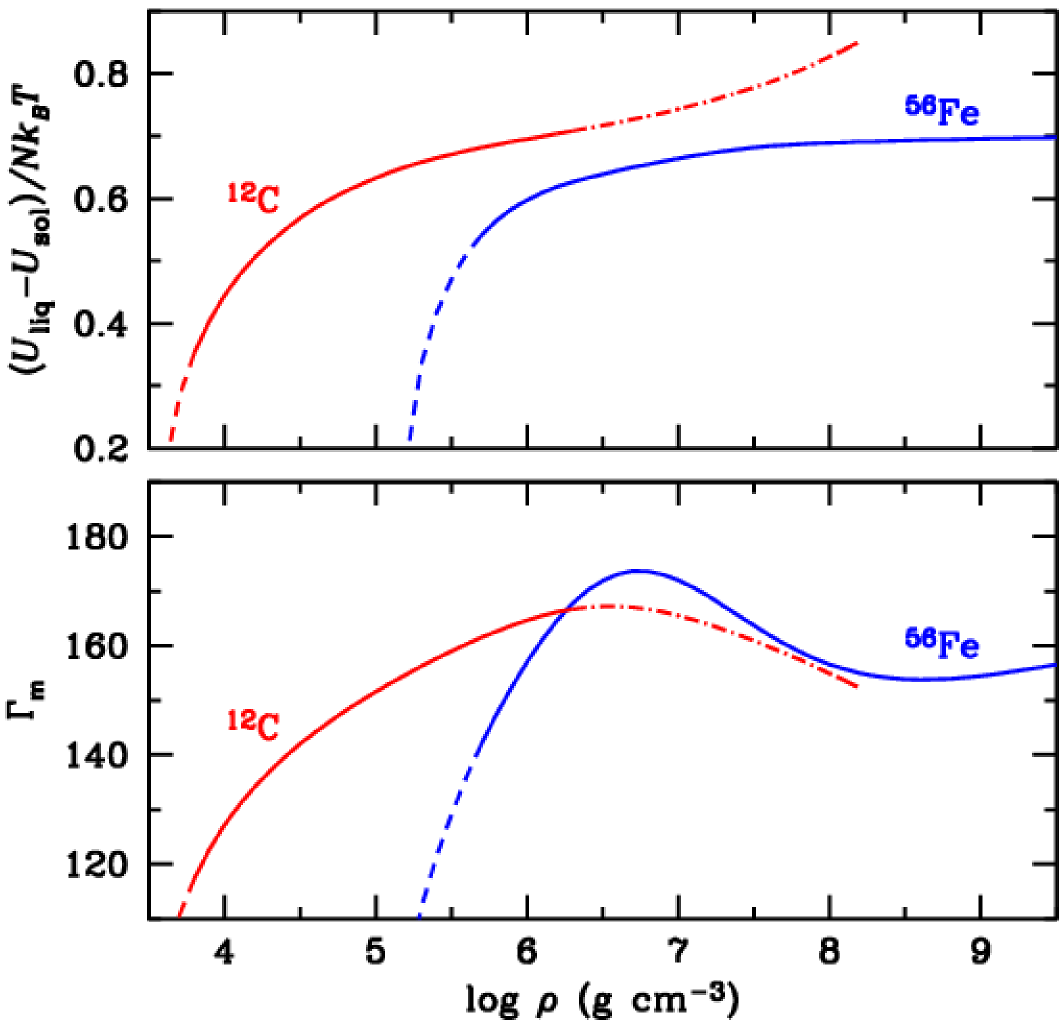
Numerical results beyond perturbation theory and beyond Yukawa-potential and harmonic models are wanted

Heat capacity of plasma in a white dwarf or a neutron star envelope



Various contributions to the heat capacity of carbon at density 10^5 g cm^{-3}

Melting of a Coulomb crystal



Top: Latent heat of carbon and iron as function of denity.
Bottom: Coulomb coupling parameter Γ value at the melting point.

Coulomb plasmas in quantizing magnetic fields

Basic parameters

$$\omega_{\rm c} = \frac{eB}{m_e c} \qquad \beta = \frac{\hbar\omega_{\rm c}}{m_e e^4/\hbar^2} = \frac{B}{2.3505\times 10^9\ {\rm G}} \qquad b = \frac{\hbar\omega_{\rm c}}{m_e c^2} = \alpha^2\beta = \frac{B}{4.414\times 10^{13}\ {\rm G}}$$

"Magnetic length" $a_{\rm m} = \sqrt{\frac{\hbar c}{eB}} = \frac{a_0}{\sqrt{\beta}}$ Landau levels $\epsilon_n = m_e c^2(\sqrt{1+2bn}-1)$

Ion cyclotron frequency: $\omega_{\rm ci} = Z\,(m_e/m_{\rm i})\,\omega_{\rm c}$

Strongly quantizing magnetic field parameters for the electrons:

$$\rho_B = 7045\,\frac{A'}{Z}\,B_{12}^{3/2} \qquad T_B = 1.343\times 10^8 B_{12}\ {\rm K} \qquad T'_B = T_B/\gamma_{\rm r}$$

$$p_F = 2\pi^2 a_{\rm m}^2 \hbar n_e \qquad x_B = 2x_{\rm r}^3/3b$$

Conditions of a direct influence of the magnetic field on the ions in a Coulomb crystal (D.A.Baiko, PhD thesis, 2000):

$$\begin{cases} \omega_{\rm ci} \gtrsim \omega_{\rm p} \\ \hbar\omega_{\rm ci} \gtrsim k_{\rm B}T \end{cases} \Leftrightarrow \begin{cases} B_{12} \gtrsim 100\,\sqrt{\rho_6} \\ B_{12} \gtrsim T/10^5\ {\rm K} \end{cases}$$

Nondegenerate nonrelativistic ions in quantizing magnetic field

$$F_{\rm id}^{\rm i} = N_{\rm i} k_{\rm B} T \left\{ \ln(2\pi a_{\rm m}^2 \lambda_{\rm i} n_{\rm i}) + \ln\left[1 - \exp\left(-\frac{\hbar\omega_{\rm ci}}{k_{\rm B}T}\right)\right] - 1 \right\} + \Delta F$$

$$\Delta F = N_{\rm i} \left\{ \frac{1}{2}\hbar\omega_{\rm ci} - k_{\rm B}T \ln\left[2{\rm ch}\left(\frac{g}{4}\frac{\hbar\omega_{\rm ci}}{k_{\rm B}T}\right)\right] \right\}$$

Partially degenerate relativistic electrons in quantizing magnetic field

$$F_{\rm id}^{(e)} = \mu_e N_e - P_{\rm id}^{(e)} V$$

$$P_{\rm id}^{(e)} = \frac{k_{\rm B}T}{\pi^{3/2} a_{\rm m}^2 \lambda_e} \sum_{n=0}^{\infty} \sum_{\sigma} (1+2bn)^{1/4} I_{1/2}(\chi_n, \tau_n)$$

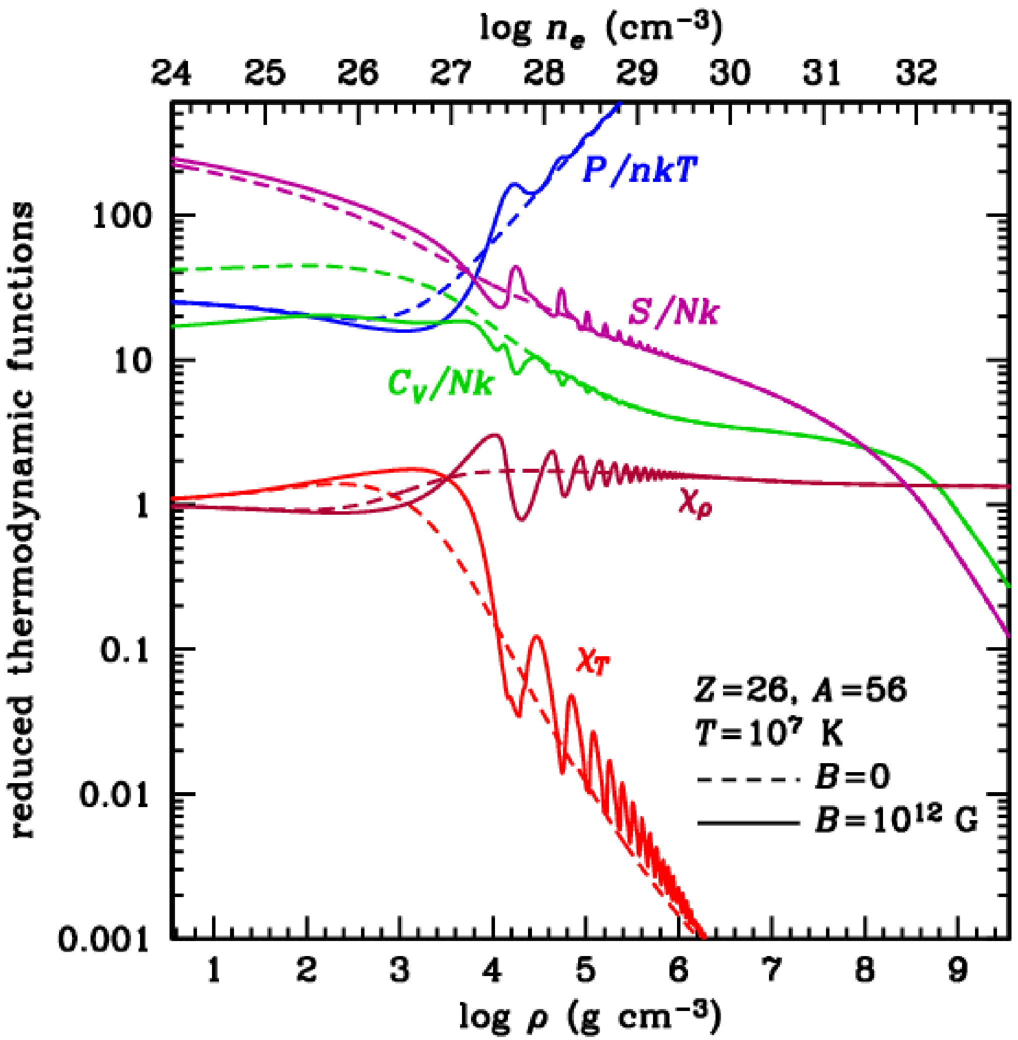
$$n_e = \frac{1}{\pi^{3/2} a_{\rm m}^2 \lambda_e} \sum_{n=0}^{\infty} \sum_{\sigma} (1+2bn)^{1/4} \frac{\partial I_{1/2}(\chi_n, \tau_n)}{\partial \chi_n}$$

$$\tau_n = \tau/\sqrt{1+2bn}, \qquad \chi_n = \chi_e + \tau^{-1} - \tau_n^{-1}$$

Exchange & correlations

Interpolation between different limiting cases:
A. Y. Potekhin, G. Chabrier, Yu. A. Shibanov, *Phys. Rev. E*, 60, 2193 (1999).

Equation of state of magnetic neutron star envelopes



Normalized thermodynamic functions of fully ionized iron without magnetic field (dashed lines) and in a strong magnetic field (solid lines)

Equation of state of multicomponent Coulomb plasmas

Strongly nonideal Coulomb plasma

For every component j one can write $f_{\rm ex} \equiv \frac{F_{\rm ex}}{N_{\rm i} k_{\rm B} T} = f_{\rm ii} + f_{\rm ie} + Z_j f_{ee}$

Linear **M**ixing **R**ule

$$f_{\rm ex}^{\rm LM}(\Gamma) \approx \sum_j x_j f_{\rm ex}(\Gamma_j, x_j = 1), \quad \Gamma_j = \Gamma \frac{Z_j^{5/3}}{\langle Z^{5/3} \rangle}$$

Weakly nonideal Coulomb plasma

Debye – Hückel approximation

$$f_{ee}^{\rm DH} = -\frac{\Gamma_e^{3/2}}{\sqrt{3}} \qquad f_{\rm ii}^{\rm DH} = f_{ee}^{\rm DH} \zeta_{\rm ii}^{\rm DH}, \quad \zeta_{\rm ii}^{\rm DH} = \frac{\langle Z^2 \rangle^{3/2}}{\langle Z \rangle^{1/2}}$$

Debye – Hückel *versus* LMR

$$f_{\rm ii}^{\rm DH} = f_{ee}^{\rm DH}\zeta_{\rm ii}^{\rm DH}, \quad \zeta_{\rm ii}^{\rm DH} = \frac{\langle Z^2\rangle^{3/2}}{\langle Z\rangle^{1/2}} \qquad f_{\rm ii}^{\rm LM} \sim f_{ee}^{\rm DH}\zeta_{\rm ii}^{\rm LM}, \quad \zeta_{\rm ii}^{\rm LM} = \langle Z^{5/2}\rangle,$$

$$f_{\rm ex}^{\rm DH} = f_{ee}^{\rm DH}\zeta_{\rm eip}^{\rm DH}, \quad \zeta_{\rm eip}^{\rm DH} = \frac{(\langle Z^2\rangle + \langle Z\rangle)^{3/2}}{\langle Z\rangle^{1/2}}. \qquad f_{\rm ex}^{\rm LM} \sim f_{ee}^{\rm DH}\zeta_{eip}^{\rm LM}, \quad \zeta_{\rm eip}^{\rm LM} = \langle Z(Z+1)^{3/2}\rangle.$$

Variants of interpolation

Д. К. Надёжин, А. В. Юдин, *Письма в Астрон. журн.*, **31**, 299 (2005)
= D. K. Nadyozhin, A. V. Yudin, *Astronomy Letters*, **31**, 271 (2005)

(a) Mean-ion model (the worst)
(b) Modified LMR

$$f_{\rm ii} = \sum_j x_j f_{\rm ii}(\Gamma_j, x_j = 1; d_j)$$

(b$_1$) $$d_j = \frac{\langle Z^2\rangle^{3/2}}{\langle Z\rangle^{1/2}\langle Z^{5/2}\rangle}$$

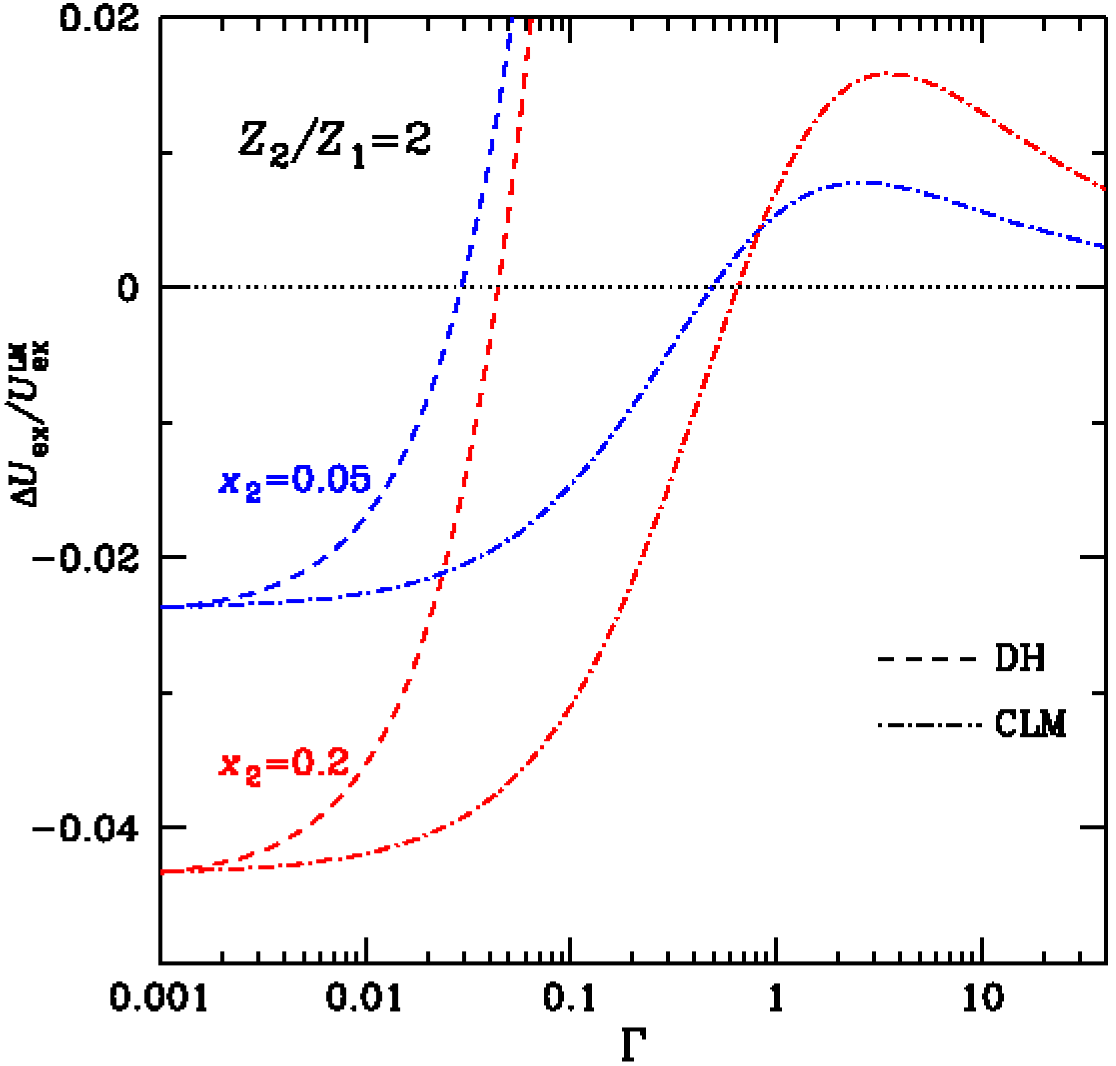
(b$_2$) $$d_j = \sqrt{\frac{\langle Z^2\rangle}{Z_j\langle Z\rangle}}$$

(c) "Complex mixing"

$$f_{\rm ii} = \frac{1}{\langle Z\rangle}\sum_{jk} x_j x_k \tilde{Z}_{jk} f_{\rm ii}(\Gamma_{jk}; d_{jk})$$

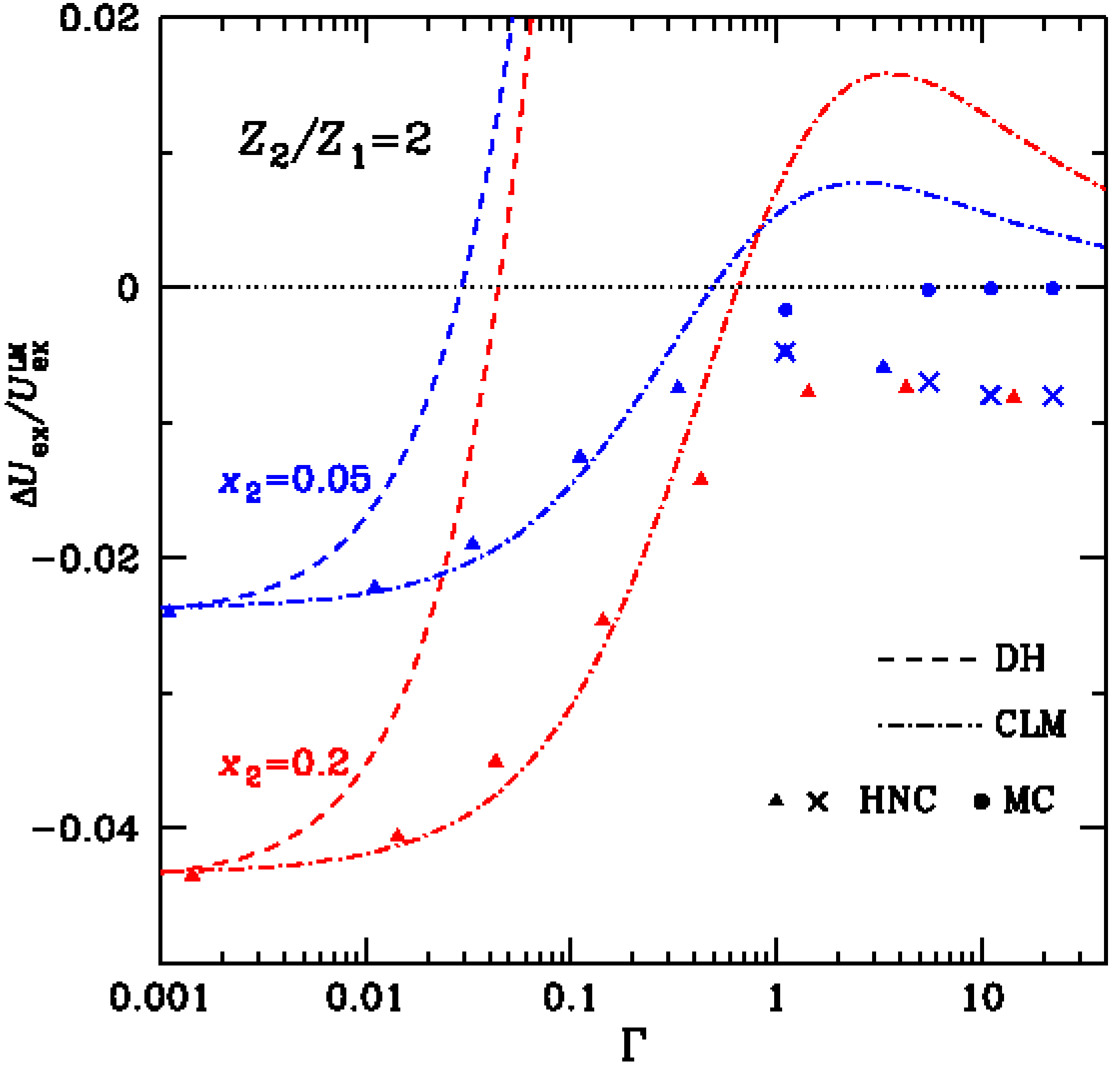
$$\Gamma_{jk} = \frac{2Z_jZ_ke^2}{(a_j + a_k)k_{\rm B}T} \qquad \tilde{Z}_{jk} = \left[\frac{Z_j^{1/3} + Z_k^{1/3}}{2}\right]^3 \qquad d_{jk} = \sqrt{\frac{Z_jZ_k\langle Z\rangle}{\langle Z^2\rangle\tilde{Z}_{jk}}}$$

Internal energy of a binary ionic mixture (BIM)



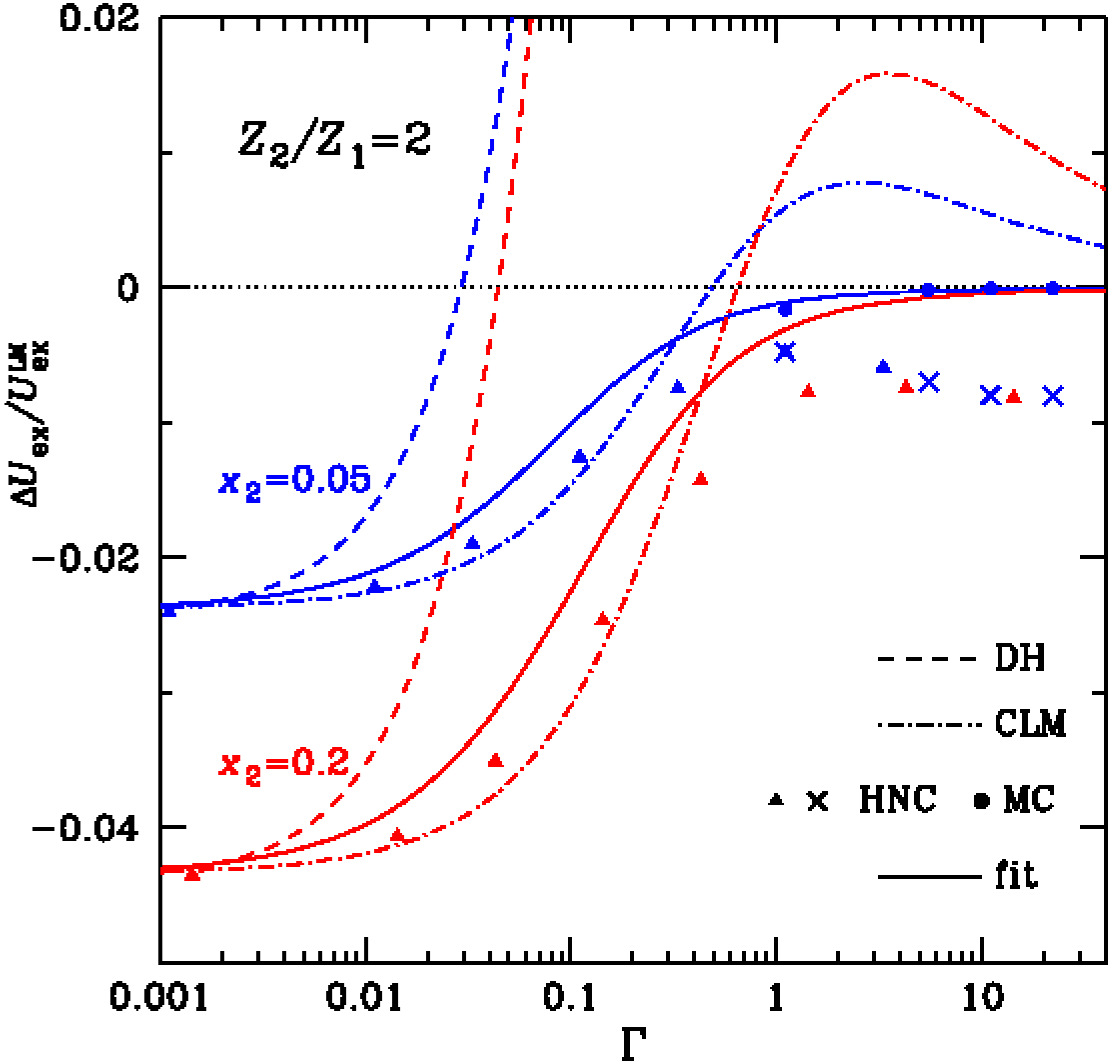
Dashed *lines*: Debye – Hückel approximation.
Dot-dashed *lines*: “modified LMR”

BIM internal energy



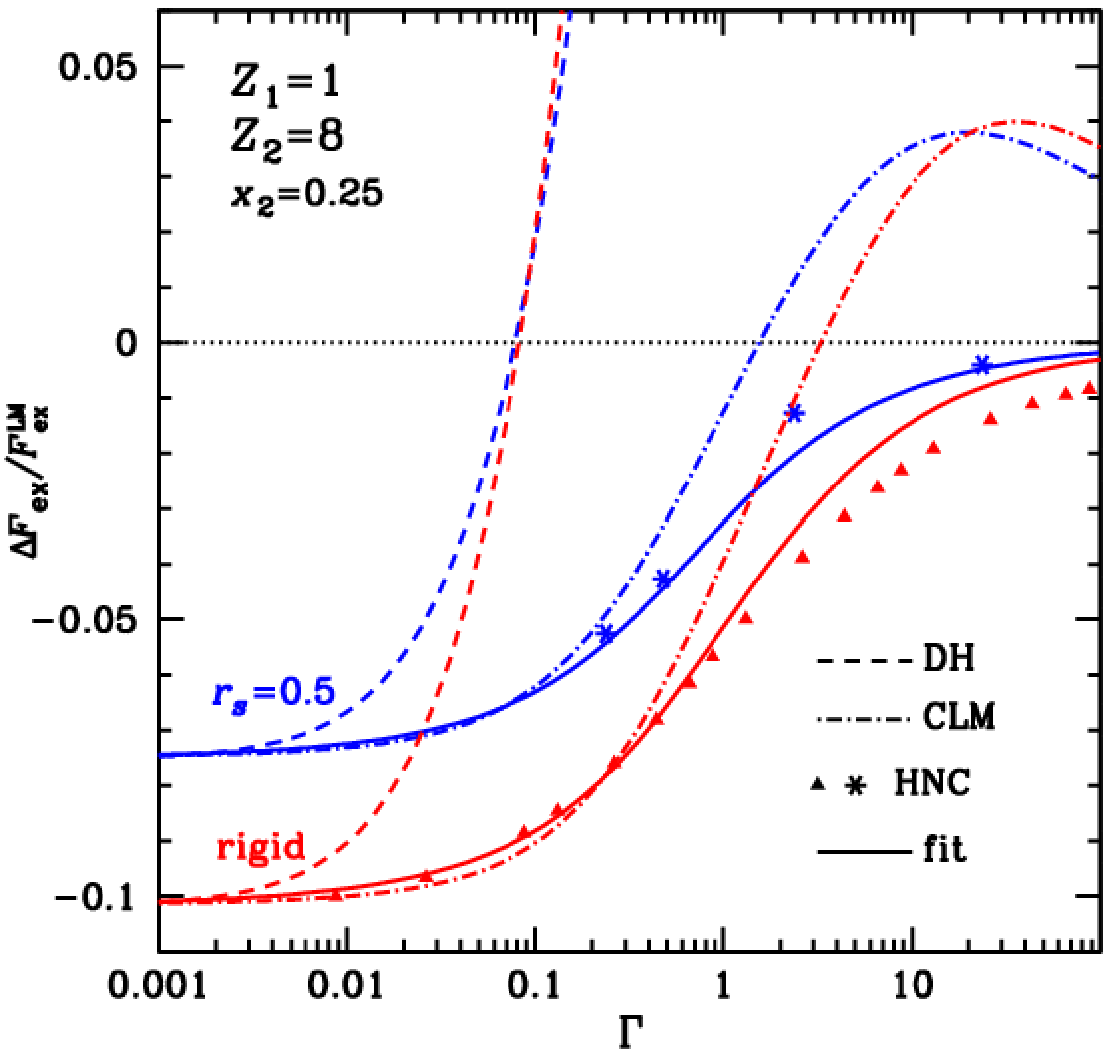
MC (●): H. DeWitt, W. Slattery, G. Chabrier, *Physica B*, **228**, 158 (1996).
HNC: ☒ – G. Chabrier, N. W. Ashcroft, *Phys. Rev. A*, **42**, 2284 (1990); ▲ – 2008.

BIM internal energy



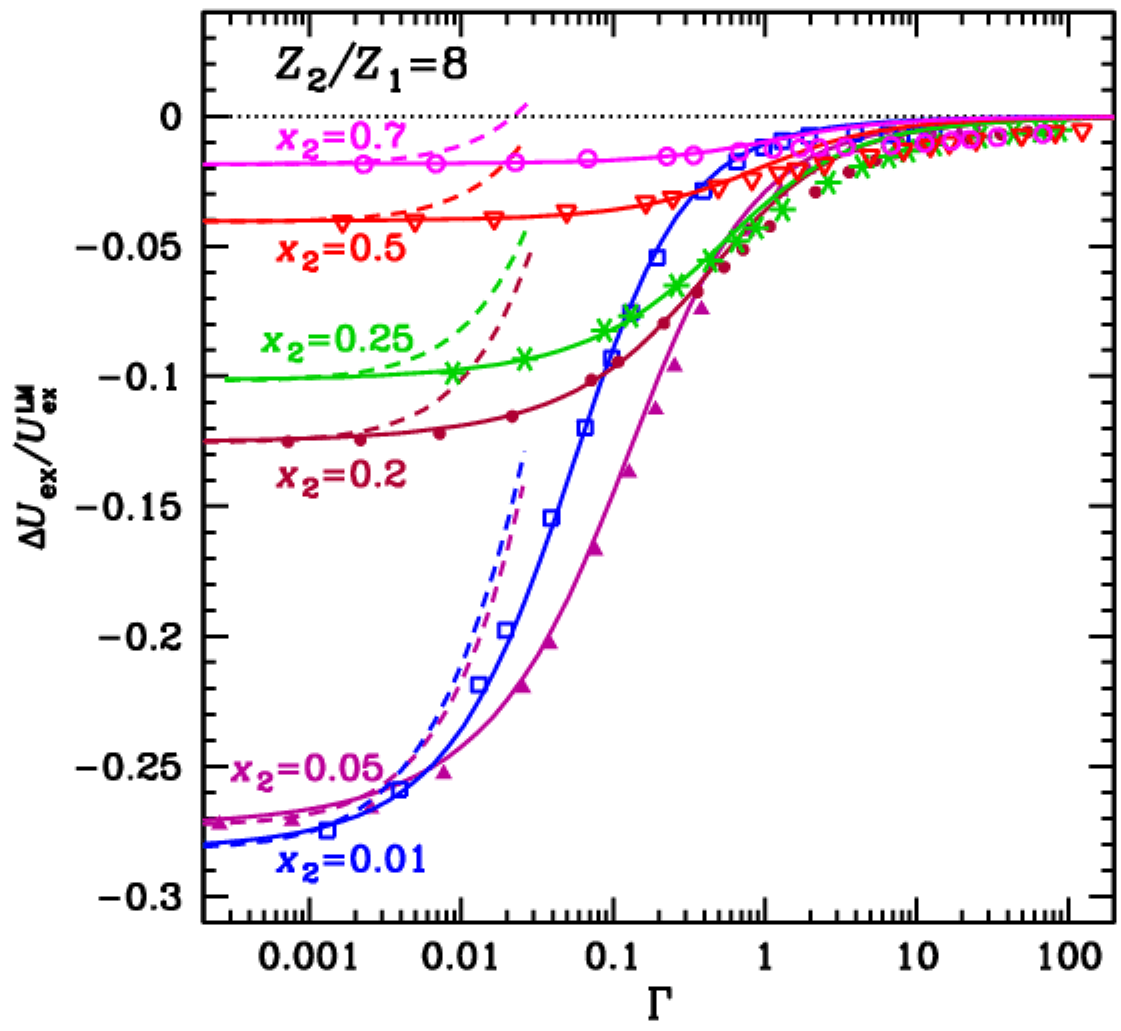
MC (●): H. DeWitt, W. Slattery, G. Chabrier, *Physica B*, **228**, 158 (1996).
HNC: ☒ – G. Chabrier, N. W. Ashcroft, *Phys. Rev. A*, **42**, 2284 (1990); ▲ – 2008.
Solid lines – present approximation.

BIM free energy

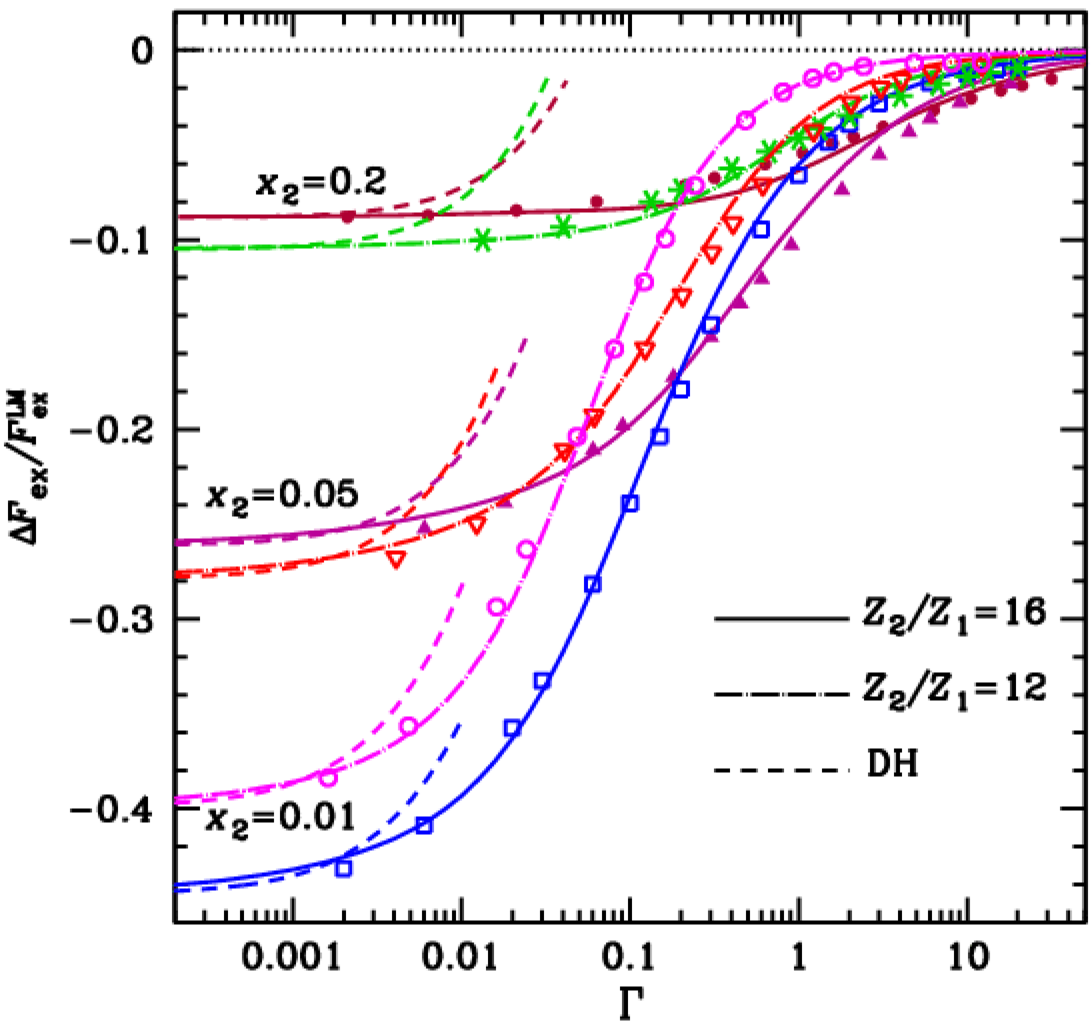


Asterisks – HNC results by G. Chabrier, N. W. Ashcroft, *Phys. Rev. A*, **42**, 2284 (1990).
Triangles – HNC results (2008).
Solid lines – present approximation.

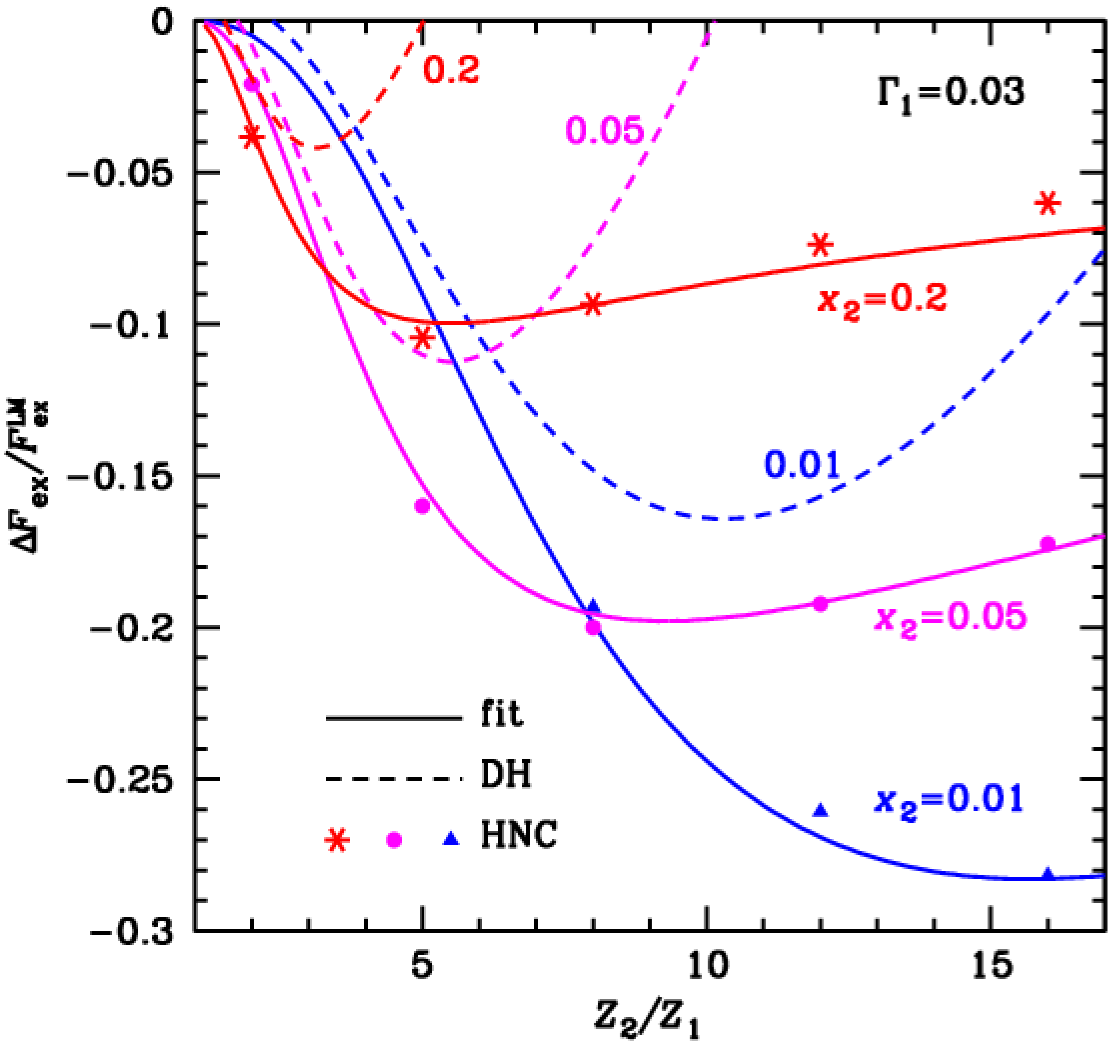
BIM internal energy



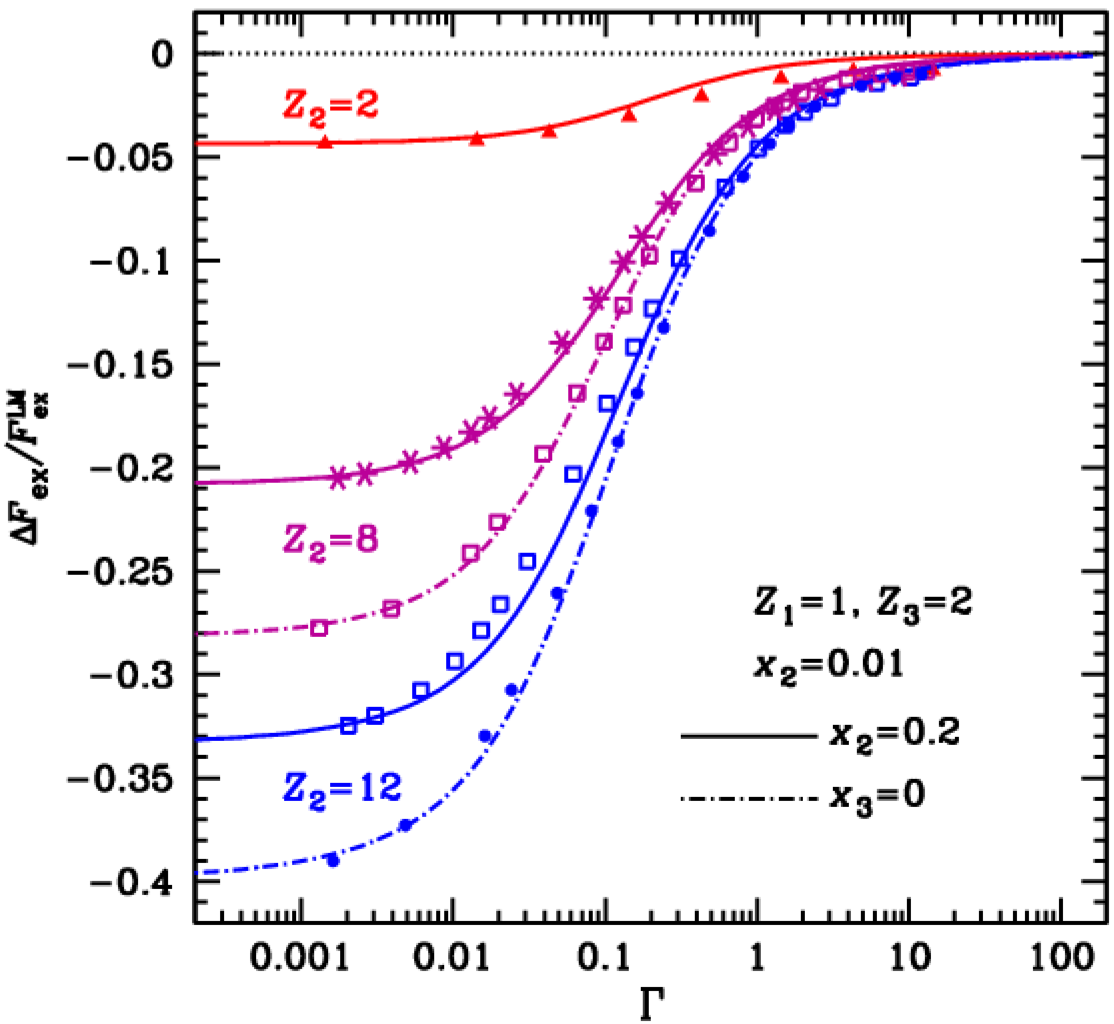
BIM free energy



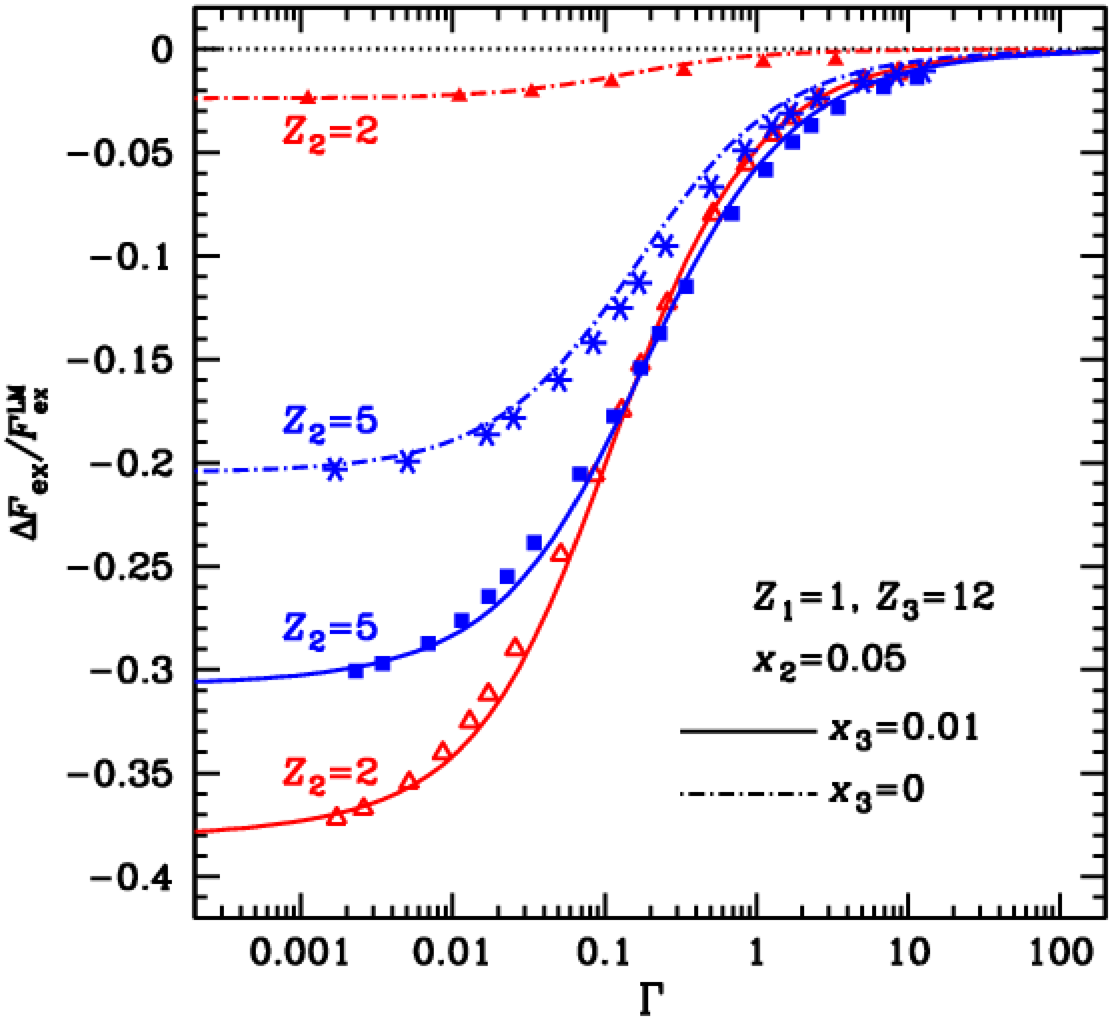
BIM free energy



Check for three-component plasmas



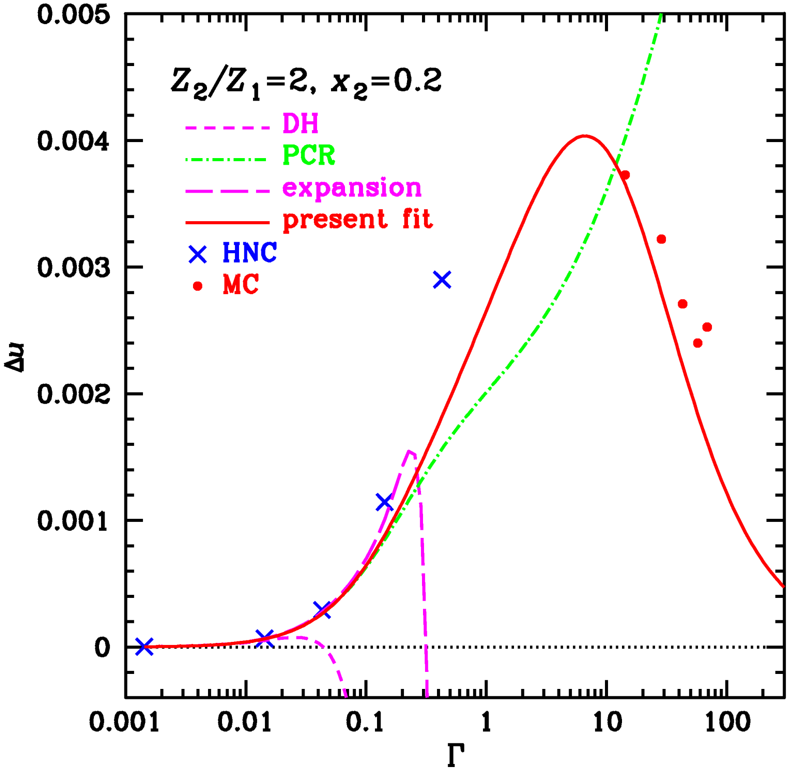
Free energy of three-component plasmas



First version of the fit: A.Y.Potekhin, G.Chabrier, F.J.Rogers, *Phys. Rev. E*, **79**, 016411 (2009)

Fine tuning at Γ > 1

A.Y.Potekhin, G.Chabrier, A. I. Chugunov, F.J.Rogers, H. E. DeWitt,
Phys. Rev. E (submitted)



Approximation of numerical results

(HNC at small to moderate Γ and MC at Γ > 1)

$$\Delta f \equiv f - f^{\mathrm{LM}} = \frac{\Gamma_e^{3/2} \langle Z^{5/2} \rangle}{\sqrt{3}} \, \frac{\delta}{(1 + a\Gamma^b)^c} \, \frac{1}{(1 + a'\Gamma^b)^{c'}}$$

$$\delta = \frac{\zeta^{\mathrm{LM}} - \zeta^{\mathrm{DH}}}{\langle Z^{5/2} \rangle} = \begin{cases} 1 - \dfrac{\langle Z^2 \rangle^{3/2}}{\langle Z \rangle^{1/2} \langle Z^{5/2} \rangle} & \text{for rigid background model} \\ \dfrac{\langle Z\,(Z{+}1)^{3/2} \rangle}{\langle Z^{5/2} \rangle} - \dfrac{(\langle Z^2 \rangle{+}\langle Z \rangle)^{3/2}}{\langle Z \rangle^{1/2} \langle Z^{5/2} \rangle} & \text{for polarizable background} \end{cases}$$

$$a = \frac{2.2\,\delta + 17\,\delta^4}{1 - b} \qquad b = d^{-0.2} \qquad c = 1 + \frac{d}{6} \qquad d = \frac{\langle Z^2 \rangle}{\langle Z \rangle^2}$$

$$a' = 0.02\, d \sqrt{\delta}\, a \qquad c' = \frac{3}{2b} - c$$

$$\Delta u = \left(\frac{3}{2} - \frac{abc\,\Gamma^b}{1 + a\Gamma^b} - \frac{a'bc'\,\Gamma^b}{1 + a'\Gamma^b} \right) \Delta f$$

$$\Delta c_V = b^2\, \Gamma^b \left(\frac{ac}{(1 + a\,\Gamma^b)^2} + \frac{a'c'}{(1 + a'\,\Gamma^b)^2} \right) \Delta f$$

Summary

- Formulae for calculations of the free energy of fully ionized nonideal Coulomb plasmas are systemized, selected, and in some cases improved.
- A simple formula is constructed for interpolation of the free energy of ion mixtures in gas and liquid phases at arbitrary coupling Γ; it agrees with HNC and MC calculations within the accuracies of these calculations.
- The expressions for the free energy and the first and second derivatives are implemented in the set of Fortran subroutines for calculation of thermodynamic functions, freely available at http://www.ioffe.ru/astro/EIP/