Annual Workshop on the Non-ideal Plasma Physics
NPP-2008

26-27 November 2008, Presidium RAS,Gagarina sq, 32a, Moscow

Influence of electrons degeneracy on bound states partition function

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Abstract

- Equation of state for a non-ideal hydrogen plasma [1] is developed to account the influence of degenerated electrons on the contribution of bound states. Derivation of corresponding partition function is presented.
- The new form of the bound states contribution to plasma pressure is compared with previously used expressions for the case of the solar plasma.
- The model EOS also includes the relativistic corrections, radiation pressure in plasma, the Coulomb interaction in the Debye-Hueckel approximation together with diffraction and exchange corrections, and the contribution of scattering states.
- Sound speed and adiabatic index values obtained with HEOS code are compared with those obtained using SAHA-S model [2].

[1]. Starostin A N and Roerich V C JETP 100(1) (2005) 165-198

[2]. Gryaznov V K, et al. J. Phys. A: Math. Gen. 39 (2006) 4459-4464

From Kadanoff-Baym technique

$$\frac{\delta\Omega_L}{V} = \sum_{i,\omega} \int_0^1 \frac{d\lambda}{2\lambda} \int \frac{d\mathbf{p}}{(2\pi)^3} G_i(\mathbf{p},\omega) S_i(\mathbf{p},\omega)$$

$$S_i(\mathbf{p}) = \frac{2}{\beta} \sum_{j,k_4} \int \frac{d\mathbf{k}}{(2\pi)^3} G_j(\mathbf{k}) G_{ij}\left(\frac{m_j\mathbf{p} - m_i\mathbf{k}}{m_i + m_j}; \frac{m_j\mathbf{p} - m_i\mathbf{k}}{m_i + m_j}; \mathbf{p} + \mathbf{k} \right)$$

$$G_{ij}(\mathbf{q},\mathbf{q}';\mathbf{P}) = \tilde{V}_{ij}(\mathbf{q} - \mathbf{q}') + (2\pi)^3 \sum_n \frac{\tilde{Y}_n(\mathbf{q}) \tilde{Y}_n^*(\mathbf{q}') \left(E_n - \frac{\hbar^2 q^2}{2\mu} \right) \left(E_n - \frac{\hbar^2 q'^2}{2\mu} \right)}{iP_4 - \frac{\hbar^2 P^2}{2M} - E_n + \mu_i + \mu_j}$$

$$\delta P = \sum_a (2S_a + 1)\hbar \int_0^1 \frac{d\lambda}{2\lambda} \int \frac{d\boldsymbol{p}}{(2\pi)^3} \int \frac{d\omega\, d\omega'}{(2\pi)^2} \frac{\Sigma_a^>\left(\boldsymbol{p},\omega\right) G_a^<\left(\boldsymbol{p},\omega'\right)}{\omega - \omega'} \left(1 - e^{-\beta(\omega-\omega')}\right)$$

Mass operator is represented using scattering amplitude

$$\Sigma_e^> \square \int \mathrm{Im}\, \Gamma_{\mathrm{ep}} \left(\omega + \Omega\right) G_{\mathrm{p}}^< \left(\boldsymbol{p}', \Omega\right) d\boldsymbol{p}'\, d\Omega$$

$$\mathrm{Im}\, \Gamma \square \sum_k \left|\tilde{\Psi}_k(\boldsymbol{q})\right|^2 (E_k - \varepsilon_q)^2 \delta_\gamma \left(\omega + \Omega - E_k - \frac{p^2}{2M} \right)$$

$$\delta\Omega_{\mathrm{ep}}^{BS} V^{-1} = \zeta_{\mathrm{e}} \zeta_{\mathrm{p}}\, \lambda_{\mathrm{ep}}^3 \int_0^1 \frac{d\lambda}{\lambda} \int \frac{d\boldsymbol{q}}{(2\pi)^3} \sum_n (E_n - \varepsilon_q)\ \left|\tilde{\Psi}_n(q)\right|^2 \left(e^{-\beta E_n} - e^{-\beta \varepsilon_q} \right)$$

Fock [1935]: $$\frac{1}{(2\pi)^3}\sum_{l,m}\left|\tilde{\Psi}_{nlm}(\boldsymbol{q})\right|^2 = \frac{8}{\pi^2 a_0^5 n^3 (q^2 + p_n^2)^4}.$$

$$p_n = (a_0 n)^{-1}, \quad a_0 = \frac{\hbar^2}{\mu e^2 \lambda}, \quad x = \frac{\hbar^2 q^2}{2\mu T}, \quad y = \beta\hbar\omega,$$

$$z = \frac{\hbar^2 p_n^2}{2\mu T} = -\beta E_n = u_n \lambda^2, \quad u_n = \frac{\alpha^2}{n^2}, \ \alpha = \alpha_{\text{ep}} = \sqrt{\frac{\mu e^4}{2\hbar^2 T}} = \sqrt{\beta Ry},$$

$$\delta P_{BS} = \zeta_{\text{e}}\zeta_{\text{p}} T\, \lambda_{\text{ep}}^3 \Sigma^{BS}, \quad \Sigma^{BS} = \sum_{n=1}^{\infty} G_n,$$

$$G_n = n^2 \int_0^{u_n} \frac{8}{\pi} z^{3/2}\, dz \int_{-\infty}^{\infty} dy \cdot \tilde{a}_n(y+z) \int_0^{\infty} \frac{\sqrt{x}(e^{-y} - e^{-x})\, dx}{(x+z)^2 (x-y)}$$

No broadening (N-B):

Starostin,Roerich,More[2003, CPP **43**(5-6) 369-372]

Starostin,Roerich[2005, JETP **100**(1) 165-198]

$$G_n = n^2 e^{u_n} F(u_n): \quad \text{if} \quad a_n(\omega) = \delta(\omega) \quad \text{then}$$

$$F(u) = F_{SRM}(u) = 1 - e^{-u}\left(4 - \frac{6}{\sqrt{\pi}} u^{1/2} + \frac{4}{\sqrt{\pi}} u^{3/2}\right) + \operatorname{erfc}\sqrt{u} \cdot \left(3 - 4u + 4u^2\right)$$

$$\Sigma^{BS} = \Sigma^{BS}_{SRM} = \sum_{k=4}^{\infty} \zeta(k-2) \frac{(-\alpha)^k}{\Gamma\left(\frac{k}{2}+1\right)} (k-2)^2 + \sum_{k=1}^{\infty} \zeta(2k+1) \frac{\alpha^{2k+3}}{\Gamma\left(k+\frac{5}{2}\right)}$$

Compare with

$$F(u) = F_{P-L}(u) = 1 - e^{-u} - u e^{-u} \quad \Rightarrow \quad \Sigma^{BS} = \Sigma^{BS}_{P-L} = \sum_{k=2}^{\infty} \zeta(2k-2) \frac{\alpha^{2k}}{\Gamma(k+1)}$$

$$\text{For } u \ll 1: \qquad F_{SRM} \approx 2u^2, \quad F_{P-L} \approx \frac{u^2}{2}$$

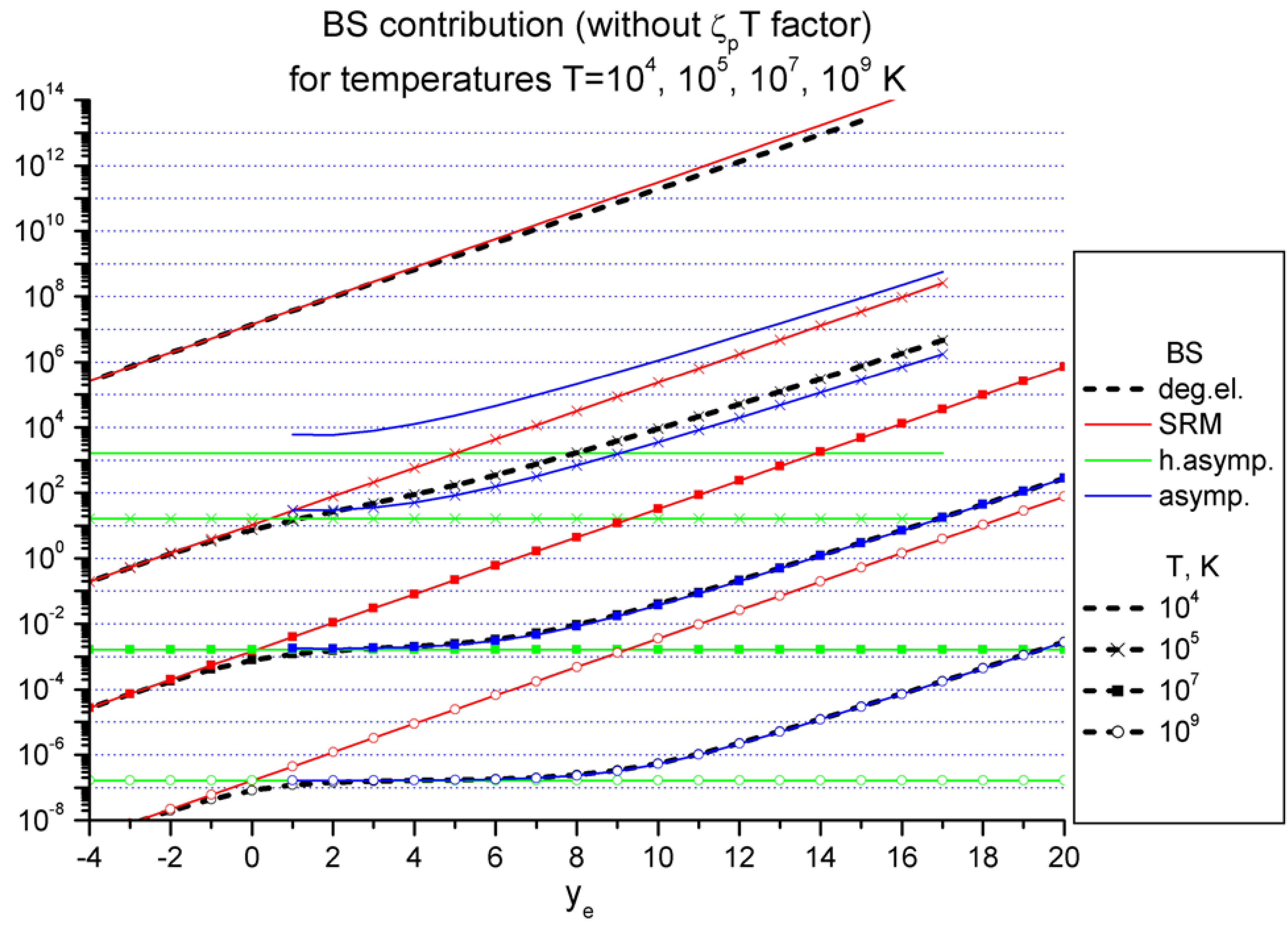
Contribution of BS with account of electrons degeneracy (X=Ry/T):

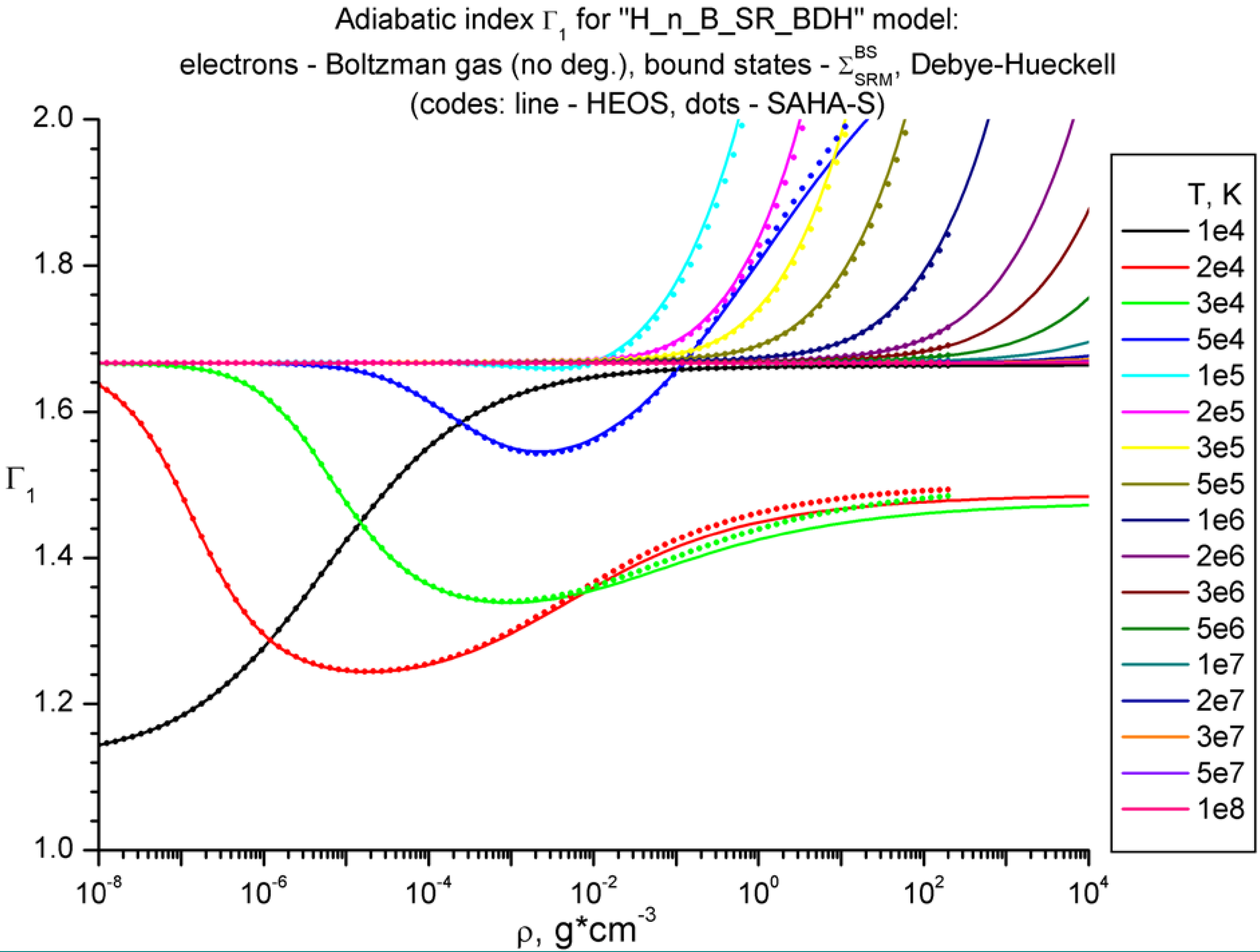
$$\frac{\delta\Omega^{BS}}{V} = -\zeta_p \frac{32}{\pi} TX \sum_{n=1}^{\infty} 2\int_0^1 \lambda d\lambda \int_0^{\infty} \frac{t^2 dt}{\left(1+t^2\right)^3} \frac{\exp\left(\frac{\lambda^2 X}{n^2}\left(1+t^2\right)\right)-1}{\exp\left(\frac{\lambda^2 X}{n^2}t^2 - y\right)+1}$$

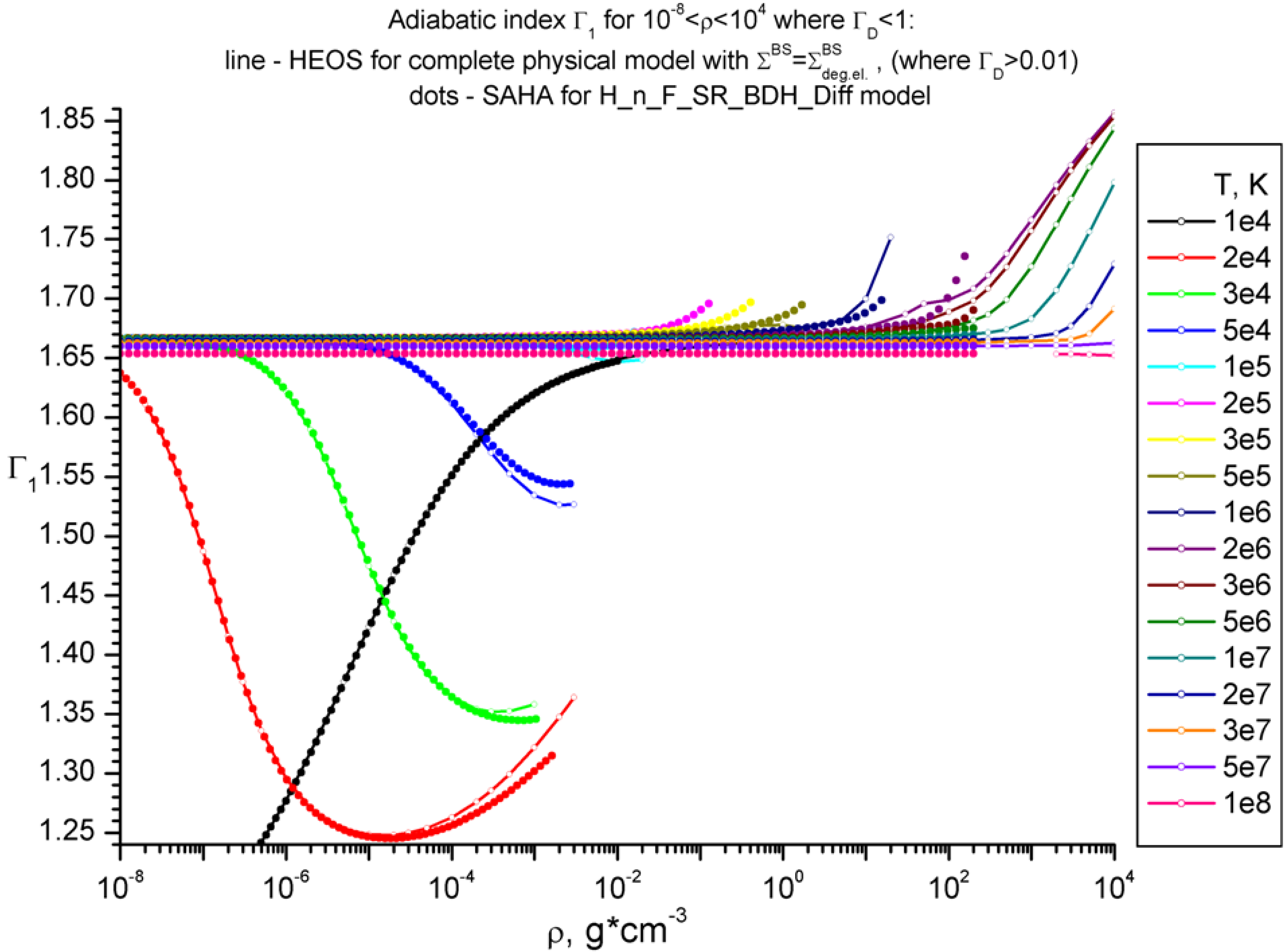
$$X \ll 1; \quad X\left(1+t^2\right)/n^2 \ll 1 < y, \quad \Rightarrow \quad \frac{\delta\Omega^{BS}}{V} \approx -\zeta_p T \frac{2\pi^2}{3}\left(\frac{\mathrm{Ry}}{T}\right)^2 \quad \text{- h.asymp.}$$

$$X \gg 1, \quad X\lambda^2 t^2/n^2 > y > 1 \quad \Rightarrow$$

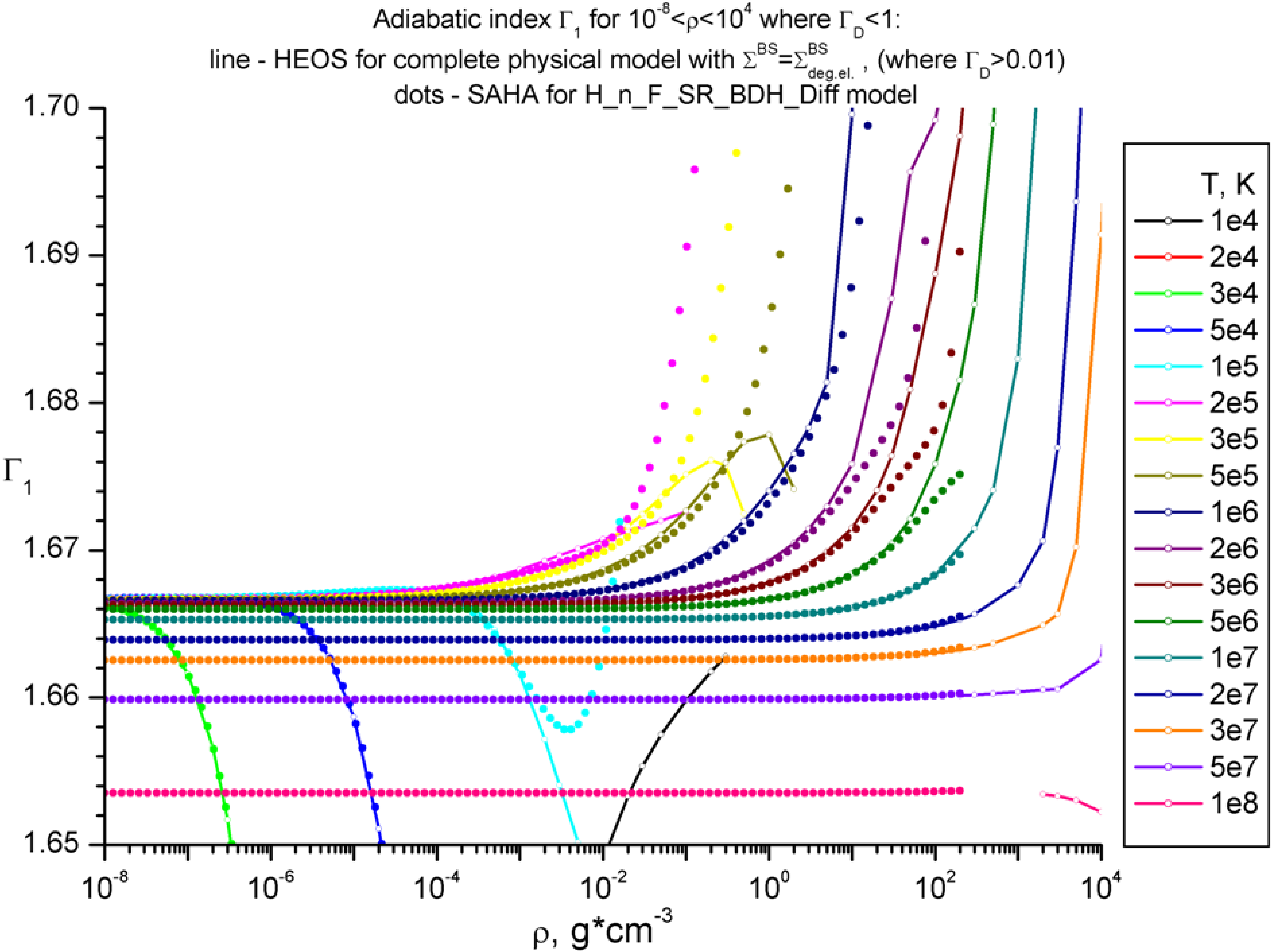
$$\frac{\delta\Omega^{BS}}{V} \to -\zeta_p T\left(\frac{2\pi^2}{3}\left(\frac{\mathrm{Ry}}{T}\right)^2 + \frac{64\zeta(3)}{15\pi}\left(\frac{\mathrm{Ry}}{T}\right)^{5/2}\frac{e^y}{y^{3/2}}\right) \quad \text{- asymp.}$$


BS contribution (without ζ_p T factor)
for temperatures T=10^4, 10^5, 10^7, 10^9 K
BS
deg.el.
SRM
h.asymp.
asymp.
T, K
10^4
10^5
10^7
10^9
y_e

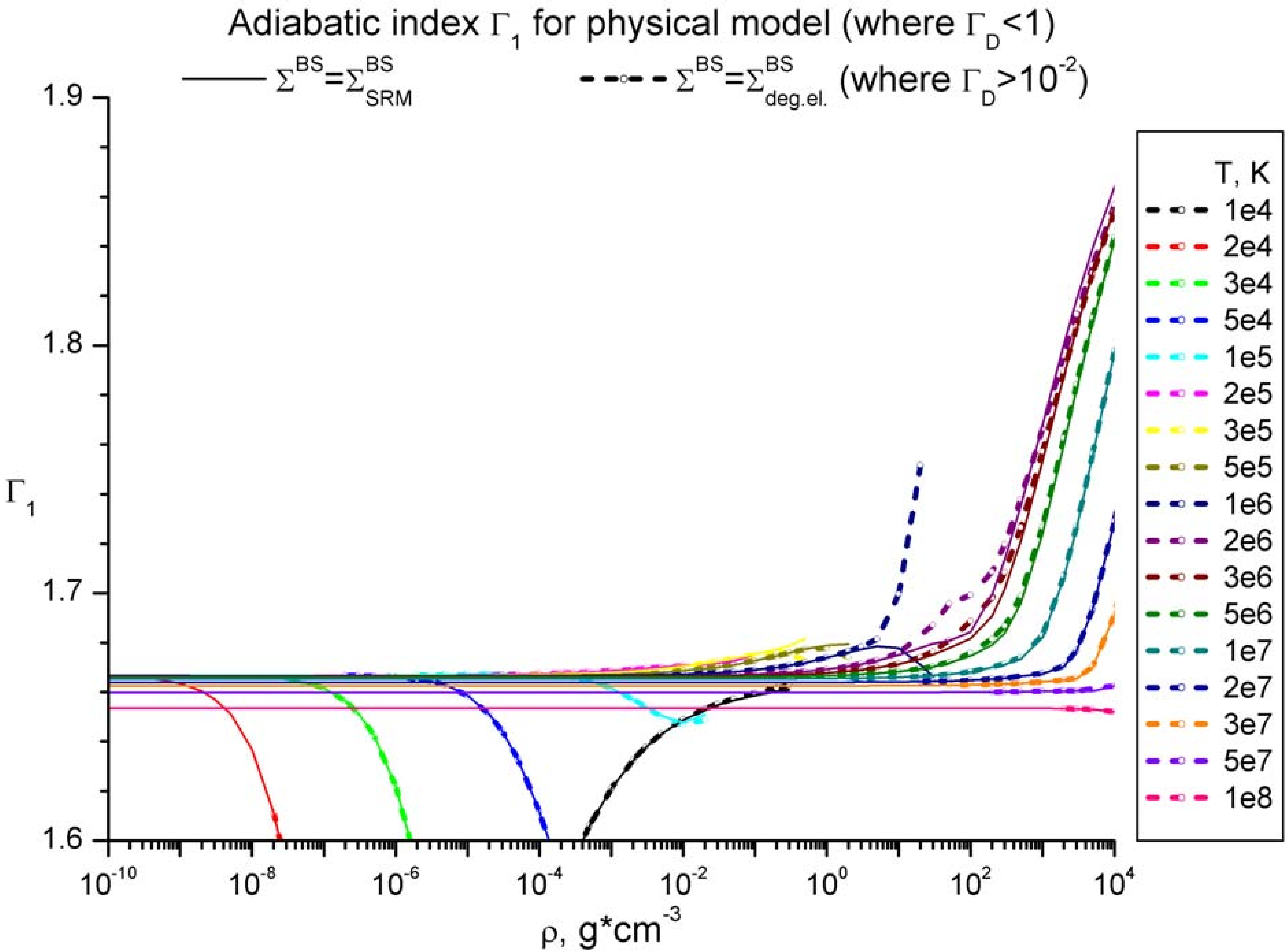

Adiabatic index Γ1 for "H_n_B_SR_BDH" model:
electrons - Boltzman gas (no deg.), bound states - Σ^BS_SRM, Debye-Hueckell
(codes: line - HEOS, dots - SAHA-S)
2.0
1.8
1.6
1.4
1.2
1.0
Γ1
10^-8
10^-6
10^-4
10^-2
10^0
10^2
10^4
ρ, g*cm^-3
T, K
1e4
2e4
3e4
5e4
1e5
2e5
3e5
5e5
1e6
2e6
3e6
5e6
1e7
2e7
3e7
5e7
1e8



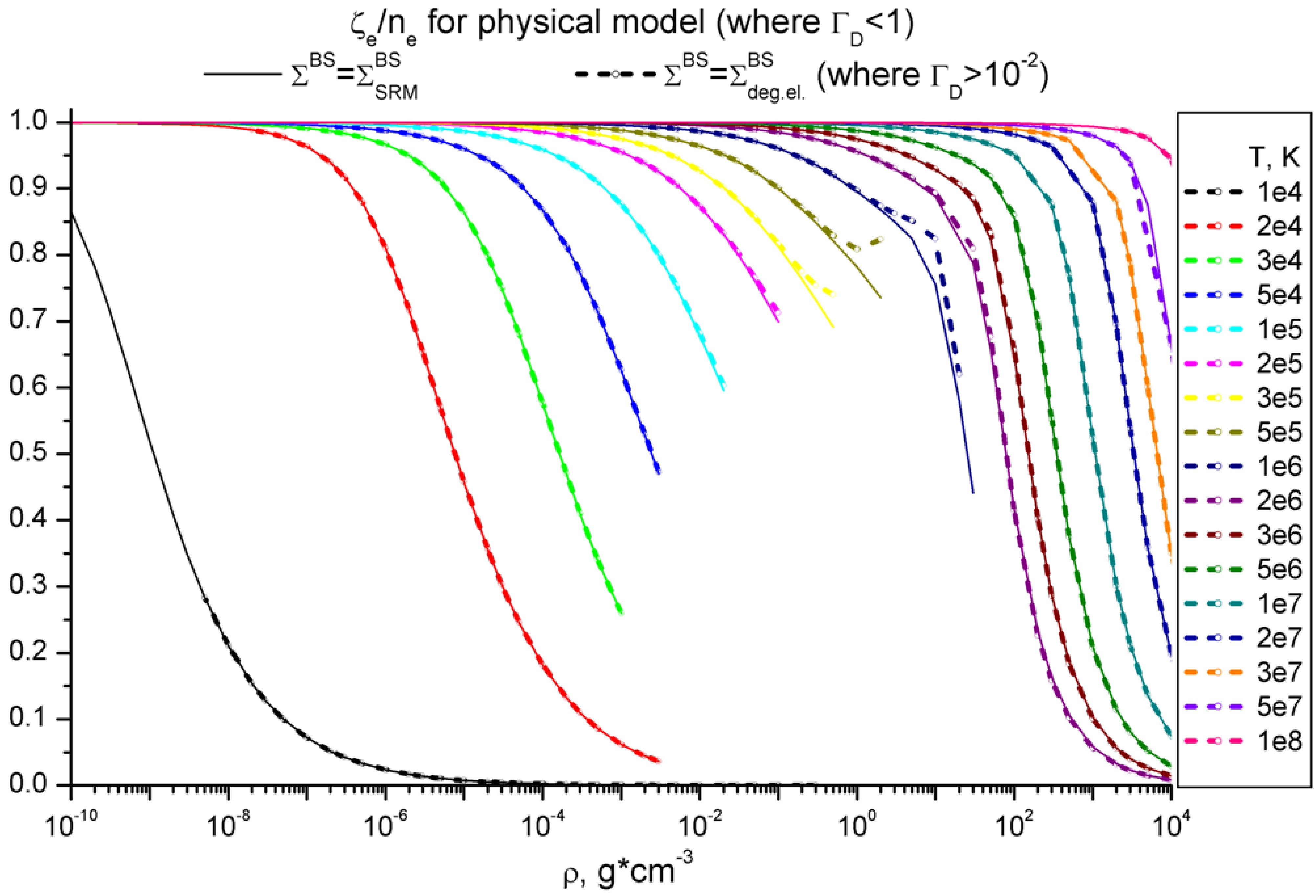
Adiabatic index Γ1 for 10^-8<ρ<10^4 where ΓD<1:
line - HEOS for complete physical model with Σ^BS=Σ^BS_deg.el. , (where ΓD>0.01)
dots - SAHA for H_n_F_SR_BDH_Diff model
Γ1
ρ, g*cm^-3
T, K
1e4
2e4
3e4
5e4
1e5
2e5
3e5
5e5
1e6
2e6
3e6
5e6
1e7
2e7
3e7
5e7
1e8



Adiabatic index Γ1 for 10^-8<ρ<10^4 where ΓD<1:
line - HEOS for complete physical model with Σ^BS=Σ^BS deg.el. , (where ΓD>0.01)
dots - SAHA for H_n_F_SR_BDH_Diff model
Γ1
ρ, g*cm^-3
T, K
1e4
2e4
3e4
5e4
1e5
2e5
3e5
5e5
1e6
2e6
3e6
5e6
1e7
2e7
3e7
5e7
1e8



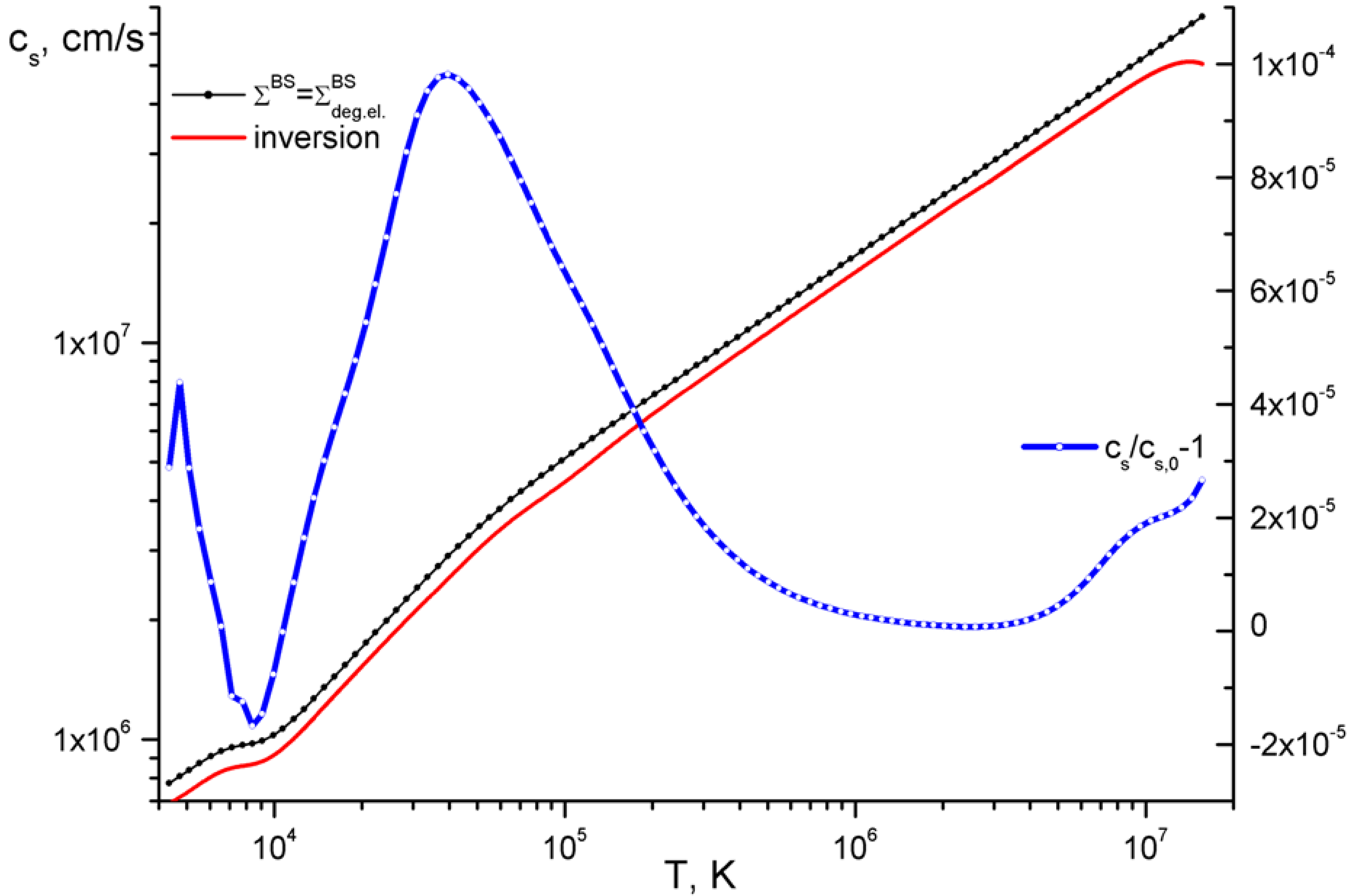
Adiabatic index Γ_1 for physical model (where Γ_D<1)
$\Sigma^{BS}=\Sigma^{BS}_{SRM}$
$\Sigma^{BS}=\Sigma^{BS}_{deg.el.}$ (where $\Gamma_D>10^{-2}$)
1.9
1.8
1.7
1.6
Γ_1
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
ρ, g*cm^{-3}
T, K
1e4
2e4
3e4
5e4
1e5
2e5
3e5
5e5
1e6
2e6
3e6
5e6
1e7
2e7
3e7
5e7
1e8



ζ_e/n_e for physical model (where Γ_D<1)
$\Sigma^{BS}=\Sigma^{BS}_{SRM}$
$\Sigma^{BS}=\Sigma^{BS}_{deg.el.}$ (where $\Gamma_D>10^{-2}$)
T, K
1e4
2e4
3e4
5e4
1e5
2e5
3e5
5e5
1e6
2e6
3e6
5e6
1e7
2e7
3e7
5e7
1e8
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
10^{-10}
10^{-8}
10^{-6}
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
ρ, g*cm^{-3}

Sound speed and relative correction to physical model with $\Sigma^{BS}=\Sigma^{BS}_{SRM}$

$(c_{s,deg.el.}/c_{s,SRM}-1)$ for conditions of the interior of the Sun



Conclusions

- estimate of BS contribution decreases by orders of magnitude due to account of electrons degeneracy (ED) in the case of large T (>10^5 K) and strong degeneracy ($\mu_e/T>>1$)
- numerical simulations show that the adiabatic index value can differ significantly from the ideal gas value $\Gamma_1=5/3$ even for moderate nonideality ($\Gamma_1\sim2$ for $\Gamma_D\sim4$)
- for hydrogen plasma and conditions of the interior of the Sun the account of ED in BS contribution leads to correction of sound speed $<10^{-4}$ in comparison to model with SRM partition function