Study on Several *Padé* Approximants for Fully Ionized Hydrogen Plasmas

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Abstract. Based on the current proposed three type *Padé* approximations of fully ionized hydrogen plasmas. Using Fortran program, we calculated the Helmholtz free energy of hydrogen plasmas and made a comparison of these Helmholtz free energy. It is concluded that the dimensionless parameter f_{ee}^{c} of W.Stolzmann's theoretical analysis presents unphysical tendency within $\Gamma_e>15$ and $r_s<4$, and f_{ie}^{c} gives an unreasonable result within $8.0<\Gamma_e<9.1$ and $7.0<r_s<8.0$ at low temperature $T=5000$K, but this range of the odd variation and the values of Γ_e (r_s) will change with the increase of temperature, when the temperature reaches super-high temperature ($T>10^7K$), f_{ie}^{c} almost is applicable to all range of the values of Γe and r_s, f_{ee}^{c} is applicable to the values of $0<\Gamma e<0.3$ and $r_s>0$. In addition, the dimensionless parameter f_{ii}^{c} of Gilles Chabrier's article and W.Stolzmann's article have a good consistency. Finally, we presented a interpolational formula for hydrogen plasmas, making up for those small odd variation. It demonstrates that the interpolation formula for hydrogen plasmas has a practical application.

Introduction

The Helmholtz free energy of the plasmas are of primary interest in understanding the thermophysical properties at high pressures and temperatures. The primary research of the plasmas is the interaction between the charged particles. The plasmas is the normal state of the matter and a good conductor of electricity, it is of great importance to the development of condensed matter physics, materials science, a planetary physics and weapons physics [1,2]. That is to say, the studies of the ionization of hydrogen at high pressures and temperatures are of practical interest, such as the development of new energy and strategic nuclear weapon [3,4,5]. Therefore, many researchers, such as W.Stolzmann, Gilles Chabrier and Setsue Ichimaru, have studied the thermophysical properties of the plasmas, and proposed relevant *Padé* approximation which provide a completely analytic, accurated description of the thermodynamic quantities of fully ionized electron-ion Coulomb plasmas.

Hydrogen atom have the most simple structure, Therefore, it seems to be an ideal example for the study of the plasma, but hydrogen's complex behavior is beyond previous imagination of scientists at high temperature and pressure. W.Stolzman [6,7,8,9], Gilles Chabrier [10,11] and Setsue Ichimaru [14,15] have studied the interaction of the charged particles using fully ionized plasmas model. W.Stolzmann presented a result of fully ionized plasmas consisting of ions and electrons which are valid in a broad range of temperatures and densities and applicable to arbitrary chemical mixtures by *Padé* approximants, however, the *Padé* approximants will be expressed by the dimensionless electronic and ionic plasmas which describe the strength of the Coulomb coupling. In Gilles Chabrier's article, he calculated the thermodynamic of fully ionized electron-ion Coulomb plasmas consisting of different species of pointlike ions and electrons which are encountered in numerous physical and astrophysical situations, and presented a completely analytic formulas for the free energy of electron-ion plasmas, basing on detailed numerical calculations for different ionic species over a wide range of density and temperatures. These *Padé* formulas provide a useful tool for various application from liquid state theory to dense stellar matter. In Setsue Ichimaru's article, he reviewed the current status of the theoretical developments describing the interparticle correlations in dense plasmas and of the knowledge on the thermodynamic properties and the transport and elementary processes, accumulated through theoretical studies since his previous review [15]. He finally presented analytical theories developed for descriptions of static and dynamic correlation in strongly coupled plasmas. We carried on the detailed calculation for all parameters by the above three authors' proposed *Padé* formulas, and obtained all variable quantities' calculatical results in a broad range of temperatures and densities, including calculatical results of electronic correlation contribution to the Helmholtz free energy f_{ee}^{c} (dimensionless parameter), electronic exchange contribution to the Helmholtz free energy f_{ee}^{X} (dimensionless parameter), ionic correlation contribution to the Helmholtz free energy f_{ii}^{c} (dimensionless parameter), ion-electron correlation contribution to the Helmholtz free energy f_{ie}^{c} (dimensionless parameter) vs. the Coulomb coupling parameter Γ and the mean distance between the electrons r_s or the mean distance between the ions ri. In this paper, we briefly illustrated advantages of their *Padé* formulas and local small variations respectively, then we obtained a analytical, detailed and comprehensive result. Finally, we summarized a interpolation formula for fully ionized hydrogen plasmas.

Theoretical Analysis

The ionization reaction of hydrogen atom will be occurred at high temperatures and pressures, it's ionization processes is

$$H \Leftrightarrow H^{+} + e \,. \tag{1}$$

This is to say, hydrogen plasmas consisting of species of H^{+} and e [3,4,5]. The interaction between the various components are expressed by *Padé* formulas.

The Helmholtz free energy F of a fully ionized hydrogen consisting of ideal part F^{id} and Coulomb free energy F^{coul}, which can be written as

$$F = F^{id} + F^{coul} \,. \tag{2}$$

where F^{id} denotes the ideal free energy of ions and electrons, F^{coul} represents the Coulomb interaction contributions to the free energy. The Coulomb part can decomposed into the following parts.

$$F^{coul} = F_{ee} + F_{ii} + F_{ie} \,. \tag{3}$$

However, W.Stolzmann, Gilles Chabrier and Setsue Ichimaru proposed different *Padé* formula for the F_{ee}, F_{ii}, F_{ie} [6][10][11][14] which are expressed by the Coulomb coupling parameter Γ_e and Γ_i, the dimensionless mean distance between the electrons r_s and temperature T.

$$\Gamma_e = \beta e^2 / a_e \,,\ \Gamma_i = \beta (Ze)^2 / a = \Gamma_e Z^{5/3} \,. \tag{4}$$

Where a_e, a are the mean distance between the electrons and between the ions, respectively.

$$a_e = (\frac{4}{3}\pi n_e)^{-1/3} \,,\ a = (\frac{4}{3}\pi n_{ion})^{-1/3} = (\frac{4}{3}\pi n_e / Z)^{-1/3} = Z^{1/3} a_e \,. \tag{5}$$

where n_{ion} is the ion density, n_e is the electron density, parameter $\beta = 1/(4\pi\varepsilon_0 k_B T)$. The temperature and the mean distance between the electrons usually are expressed by the dimensionless τ and r_s.

$$\tau = \frac{k_B T}{Ryd} \,,\ 1Ryd = 13.6058eV \,,\ r_s = \frac{a_e}{a_B} \ (a_B \text{ is Bohr radius}). \tag{6}$$

Results and Discussion

In this section, we give a systematic comparison of *Padé* formulas of the Helmholtz free energy F_{ee}, F_{ii}, F_{ie}. we calculated all Helmholtz free energy of the fully ionized hydrogen plasmas from low temperature to super-high temperature, but mainly listed four typical isotherms of the Helmholtz free energy *f* (dimensionless parameter) vs. the Coulomb coupling parameter Γ ($\Gamma_e = \Gamma_i$, for hydrogen) and the mean distance between the electrons r_s ($r_s = r_i$, for hydrogen).

Electron-electron Interaction Contribution to the Helmholtz Free Energy F_{ee} (Γ_e, r_s, T)

Electron-electron interaction contribution to the Helmholtz free energy F_{ee} of W.Stolzmann's article is expressed by the dimensionless electronic plasmas parameters(Γ_e, r_s, T), which describe the strength of the Coulomb coupling [8,14]

$$F_{ee} = F_{ee}^{c} + F_{ee}^{x} \cdot \tag{7}$$

$$f_{ee}^{c} = \frac{F_{ee}^{c}}{N_e k_B T} = -\frac{a_0 \Gamma_e^{3/2} - a_2 \Gamma_e^{6} [\varepsilon_c(R_s) + \Delta\varepsilon_c(R_s, \tau)] / \tau}{1 + a_1 a_3 \Gamma_e^{3/2} + a_2 \Gamma_e^{6}}, \tag{8}$$

$$f_{ee}^{x} = \frac{F_{ee}^{x}}{N_e k_B T} = -\frac{2e^2}{\Lambda_e^4 n_e k_B T} \int_{-\infty}^{\Psi} d\Psi' I_{-1/2}^{2}(\Psi') \cdot \tag{9}$$

where Λ_e is the thermal De Broglie-wavelength ($\Lambda_e = 2\pi\hbar\sqrt{2m_e \pi k_B T}$), other parameters are given in Ref. [6].

While electron-electron interaction contribution to the Helmholtz free energy f_{ex} of Setsue Ichimaru's article[14] is given by

$$\begin{aligned} -f_{ex} = \frac{F_{ex}}{N k_B T} &= \frac{c}{e}\Gamma + \frac{2}{e}\left(b - \frac{cd}{e}\right)\Gamma^{1/2} + \frac{1}{e}\left[\left(a - \frac{c}{e}\right) - \frac{d}{e}\left(b - \frac{cd}{e}\right)\right]\ln\left|e\Gamma + d\Gamma^{1/2} + 1\right| \\ &- \frac{2}{e(4e - d^2)^{1/2}}\left[d\left(a - \frac{c}{e}\right) + \left(2 - \frac{d^2}{e}\right)\left(b - \frac{cd}{e}\right)\right] \times \left[\tan^{-1}\frac{2e\Gamma^{1/2} + d}{(4e - d^2)^{1/2}} - \tan^{-1}\frac{d}{(4e - d^2)^{1/2}}\right] \end{aligned} . \tag{10}$$

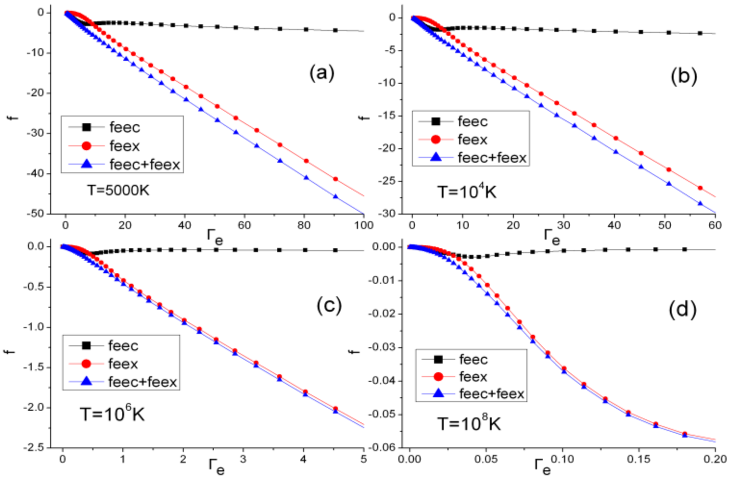

Fig.1 The Helmholtz free energy f_{ee}^{c}, f_{ee}^{x}, $f_{ee}^{c} + f_{ee}^{x}$ vs. the electron coupling parameter Γ_e for four isotherms of hydrogen plasma from W.Stolzmann's theoretical analysis [6] at the temperatures values of $T=5000$K, 10^4K, 10^6K, 10^8K

Based on several proposed *Padé* formulas of W.Stolzmann's theoretical analysis [6], using calculational results, we made a comparison for four isotherms with the Helmholtz free energy f_{ee}^{c}, f_{ee}^{x}, $f_{ee}^{c} + f_{ee}^{x}$, the electron coupling parameter Γ_e in a broad range of temperature, as shown in Fig.1. We find that the value of f_{ee}^{c} is small, while the value of f_{ee}^{x} is very big and mainly play an important role at the strongly coupling limit, but with the decrease of the value of the electron coupling parameter Γ_e and the increase of the value of the mean distance between the electrons r_s, f_{ee}^{c} and f_{ee}^{x} tend to get balance. Such as at low temperatures $T=5000$K, f_{ee}^{c} can be ignored comparing with f_{ee}^{x} within $\Gamma_e>15$ and $r_s<4$, but the difference between the value of f_{ee}^{c} and f_{ee}^{x} get bigger with the increase of Γ_e at high temperatures. Detailed quantitative analysis is as following, as shown in picture (b) ($T=10^4$K), when $\Gamma_e>6$ ($r_s<5$), the value of f_{ee}^{c} much smaller than the value of f_{ee}^{x}, so f_{ee}^{c} can be ignored, the curves of f_{ee}^{x} and $f_{ee}^{c}+f_{ee}^{x}$ get very close, but with the increases of temperature, the value of this range also is being changed. As shown in the picture (c), this range becomes $\Gamma_e>0.4$ ($r_s<0.6$). When the temperature reaches the values $T=10^8$K, as shown in the picture (d), the electron coupling parameter approximately reaches the values $\Gamma_e>0.025$, while the mean distance between the electrons approximately reaches the values $r_s<0.08$.

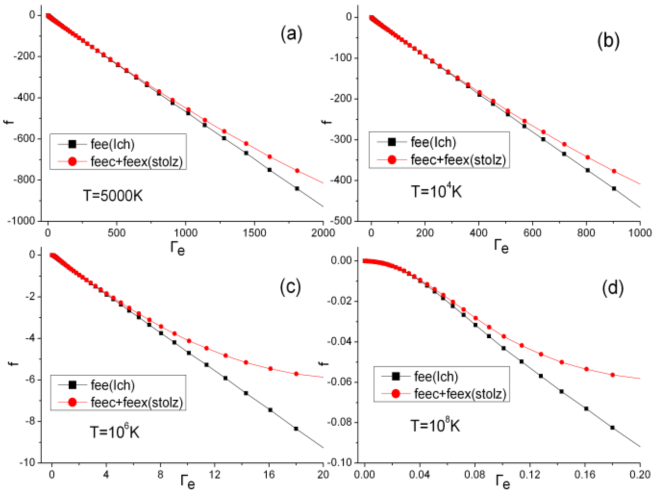

Fig.2 The Helmholtz free energy fee of Setsue Ichimaru's article and $f_{ee}^{c}+f_{ee}^{x}$ of W.Stolzmann's article vs. the electron coupling parameter Γ_e at the temperatures values of $T=5000$K , 10^4K, 10^6K, 10^8K. The filled circles refers to the *Padé* approximant of $f_{ee}^{c}+f_{ee}^{x}$ from Stolzmann [6], the filled squares show the Padé approximant of f_{ee} from Ichimaru [10].

We also made a comparison between f_{ee} of Setsue Ichimaru's article [14] and $f_{ee}^{c}+f_{ee}^{x}$ of W.Stolzmann's article [6], as shown in Fig.2. By calculating, we obtained that two curves of f_{ee} and $f_{ee}^{c}+f_{ee}^{x}$ have very good consistency at the small of Γ_e and the big of r_s at the temperatures ranging from $T=5000$K to $T=10^8$K, but we will adopt f_{ee} of Setsue Ichimaru's article [14] if calculate the value of f_{ee}, because it can be more accurately express the value of f_{ee} while the value of $f_{ee}^{c}+f_{ee}^{x}$ gives an unreasonable result at the big region of Γ_e and the small region of r_s. By comparison, we can see that the unreasonable result of electronic correlation contribution to the Helmholtz free energy f_{ee}^{c} cann't be neglected if calculate $f_{ee}^{c}+f_{ee}^{x}$ (equal to f_{ee}) at the big region of Γ_e and the small region of r_s, and the value of f_{ee}^{c} almost has effects on f_{ee} or $f_{ee}^{c}+f_{ee}^{x}$ at the big region of Γ_e and the small region of r_s. This also shows that f_{ee}^{c} has effects on f_{ee}^{x} within a certain some range of Γ_e and r_s.

Ion-ion Correlation Contribution to the Helmholtz Free Energy F_{ii}^{c} (Γ_e)

Ion-ion correlation contribution to the Helmholtz free energy F_{ii}^{c} of W.Stolzmann's article [6] is given by

$$f_{ii}^{c}=\frac{F_{ii}^{c}}{N_i k_B T}=-\frac{b_0\Gamma_i^{3/2}+b_2\Gamma_i^{9/2}\varepsilon_{ii}}{1+b_1\Gamma_i^{3/2}+b_2\Gamma_i^{9/2}}\,. \tag{11}$$

while ion-ion correlation contribution to the Helmholtz free energy F_{ii}^{c} of Gilles Chabrier's the first article [10] is given by

$$\begin{aligned}f_{ii}^{c}(\Gamma_i)=&A_1[\sqrt{\Gamma_i(A_2+\Gamma_i)}-A_2\ln(\sqrt{\Gamma_i/A_2}+\sqrt{1+\Gamma_i/A_2})]\\&+2A_3[\sqrt{\Gamma_i}-\arctan(\sqrt{\Gamma_i})]\end{aligned}\,. \tag{12}$$

Using the above *Padé* formulas, we mainly introduced ionic correlation contribution to the Helmholtz free energy f_{ii}^{c} of Gilles Chabrier's two article [10], and compared with the *Padé* approximant of f_{ii}^{c} from Stolzmann's article [6]. As shown in Fig.3, we give a comparison between f_{ii}^{c} of Gilles Chabrier's articles [10] and f_{ii}^{c} of W.Stolzmann's article [6]. It is concluded that the ionic correlation contribution to the Helmholtz free energy f_{ii}^{c} of W.Stolzmann's article and f_{ii}^{c} of Gilles Chabrier's articles[10] have a very good Consistency and the curve of them almost completely close at different temperatures ranging from $T=5000$K to $T=10^8$K. Therefore, f_{ii}^c of Gilles Chabrier's articles and W.Stolzmann's article are very reasonable for ion-ion interaction.

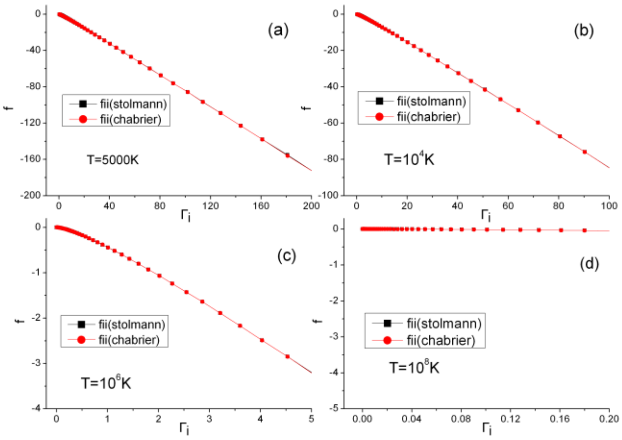

Fig.3 The ionic correlation contribution to the Helmholtz free energy f_{ii}^c vs. the ion coupling parameter Γ_i by with the datas given by Gilles Chabrier's theoretical analysis and W.Stolzmann's article for different temperatures ranging from $T=5000$K to $T=10^8$K. The filled squares refers to the Padé approximant of f_{ii}^c from Stolzmann's articles [6], the filled circles show the *Padé* approximant of f_{ii}^c from Gilles Chabrier's articles [10].

Ion-electron Correlation Contribution to the Helmholtz Free Energy F_{ie}^c (Γ_e, r_s)

Ion-electron correlation contribution to the Helmholtz free energy F_{ie}^c of W.Stolzmann's article [6] is expressed by

$$f_{ie}^c=\frac{F_{ie}^c}{N_i k_B T}=-\frac{c_0\Gamma_i^{3/2}+c_2\Gamma_e^{9/2}\varepsilon_{ie}}{1+c_1\Gamma_i^{3/2}+c_2\Gamma_e^{9/2}+2c_4\Gamma_i^{3/2}\ln[1+(c_5/\Gamma_i^3)^{1/2}]}. \tag{13}$$

Ion-electron correlation contribution to the Helmholtz free energy F_{ie}^c of Gilles Chabrier's the article [10,11] is expressed by

$$f_{ie}^c=\frac{F_{ie}}{N_i k_B T}=-\Gamma_e\frac{c_{DH}\sqrt{\Gamma_e}+c_{TF}a\Gamma_e^{v}g_1h_1}{1+[b\sqrt{\Gamma_e}+ag_2\Gamma_e^{v}/r_s]h_2}. \tag{14}$$

As shown in Fig.4, by calculating, we obtained the following conclusion by above *Padé* formulas. There are three major issues. First, we made a comparison between ion-electron correlation contribution to the Helmholtz free energy f_{ie}^c of Gilles Chabrier's article [10] and W.Stolzmann's article [6] at different temperatures of $T=5000$K, 10^4K, 10^6K, 10^8K. As shown in Fig.4, there are differences between them in small region of Γ_e and r_s at different temperatures ranging from $T=5000$K to $T=10^8$K, but with increase of the temperature, this region of difference get smaller and smaller, however, they have very good agreement at smaller region of Γ_e and bigger region of r_s at all temperatures. Second, it showed that ion-electron correlation contribution to the Helmholtz free energy f_{ie}^c vs. the electron coupling parameter Γ_e by with the datas given by Gilles Chabrier's theoretical analysis[10] for different temperatures ranging from $T=5000$K to $T=10^8$K. As shown in Fig.4, our calculation is suitable for the value of $\Gamma_e>0$ and $r_s>0$, the curve of f_{ie}^c doesn't present any unreasonable result and is very smooth in all region of Γ_e and r_s at different temperatures of $T=5000$K, 10^4K, 10^6K, 10^8K. Three, it described ion-electron correlation contribution to the Helmholtz free energy f_{ie}^c vs. the electron coupling parameter Γ_e by with the datas given by W.Stolzmann's theoretical analysis for different temperatures ranging from $T=5000$K to $T=10^8$K. As shown in Fig.4, f_{ie}^c gives an unreasonable result within $8.0<\Gamma_e<9.1$ and $7.0<r_s<8.0$ at low temperature $T=5000$K, but this range of the unphysical tendency and the values of r_s get small with the increase of temperature, when the temperature reaches the values $T>10^5$K, the unphysical tendency disappears, f_{ie}^c almost is applicable to all range of Γ_e and r_s, and the curve of f_{ie}^c is very smooth at all the region of Γ_e and r_s.

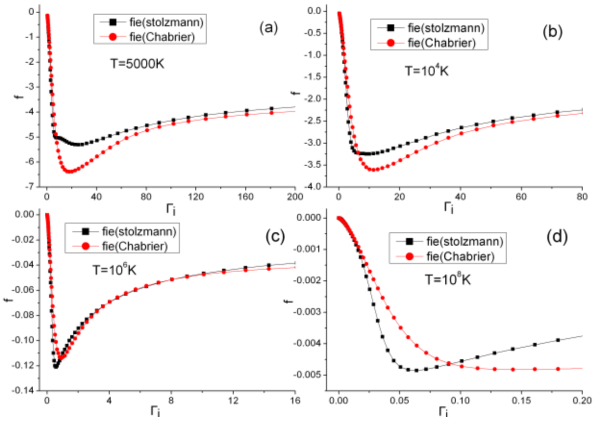

Fig.4 The ion-electron correlation contribution to the Helmholtz free energy $f_{ie}{}^{c}$ of Gilles Chabrier's article[10] and $f_{ie}{}^{c}$ of W.Stolzmann's article [6] vs. the electron coupling parameter Γ_e for different temperatures ranging from $T=5000$K to $T=10^8$K. The filled circles refers to the *Padé* approximant of $f_{ie}{}^{c}$ from Stolzmann's articles [6], the filled squares show the *Padé* approximant of $f_{ie}{}^{c}$ from Chabrier's articles [10].

From the above calculative results of several *Padé* approximants (as shown in Fig.1~4), We can see that their *Padé* formulas present odd variation in some regions. Their *Padé* formulas have its own advantages, but there are some drawwbacks in small regions (it were pointed out in the above figure). Therefore, we obtained a interpolation formula in the following conclusion, making up the local shortcomings.

Conclusion

We have calculated the Helmholtz free energy of the fully ionized electron-ion Coulomb plasmas of W.Stolzmann, Gilles Chabrier and Setsue Ichimaru's theoretical analysis by using *Padé* approximants. These approximants is realistic in various conditions at a wide range of temperatures or densities. Furthermore, these approximants were applicable to any chemical mixtures. Finally, We found out some regions of odd variation by calculation, and obtained their respective advantages and disadvantages by compare with several the author's theoretical analysis. Therefore, we used the following interpolational formula if calculating the excess free energy of hydrogen plasmas.

$$F_{ex} = F_{ee} + F_{ii}^{c} + F_{ie}^{c},$$

where F_{ee} denotes the interaction between electronic and electronic, coming from Setsue Ichimaru's article[14], and it's dimensionless is expressed as

$$\begin{aligned}-f_{ex} = -\frac{F_{ee}}{N_e k_B T} &= \frac{c}{e}\Gamma + \frac{2}{e}\left(b - \frac{cd}{e}\right)\Gamma^{1/2} + \frac{1}{e}\left[\left(a - \frac{c}{e}\right) - \frac{d}{e}\left(b - \frac{cd}{e}\right)\right]\ln\left|e\Gamma + d\Gamma^{1/2} + 1\right| \quad , \\ &- \frac{2}{e(4e-d^2)^{1/2}}\left[d\left(a - \frac{c}{e}\right) + \left(2 - \frac{d^2}{e}\right)\left(b - \frac{cd}{e}\right)\right] \times \left[\tan^{-1}\frac{2e\Gamma^{1/2} + d}{(4e-d^2)^{1/2}} - \tan^{-1}\frac{d}{(4e-d^2)^{1/2}}\right]\end{aligned}$$

$F_{ee}{}^{c}$ denotes the interaction between ion and ion, coming from W.Stolzmann's article, and it's dimensionless is expressed as

$$f_{ii}^{c} = \frac{F_{ii}^{c}}{N_i k_B T} = -\frac{b_0 \Gamma_i^{3/2} + b_2 \Gamma_i^{9/2} \varepsilon_{ii}}{1 + b_1 \Gamma_i^{3/2} + b_2 \Gamma_i^{9/2}},$$

$F_{ie}{}^{c}$ denotes the interaction between ion and electronic, coming from Gilles Chabrier's article, and it's dimensionless is expressed as

$$f_{ie}^{c} = \frac{F_{ie}}{N_i k_B T} = -\Gamma_e \frac{c_{DH}\sqrt{\Gamma_e} + c_{TF} a \Gamma_e^{\nu} g_1 h_1}{1 + [b\sqrt{\Gamma_e} + a g_2 \Gamma_e^{\nu} / r_s] h_2} \cdot$$

Finally, we give several curves of the coulomb interaction contribution to the Helmholtz free energy $f_{ee}{}^{c}$, $f_{ie}{}^{c}$, $f_{ie}{}^{c}$ between charged particles of fully ionized hydrogen plasma at low temperature $T=5000$K.

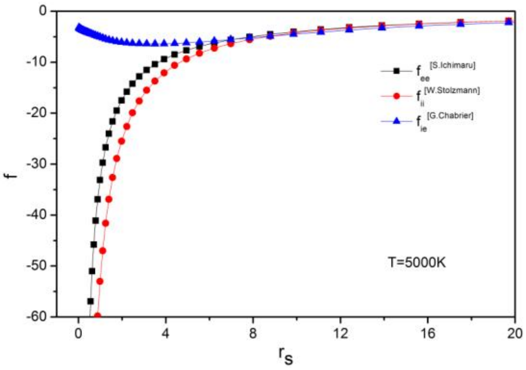

Fig.5 The coulomb interaction contribution to the Helmholtz free energy between charged particles of fully ionized hydrogen plasma at low temperature *T=5000*K.

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