Electron transport in hydrogen thermal plasmas

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The transport coefficients of hydrogen thermal plasma have been usually evaluated by using higher-order approximations of the Chapman-Enskog method and have shown a strong dependence on the presence of electronically excited states (EES) especially at high pressures. Even small concentrations of EES affect the transport properties significantly. Within the framework of Chapman-Enskog method, higher-order contributions to the electron transport in hydrogen thermal plasma have been computed with and without excited states. Effect of EES on the higher-order contributions for electron diffusion and thermal diffusion ratio have been worked out. It has been observed that EES affect the electron diffusion coefficient modestly as compared to thermal diffusion ratio. The higher-order contributions to thermal diffusion ratio show a unique behavior especially at high pressures thereby emphasizing the role of e-H (n) interactions.

1. Introduction

The effect of electronically excited states (EES) on the transport coefficients of LTE thermal plasmas have been studied recently due to their importance in technological applications [1-8]. Within the framework of Chapman-Enskog method, the importance of including higher-order contributions while evaluating the transport properties has been emphasized in our recent work [7] on viscosity as well as in the works of Capitelli et al [3 ,4] for hydrogen thermal plasmas by taking EES into account. Higher-order contribution to a given transport property is defined by $f_t^{(k)} = t^{(k)}/t^{(1)}$,where $t^{(k)}$ is the contribution to the given transport coefficient up to k orders. Proceeding on the similar lines as in our previous work on electron thermal conductivity and electrical conductivity [8] , a need was felt to evaluate the role of EES in electron-electron diffusion D_{ee} and thermal diffusion ratio k_e^T for hydrogen thermal plasma. It may be pointed out that $f_{D_{ee}}^{(2)}$ contributes 52% to diffusion D_{ee} at 30000 K for p = 1 atm, where $f_{D_{ee}}^{(2)}$ represents second-order contribution to electron-electron diffusion. How these contributions change with pressure when EES

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are taken into account and this has been attempted in the present work. Two cases of hydrogen thermal plasmas have been considered (i) (H, H^+, e) plasma and (ii) (H^+, H (n) n=1, 12, e) plasmas by including the EES of hydrogen (Sec.2). Section 3 presents first-order electron transport as well as their higher-order contributions along with the role of EES on higher-order contributions to the electron diffusion coefficient and thermal diffusion ratio , which is explained with the help of relative error RE (= $\left| t_e^{(3)}(b) - t_e^{(3)}(a) \right| \times 100 / t_e^{(3)}(b))$ where $t_e^{(3)}(a)$ and $t_e^{(3)}(b)$ represent third-order electron transport properties for case (i) and case (ii) respectively. The unusual behaviour of $f_{k_e^T}^{(m)}$ (m=2,3) at p = 100 atm. has been observed which signifies the strong dependence of higher-order contribution on e-H(n) interactions and the same has been discussed in section 4.

2. Expressions:

2.1 Electron-Electron Diffusion Coefficient:

Within the framework of Chapman-Enskog method, the nth order electron-electron diffusion coefficient given by [11, 12].

$$D_{ee}^{(n)} = D_{ee}^{(1)} f_{D_{ee}}^{(n)}$$

where $D_{ee}^{(1)} = \dfrac{1.5}{x_e n} \left(\dfrac{2\pi k T_e}{m_e} \right)^{1/2} \dfrac{1}{q^{00}}$

$$D_{ee}^{(2)} = D_{ee}^{(1)} \frac{q^{00} q^{11}}{q^{11} q^{00} - (q^{01})^2}$$

$$D_{ee}^{(3)} = D_{ee}^{(1)} \frac{q^{11} q^{22} - (q^{12})^2}{q^{00}[q^{11} q^{22} - (q^{12})^2] + q^{01}(q^{12} q^{02} - q^{01} q^{22}) + q^{02}(q^{01} q^{12} - q^{02} q^{11})}$$

2.2 Electron Thermal Diffusion Ratio:

The nth order electron thermal diffusion ratio is

$$k_e^{T(n)} = k_e^{T(1)} f_{k_e^T}^{(n)}, \text{ where}$$

$$k_e^{T(1)} = \frac{5}{2} x_e \frac{q_{ee}^{01}}{q_{ee}^{11}}$$

and $\qquad k_e^{T(2)} = \dfrac{5}{2} x_e \dfrac{\begin{vmatrix} q_{ee}^{01} & q_{ee}^{02} \\ q_{ee}^{21} & q_{ee}^{22} \end{vmatrix}}{\begin{vmatrix} q_{ee}^{11} & q_{ee}^{12} \\ q_{ee}^{21} & q_{ee}^{22} \end{vmatrix}}$

$$k_e^{T(3)} = \frac{5}{2} x_e \frac{\begin{vmatrix} q_{ee}^{01} & q_{ee}^{02} & q_{ee}^{03} \\ q_{ee}^{21} & q_{ee}^{22} & q_{ee}^{23} \\ q_{ee}^{31} & q_{ee}^{32} & q_{ee}^{33} \end{vmatrix}}{\begin{vmatrix} q_{ee}^{11} & q_{ee}^{12} & q_{ee}^{13} \\ q_{ee}^{21} & q_{ee}^{22} & q_{ee}^{23} \\ q_{ee}^{31} & q_{ee}^{32} & q_{ee}^{33} \end{vmatrix}}$$

where m_e, T_e, n_e represents mass, temperature and density of electrons. The expressions for $q^{00}, q^{01}, q^{02}, q^{11}, q^{12}, q^{13}, q^{22}, q^{23}, q^{33}$ are given elsewhere[12].

In present work, we have considered hydrogen plasma of 14 components viz. electron, H^+ and the electronically excited states H(n), n=1,12. The interactions involved are e-e, e-H^+, e-H(n). As there is decrease in the number of excited states with the increase of pressure, a simple cut off criterion [3] for estimating their number has been used. For obtaining the equilibrium composition of the mixture Saha and Boltzmann laws have been used. The collision integrals for the interactions e-e, e-H^+, have been taken from [3] and e-H(n) from [11].

3. Computation and Results:

We have considered two cases viz (i) thermal plasma (H, H^+, e) where all the atomic hydrogen has been assumed to be in the ground state and (ii) hydrogen thermal plasma with 14 components (e , H (n), n=1,12 & H^+). To study the temperature dependence in the two cases the first, second and third-order electron diffusion coefficient and thermal diffusion ratio have been calculated for a wide range of pressures using the method described in Section 2. Table I presents values of $D_{ee}^{(1)}$ vs. temperature at p = 1, 10 & 100 atm respectively for case (ii). Fig. 1 depicts the variation of $f_{D_{ee}}^{(3)}$ vs. temperature for the cases (i) and (ii) at p = 1, 10 & 100 atm respectively.

Table I: First-order electron Diffusion coefficient $D_{ee}^{(1)}$ (natm^{-1}m^{2}s^{-1}) in the temperature range $(10^4 - 3\times10^4\,\text{K})$ for different number of atomic excited states, where natm is number of atmospheres.

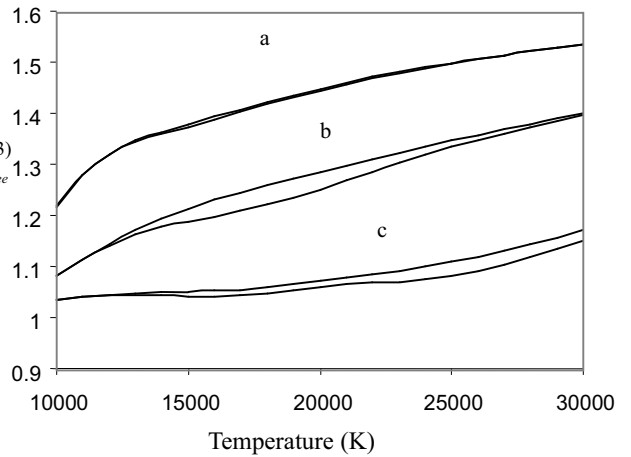| Temperature (K)	p=1 atm n=12	p=10atm n=12	p=100 atm n=7
10000	0.53711	0.92536	1.14285
12000	0.38318	0.92650	1.51943
14000	0.31146	0.83131	1.81033
16000	0.31581	0.76101	2.01118
18000	0.37913	0.76425	2.15361
20000	0.48552	0.85440	2.29291
22000	0.62583	1.02407	2.48695
24000	0.79778	1.25681	2.77256
26000	1.00232	1.54057	3.15885
28000	1.24165	1.87119	3.63734
30000	1.51845	2.24942	4.19650

Fig. 1: Variation of $f_{D_{ee}}^{(3)}$ with temperature. Curve pairs a, b, c refer to $f_{D_{ee}}^{(3)}$ for p = 1, 10 and 100 atm respectively. Lower and upper curves in each pair represent cases (i) and (ii) respectively.

$D_{ee}^{(1)}$ and $D_{ee}^{(3)}$ first decrease and then increase with temperature at p = 1 atm and at p = 10 atm for both case (i) and case (ii).Third -order contribution $f_{D_{ee}}^{(3)}$ increases with temperature whereas for the case (ii) these values are a little higher with maximum deviation between them shifting to high temperatures. At p = 100 atm, $f_{D_{ee}}^{(3)}$ shows a slight decrease and then increases for both cases.

The relative error RE for e-e diffusion has been observed to be 1.2% , 9.3% and18.6% for p = 1,10 and 100 atm respectively thereby indicating the role of EES at high pressure.

Table II presents values of $k_e^{T(1)}$ vs. temperature at p = 1, 10 & 100 atm respectively for case (ii). Fig. 2 depicts the variation of $f_{k_e^T}^{(3)}$ with temperature for the cases (i) and (ii) at p = 1, 10. respectively. Fig 4(b) presents the same at p = 100atm for different numbers of excited states. For the case (i) and case (ii) $f_{k_e^T}^{(2)}$ and $f_{k_e^T}^{(3)}$ first increases then decreases with temperature for p= 1 atm and p = 10 atm but at p = 100 atm both $f_{k_e^T}^{(2)}$ and $f_{k_e^T}^{(3)}$ shows a sharp dip at around 21000K for case(i) .

RE for electron thermal diffusion ratio (Fig 3) assumes maximum values of 0.7% and 6.9% and 34.1% for p = 1 , 10 and 100 atm respectively. Even much more deviations have been observed for $k_e^{T(3)}$ indicating the effect of EES at high pressures.

Table II: First-order thermal diffusion ratio coefficient $k_e^{T(1)}$ in the temperature range ($10^4 - 3 \times 10^4$ K) at different pressures and for different number of atomic excited states.

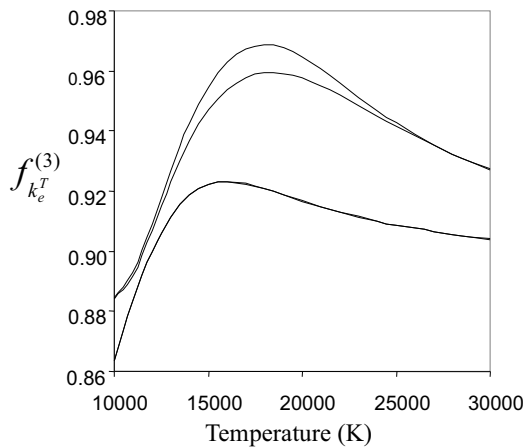| Temperature (K)	p=1 atm n=12	p=10 atm n=12	p=100 atm n=7
10000	0.01190	0.00271	0.00061
12000	0.05726	0.01529	0.00316
14000	0.14857	0.04891	0.01002
16000	0.24608	0.10790	0.02299
18000	0.30316	0.17936	0.04354
20000	0.32739	0.23922	0.07276
22000	0.33818	0.27681	0.10893
24000	0.34409	0.29800	0.14697
26000	0.34799	0.31065	0.18184
28000	0.35091	0.31910	0.21105
30000	0.35325	0.32532	0.23444

Fig.2: Variation $f_{k_e^T}^{(3)}$ of with temperature. The lower and upper curves of the upper pair depict this variation for p=10 for both the cases (i) & (ii) whereas the lower merged pair represents the same for p=1 atm
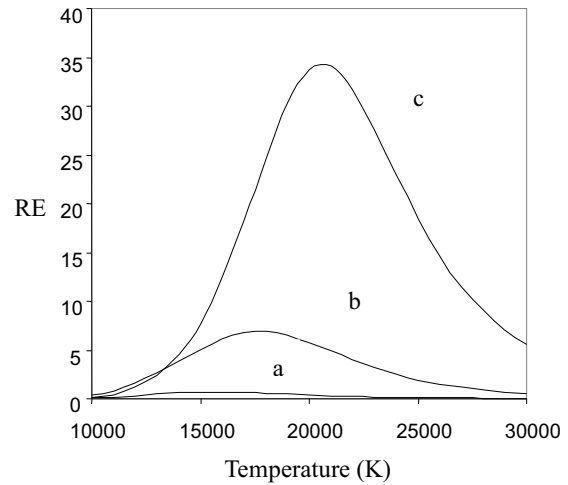
Fig.3: Variation of relative error RE (= $\left| k_e^{T(2)}(b) - k_e^{T(2)}(a) \right| \times 100 / k_e^{T(2)}(b)$) with temperature for different pressures, where $k_e^{T(2)}(a)$ and $k_e^{T(2)}(b)$ refer to cases (i) and (ii) respectively. Curves a, b and c refer to p = 1, 10 and 100 atm respectively.

4. EES dependence at high pressures:

In order to explain the strange behavior of $f_{k_e^T}^{(m)}$ (*m=2,3*) at high pressures(i,e at p=100 atm) , hydrogen thermal plasmas with different number of EES has been considered viz. n=1, 3, 5 and 7. Its results are depicted in figs 4(a) & 4(b) and to know the dominance of EES , concentrations of the ground state atoms at different temperatures are displayed in Fig 5.
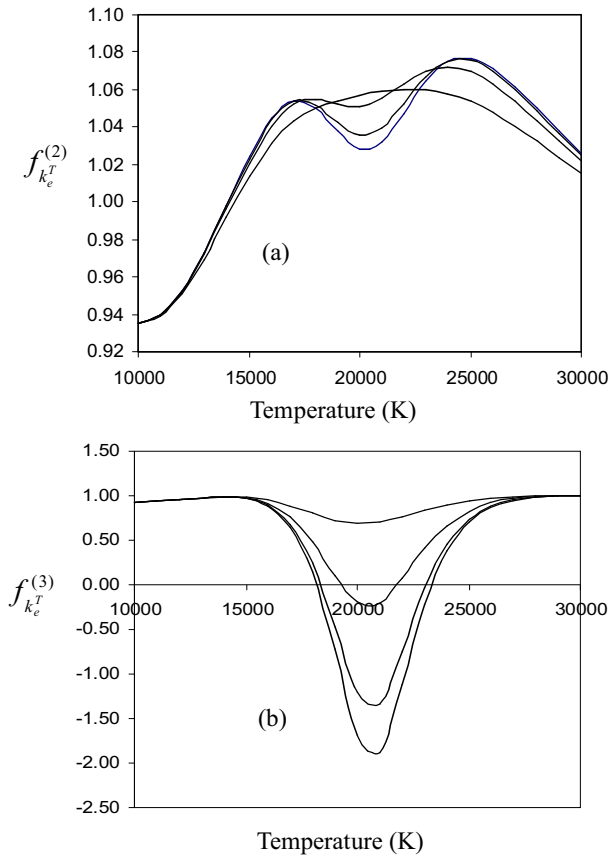

Fig. 4: (a) Variation of $f_{k_e^T}^{(2)}$ with temperature for different values of *n*. The curves from lower to upper represent n = 1, 3, 5 & 7 respectively at p =100 atm.(b) Similar variation for $f_{k_e^T}^{(3)}$

Here it is worth pointing that concentration of atoms in ground state $X_{H(1)}$ depends upon population of excited states viz. $X_{H(1)} = X_H - \sum_{i=2}^{n} X_i$, where X_i and X_H denote the concentration of atoms in the ith excited state and the total concentration of the H atoms in (H (n), H$^+$, e) plasma respectively. It is evident from the Fig.4 that as the number of excited states increases the peaked

behavior of $f_{k_e^T}^{(m)}$ (*m=2,3*) disappears. The above can be explained by the fact that EES must be taken into account while evaluating higher-order contributions.
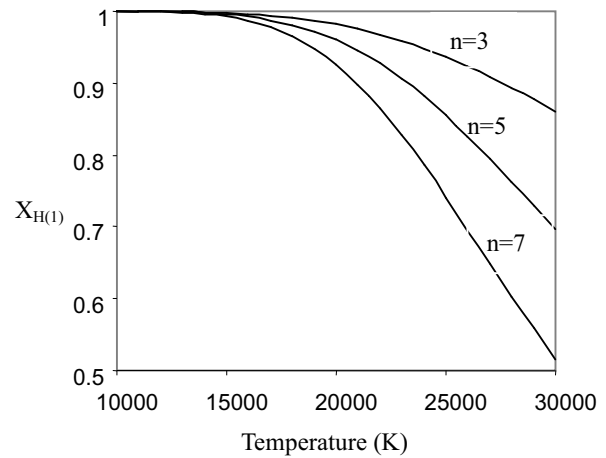

Fig. 5: Variation of ground state concentration $X_{H(1)}$ with temperature for hydrogen plasmas with 3, 5 and 7 excited states respectively at p = 100 atm.

Therefore we conclude that only at high pressures the EES strongly affect the electron transport properties thereby indicating their dominance.

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