Ionization in Hydrogen Plasmas; Comparison of Two Methods of Calculation

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This paper reports the results that are obtained by two methods for calculating the density of ionization in hydrogen plasmas. In a limited, low-density range, the density of ionization may be calculated by use of the Saha equation and the perfect gas law. This method is limited to the low-density range by the requirements for equilibrium in the plasma. As the density of the plasma increases, the overlapping fields from the products of ionization give rise to microfields which reduce the ionization potential and make it necessary to use a more complex equation of state.

One method to calculate the lowering of the ionization potential and the increase in the density of ionization was proposed by Ecker and Kröll (1963). This method is applicable to all atomic species but it is an approximate calculation. When the method was applied to a dense plasma (Bruce and Todd, 1964), the calculated density of ionization was between one and two orders of magnitude higher than that predicted from the perfect gas law; a more thorough study of the problem is accordingly indicated. The second method is designated as the Yukawa method because it consists of substituting the Yukawa potential in the Schröedinger equation to obtain the effective ionization of hydrogen. This is an exact calculation which can be made over a limited range of moderate densities. From the calculated density of ionization, other thermodynamic constants are to be detemined. The methods for calculating these constants are being developed. In the present paper, the changes in pressure will be calculated and used to illustrate the applicability of the method.

Calculations of Electron Density

For comparison and discussion of their relative merits, three methods are presented and compared for calculation of the density of ionization. The first and simplest method is to assume an ideal gas that is described by the perfect gas law. The density of ionization is calculated by the application of the Saha equation. The results are applicable for a diffuse plasma provided complete equilibrium is attained. As the density increases, the error becomes larger.

The preceding method neglects the interaction of the fields of the electrons and ions with the components of the plasma. These fields are referred to as the microfields and they become very important as the density of the plasma increases. They have the effect of lowering the ionization potential and of storing energy in the microfields. The stored energy reduces the pressure in the plasma and requires a modification of the perfect gas law in order to have an applicable equation of state. The reduced ionization potential, I^*, is defined in the first table of equations (Fig. 1) and the value is always less than the ionization potential in free space, I. In order to calculate the amount of ionization, the reduced ionization potential, I^*, is employed in the Saha equation (Ecker and Weizel, 1956; Margenau and Lewis, 1959). An approximate method for calculating the lowering of the ionization potential was suggested by Ecker and Kröll (1963). They employ two equations, one for densities less than a critical density and the other for densities in execess of this density. The critical density is defined by equation 4 and is the limit of validity of the Debye theory (Debye and Hückel, 1923; Kirkwood and Poirier, 1954). The relations are presented in equations 5, 6, 7 and 8. The results are approximate over the entire range of densities. They are rather accurate for

EQUATIONS I

1 SAHA EQUATION $\frac{N_i N_e}{N_0} = \frac{2(2\pi m_e kT)^{3/2}}{h^3} \frac{Q_i}{Q_0} \exp(-I^*/kT)$

2 EFFECTIVE IONIZATION POTENTIAL $I^* = I - \Delta I$

3 DEBYE RADIUS $D = \left[\frac{\varepsilon_0 kT}{8\pi e^2 N_e}\right]^{1/2}$

4 CRITICAL DENSITY $n_{cr} = (3/4\pi)\left[\frac{kT}{e^2}\right]^3$

5 ΔI FOR $N_T \leq n_{cr}$ $\Delta I = + e^2/\varepsilon_0 D$

6 ΔI FOR $N \geq n_{cr}$ $\Delta I = + C e^2/\varepsilon_0 R_0$

7 CONSTANT C IN 6 $C = 2.2 e (2 N_{e_{cr}})^{1/2} / \left[(kT)^{1/2} n_{cr}^{1/3}\right]$

8 AVERAGE PARTICLE DISTANCE $R_0 = \left[3/4\pi N_T\right]^{1/3}$

SYMBOLS DEFINED

N_0 – UNIONIZED PARTICLE DENSITY

N_i – ION DENSITY

N_e – ELECTRON DENSITY

N_T – TOTAL PARTICLE DENSITY

$N_{e_{cr}}$ – ELECTRON DENSITY AT CRITICAL DENSITY

Q_i – ELECTRONIC PARTITION FUNCTIONS

T – TEMPERATURE

e – ELECTRONIC CHARGE

h – PLANCK'S CONSTANT

k – BOLTZMANN'S CONSTANT

m_e – ELECTRON MASS

ϵ_0 – DIELECTRIC CONSTANT

Fig. 1. Equations.

EQUATIONS II

9. YUKAWA POTENTIAL $V(r) = \frac{e^2 \exp(-r/D)}{\varepsilon_0 r}$

10 EIGENVALUE EQUATION $\frac{d^2 u(x)}{d x^2} + \left[C_1 + \frac{C_2 e^{-x}}{x} \right] u(x) = 0$

11. C_1 IN "10" $C_1 = 2.0 \; m_e D^2 I^* / \hbar^2$

12. C_2 IN "10" $C_2 = 2.0 \; e^2 m_e D / \hbar^2$

13. EFFECTIVE IONIZATION POTENTIAL

$$I^* = (C_1 / C_2^2) \; (2 e^4 m_e / \hbar^2)$$

PRESSURE EQUATIONS

14. TOTAL PRESSURE $P_{TOT} = P_{PER} + P_{DEB} + P_{MA} + P_{DEG}$

15. IDEAL GAS PRESSURE $P_{PER} = N_T k T$

16. DEBYE CORRECTION $P_{DEB} = - e^2 N_e / (3 D \varepsilon_0)$

17. MAYER CORRECTION

$$P_{MA} = -k T N_e \sum_{\nu=1}^{16} \sum_{m=1}^{2} (-1)^{m+1} \frac{a_T}{(-a_T)^{\nu}} \left[b_{\nu}(\phi_D) - g_{\nu}(\phi_D) \right]$$

18. a_T IN "17" $a_T = a \varepsilon_0 k T / e^2$

19 ϕ_D IN "17" $\phi_D = a / D$

20. a IN "18" AND "19" $a = \left[-\frac{D}{2} + \left[\frac{D^2}{4} + A \cdot D \right]^{1/2} \right]$

21. A IN "20" $A = e^2 / \varepsilon_0 k T$

22 DEGENERACY CORRECTION

$$P_{DEG} = N_e k T \sum_{y=1}^{\infty} C_y (W/k T)^{3y/2}$$

23. W IN "22" $W = (h^2 / 2 m_e) \left[(3 N_e)/(8 \pi) \right]^{2/3}$

Fig. 2. Equations.

low densities as long as equilibrium exists. The high density equation is made to correspond to the low density solution at the Debye limit. It fails at high densities when the microfields interact strongly. The density at which the equation fails is not clearly established.

There are equations for an exact calculation of the effective ionization potential for hydrogen provided the density of the plasma is not too great and provided equilibrium exists. In this method the value of I^* is obtained by solving Schröedinger's equation with the Yukawa potential function inserted into that equation. The resulting eigen-value problem, equation 10, has been studied by several authors (Sachs and Goeppert-Meyer, 1938; Hulthén, 1942). Hulthén and Laurikainen (1951) have published numerical values for the eigen-functions and the eigen-values that correspond to C_1 and C_2. The effective ionization potential for the hydrogen atom, equation 13, is obtained in terms of the values of C_1 and C_2. The magnitude of the ionization potential decreases with the Debye length, D, as is illustrated by the curve in Fig. 3. The very steep slope for small Debye lengths is indicative of pressure ionization. The Yukawa potential fails at high densities. The range of applicability is certainly as great as that of the Debye theory, which is discussed by Kirkwood and Poirier (1954).

Comparisons between the density of ionization that is predicted by the three methods assist in evaluating the range of applicability and the accuracy of the different solutions. The variation of the ionization with density was investigated for isotherm curves with energies of the particles of 2 ev and 5 ev. The results from the three methods are shown in the inserted curves in Figs. 7 and 8. The results for the perfect gas law were taken from Rouse (1962). Deviations between the three methods become larger as the densities increase and the temperature decrease.

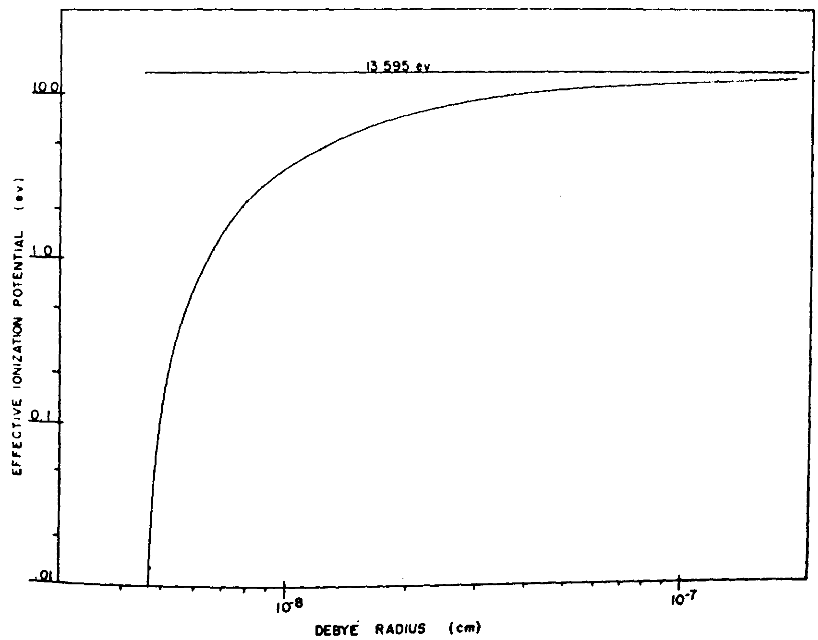

Fig. 3. Effective ionization potential for hydrogen as a function of the Debye length.

CALCULATION OF THE PRESSURE-DENSITY RELATION FOR CONSTANT TEMPERATURE

The energy that is stored in the microfields reduces the pressure below the value that is predicted by the perfect gas law. In this paper the corrections to the perfect gas law from the energy in the microfields and from the degeneracy correction are considered. The correction for degeneracy is introduced to account for the approach to Fermi statistics for the electrons at high densities. The total pressure is divided into four parts for calculation as indicated by equation 14. These are: (a) the pressure from the perfect gas law, P_{PER}; (b) the decrease in pressure from the Debye-Hückel limiting law, P_{DEB}; (c) the increase in pressure from the Mayer correction, P_{MA}; and (d) the increase in pressure from the degeneracy correction, P_{DEG}. The part of the pressure from the two terms, P_{DEB} and P_{MA}, is currently designated as the Mayer Cluster Integral correction but tabulated values are available for P_{MA} (Poirier, 1953). The partial pressure, P_{DEB}, is the Debye-Hückel limiting pressure and is described in an early paper (Debye and Hückel, 1923). This term is always negative and may have a larger absolute value than the perfect gas pressure. The numerical value is calculated from equation 16. The partial pressure, P_{MA}, is a positive pressure but only includes the correction for the Coulomb potential. The value is calculated from equation 17 with numerical values of the terms within the square brakets for various values of a and ν that are taken from the paper by Poirier (1953). The basic considerations for the derivation of the particular degeneracy correction that is employed for P_{DEG} was derived by Stoner. The equations in the form of equations 22 and 23 were presented in a form for computation in a later paper (McDougall and Stoner, 1939).

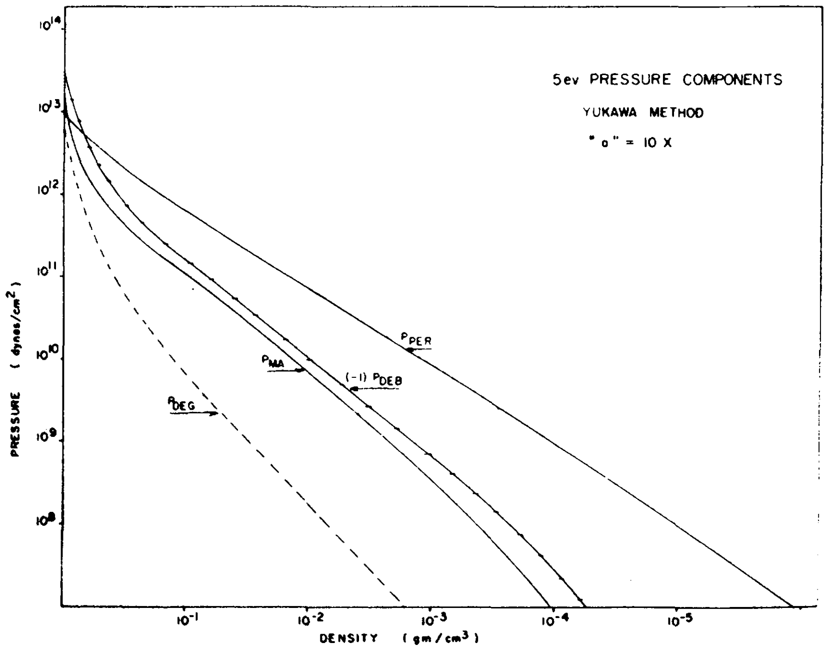

Fig. 4. Components of pressure for the 5 ev isotherm by the Yukawa method.

Only the Coulomb potential is explicitly introduced in the equation to determine the effect of the microfields, but Mayer has suggested that all "other interactions" between the particles may be approximated by a proper choice of the distance of closest approach, a. The "other interactions" would include all short range forces and, in particular, the short range repulsive forces between the cores of the ions and electrons. From the complexity of the interaction, no single numerical value of a can be valid for all ranges of density and temperature. Duclos and Cambel (1962) suggest that the parameter, a, may be made a function of the Debye length which is given in equation 20. This is equivalent to introducing a dependence of a on the temperature in order to extend the range of applicability.

The relative magnitude of the different components of the pressure was investigated for 5 ev-particles in the plasma over a wide range of densities. The Yukawa method was employed and equation 20 was used for the distance of closest approach. The components of the pressure are shown in Fig. 4 and the total pressure is given as the curve that is labeled Yukawa in Fig. 8. The perfect gas pressure, P_{PER}, is positive and is a straight line. The limiting Debye-Hückel pressure is negative and the absolute value is greater than the perfect gas pressure for dense plasmas where the accuracy is becoming questionable. Both the pressure from the Mayer effect, P_{MA}, and the pressure from the degeneracy, P_{DEG}, are positive. The magnitude of P_{MA} depends on the value of a and the total pressure will be negative with a small value a. A small value of a has the effect of storing too much energy in the microfields. The slope of the P_{MA}

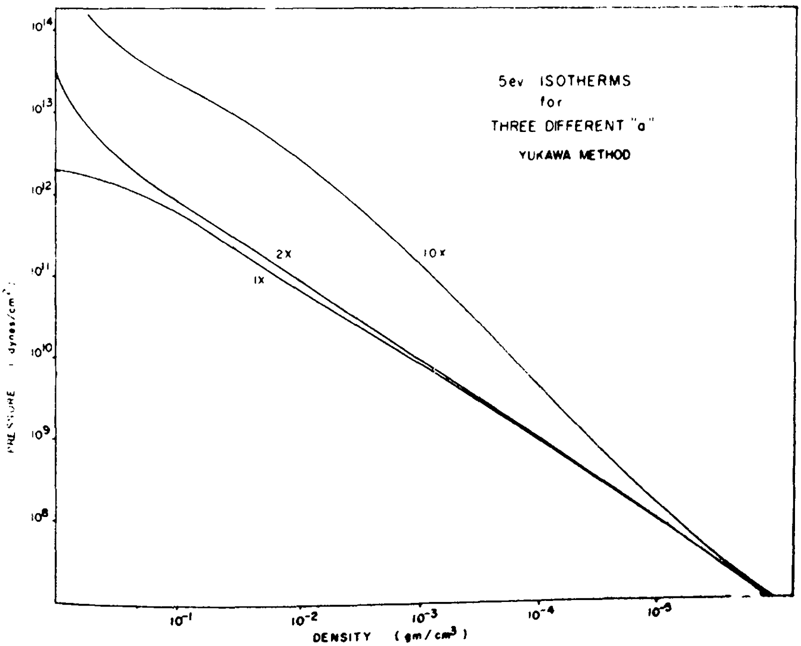

Fig. 5. Isotherms for 5 ev by the Yukawa method using three values for the distance of closest approach.

curve depends on whether a is a true constant or is a function of the temperature through equation 20. The latter choice appears more realistic and gives a lower pressure in dense plasmas. There does not appear to be definitive experimental evidence on the proper choice in the range of density that is of interest to this project.

The distance of closest approach affects P_{MA} so significantly that the subject was investigated analytically by both the Yukawa and the Ecker and Kröll methods. The analytical comparison consisted of calculating the relation between the pressure and density for three distances of closest approach in a plasma with particles that are in equilibrium with an energy of 5 ev; i.e. to calculate the 5 ev isotherm. The isotherms by the Yukawa method were calculated for the distance that is given by equation 20, by twice this distance and by ten times this distance. Duclos recommended that latter value for the closest approach in order to obtain results that are believed to exist in the plasma. The results of these calculations are presented in Fig. 5. The isotherms by the Ecker and Kröll method were calculated for the same three distances of closest approach and the results are presented in Fig. 6. There is no practical dilfference in the predictions of the Yukawa method and of the Ecker and Kröll method at densities that are less than 10^{-3} g/cm^3 and there is only a minor difference in the very high density range from 10^{-2} to 1. The minor differences between the two methods of calculation do show a difference in the slope with which the curves approach the highest density.

The effect of temperature on the pressure-density relations is indicated by the calculation of the isotherms for particles in the plasma with an energy of 2 and of 5 ev. The calculations were made by the three available

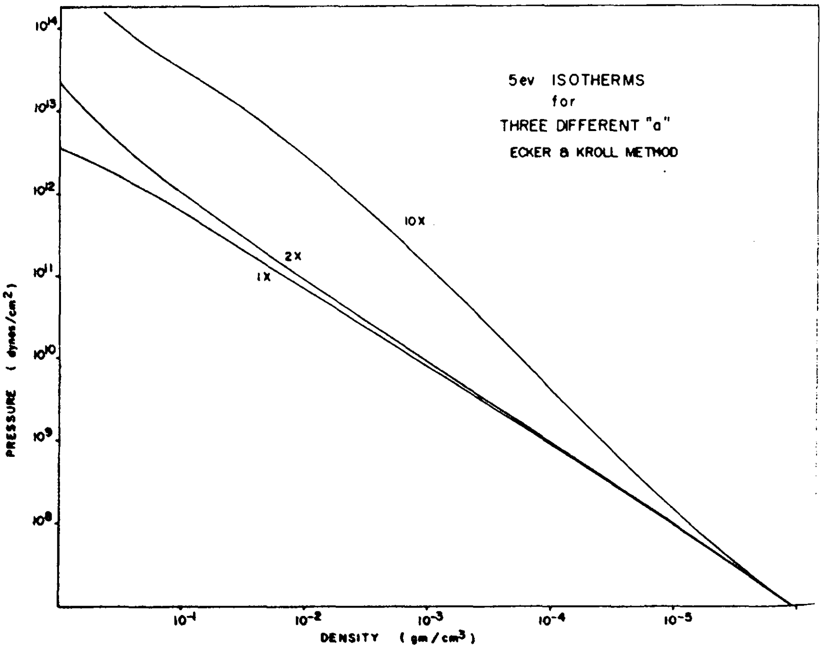

Fig. 6. Isotherms for 5 ev by the Ecker and Kröll method using three values for the distance of closest approach.

methods: the perfect gas law approximation, the Yukawa method and the Ecker and Kröll method. For the latter two calculations, the distance of closest approach was assumed to be 10 tmes the distance that is given by equation 20; i.e. by the distance that is recommended by Duclos. The isotherms for 2 ev that were calculated by the three methods are presented in Fig. 7. The inserted curves in the upper right show the ionization vs. the density for the same three methods. The isotherms for 5 ev by the same three methods are presented in Fig. 8. In comparing the curves in these two figures, the most interesting difference is the rapid increase in ionization with density for the 2 ev isotherms as compared with the 5 ev electron volt group. The difference occurs since the ionization is practically complete for all densities in the 5 ev plasma while the ionization is increasing rapidly with the pressure at high densities in the 2 ev plasma. This effect is designated "pressure ionization" at an earlier position in this paper.

In conclusion, the difference between the 1x and the 10x curves in Figs. 5 and 6 represents an approximation for the short range repulsive forces which has not yet been calculated. There is not much reason for a choice between the Yukawa and the Ecker and Kröll results. Since the latter method is applicable for all ions, the nearness of the Yukawa and Ecker and Kröll results yields confidence for the application to other ions.

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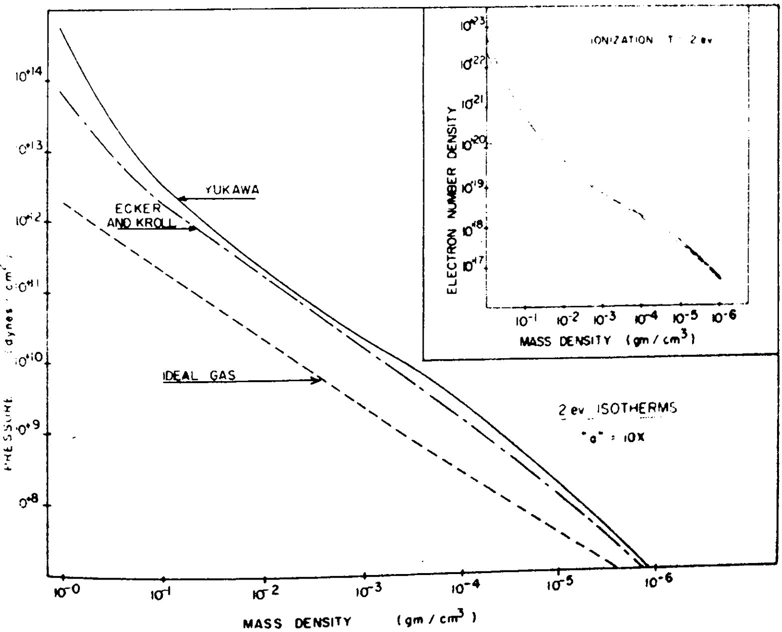

Fig. 7. Comparison of the Yukawa, the Ecker and Kröll and the ideal gas isotherms for 2 ev particles. Corresponding ionization curves are shown in the upper right.

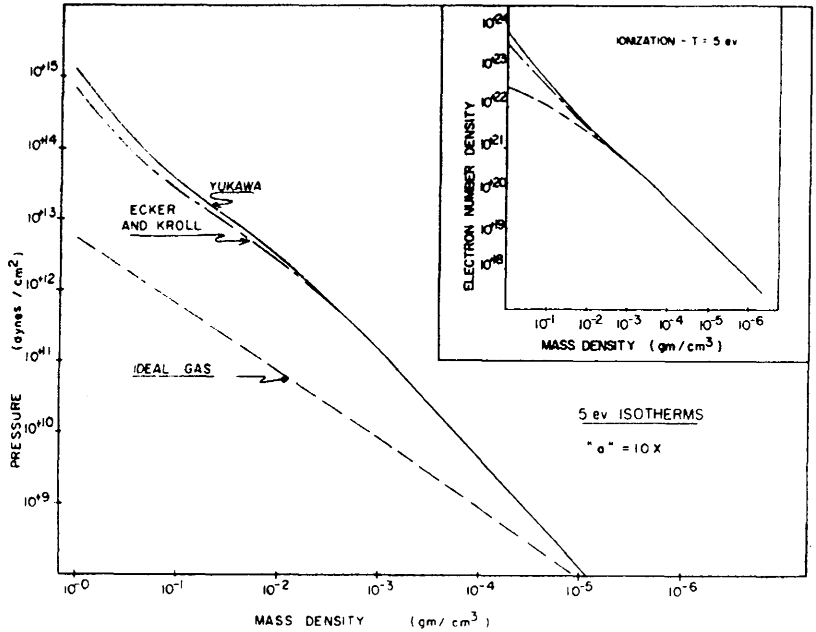

Fig. 8. Comparison of the Yukawa, the Ecker and Kröll, and the ideal gas isotherms for 5 ev particles. Corresponding ionization curves are shown in the upper right.

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