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FIRST-ORDER ESTIMATE OF THE SAHA EQUATION FOR A HELIUM PLASMA

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Closed forms for the ratios $n_e n_i/n_0(q)$ and $n_e^2 n_\alpha/n_0(q)$ are obtained for a high temperature helium plasma; they include approximate expressions for electrostatic interaction. The analysis further assumes that ground state contributions dominate partition function summations. In the above expressions, n_e is the electron number density, n_i is the ion number density, n_α is the alpha particle number density, and $n_0(q)$ is the number density of helium atoms excited to the q-quantum number state. These ratios are found to be maximum at the quantum state $q \approx \sqrt{R/k_B T}$, where R is the Rydberg constant, k_B is Boltzmann's constant and T is the temperature.

ОЦЕНКА ПЕРВОГО ПОРЯДКА ДЛЯ УРАВНЕНИЯ САХА, ОПИСЫВАЮЩЕГО ГЕЛИЕВУЮ ПЛАЗМУ

В работе получены близкие выражения для отношений $n_e n_i/n_0(q)$ и $n_e^2 n_\alpha/n_0(q)$ в случае высокотемпературной гелиевой плазмы, причем использованы приближенные выражения для электростатического взаимодействия. Последующий анализ позволяет сделать вывод, что вклады от основных состояний влияют на сложение функций распределения. В указанных выше выражениях n_e — это плотность электронов, n_i — плотность ионов, n_α — плотность альфа частиц и $n_0(q)$ — плотность атомов гелия, возбужденных до состояния с квантовым числом q. Найдено, что эти выражения достигают максимума при значении $q = \sqrt{R/k_B T}$, где R — постоянная Ридберга, k_B — постоянная Больцмана и T — температура.

I. INTRODUCTION

Recent attempts at producing an X-ray laser as well as the general study of onizing and reacting plasma have stimulated anew the interest in the Saha equation [1]. Early among such investigations is that of McWhirter and Hearn [2], which deals with a Hydrogen plasma and seeks to find the population densities

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of atoms in excited states as a function of time. The authors find that a quasi steady state maintains for a given excited state when bound bound-transitions are far more probable than transitions to and from the continuum. For such cases the Saha equation becomes relevant. The numerical analysis reveals a population inversion between the 3rd and 4th quantum states.

Recent experiments have exhibited a population inversion in an aluminium plasma [3] during its free expansion and cooling between the $n=3$ and $n=4$ quantum levels corresponding to radiation at the wavelength 12.97 nm. The plasma is produced by bombarding an aluminium surface with a 50 GW laser. A theoretical study of this experiment is modeled after a Helium plasma [4], in which the Saha equation plays an important role relevant to the high quantum levels of the atom. In this note we consider the appropriate forms of this equation relevant to a Helium plasma.

II. ANALYSIS

IIa. Energy states

Eigenenergies of the excited states of the helium atoms are conveniently obtained from the Heisenberg unsymmetric forms for the Hamiltonian [5],

$$H = H_{0a} + \varepsilon H_{1a} = H_{0b} + \varepsilon H_{1b},$$

where H_1 denotes the electrostatic perturbation component. In the unperturbed Hamiltonian, H_{0a}, electron no. 1 'sees' the bare nucleus and electron no. 2 'sees' a shielded nucleus. Assuming for the moment a nuclear charge of eZ, we have

$$H_{0a} = P_1^2/2m_1 + P_2^2/2m_2 + Ze^2/r_1 + (Z-1)e^2/r_2. \qquad (1)$$

In the excited states of H_{0a} one assumes that electron no. 1, which is closer to the nucleus, remains in its ground state. In H_{0b} the roles of electrons are reversed. Eigenfunctions of H_{0a} and H_{0b} are in the product form

$$\begin{aligned} u_{0a} &= \Psi^{(2)}_{100}(1)\ \Psi^{(1)}_{qlm}(2) \\ u_{0b} &= \Psi^{(2)}_{100}(2)\ \Psi^{(1)}_{qlm}(1), \end{aligned} \qquad (2)$$

where $\Psi^{(Z)}_{qlm}$ denote hydrogenic wavefunctions corresponding to the nuclear charge eZ. These states satisfy the equations

$$\begin{aligned} H_{0a}u_{0a} &= E_0 u_{0a} \\ H_{0b}u_{0b} &= E_0 u_{0b} \\ E_0 &= -4R(1+1/4q^2). \end{aligned} \qquad (3)$$

The reason that the value of the unperturbed ground state

$$E_{0,G} = -4(1.25)R$$

is more positive than the canonical value [6] $E^1_{0,G} = -8R$, is due to the unsymmetric form of the Hamiltonian (1) in which one electron is shielded. Thus E_{0G} exceeds $E^1_{0,G}$ by $3R$, which gives the ground state energy $E_{0,G} = -74.8$ eV.

In these expressions R is the Rydberg constant, $R = e^2/2a_0^2 = 13.6$ eV, $a_0 = = n^2/me^2 = 0.0529$ nm.

Returning to the representation (2), space-spin wavefunctions of the unperturbed Hamiltonian $H_{0a} + H_{0b}$ appear as

$$^3\Psi_{qlm} = \frac{1}{\sqrt{2}}(u_{0a} - u_{0b})\xi_S(1,2) \qquad (4a)$$

$$^1\psi_{qlm} = \frac{1}{\sqrt{2}}(u_{0a} + u_{0b})\xi_A(1,2). \qquad (4b)$$

The spin wavefunctions $\xi_{A,S}$ are given by

$$\xi_A = \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) - \beta(1)\alpha(2)] \qquad (5a)$$

$$\xi_S^{(1)} = \alpha(1)\alpha(2) \qquad (5b)$$

$$\xi_S^{(0)} = \frac{1}{\sqrt{2}}[\alpha(1)\beta(2) + \beta(1)\alpha(2)] \qquad (5c)$$

$$\xi_S^{(-1)} = \beta(1)\beta(2). \qquad (5d)$$

In these equations the spinors α and β satisfy the eigenvalue equations

$$\hat{S}_1^2\alpha(1) = \frac{3}{4}\hbar^2\alpha(1)$$

$$\hat{S}_{z1}\alpha(1) = \frac{\hbar}{2}\alpha(1)$$

$$\hat{S}_1^2\beta(1) = \frac{3}{4}\hbar^2\beta(1)$$

$$\hat{S}_{z1}\beta(1) = -\frac{\hbar}{2}\beta(1)$$

etc.

As it is well known, when the electrostatic interaction $e^2/|r_1 - r_2|$ is brought into play, energies corresponding to the triplet states lie lower than those of the singlet states. It has been further established that less energy is required to ionize a Helium atom (from the ground state) than is required to raise both electrons to excited levels.

With these observations in mind we may conclude that excited states of Helium are predominantly of the form given by the triplet states (4a). The corresponding eigenenergy, with correction due to the electrostatic interaction written $4R\Lambda(q)$, appears as

$$W(q) = -4R\left(1+\frac{1}{4q^2}\right)+4R\Lambda(q). \tag{7}$$

The calculated [5] value of $4R\Lambda \simeq -10.9$ eV. The degeneracy of the eigenenergy $W(q)$ is $2\times q^2\times 3$, where the factor of 2 corresponds to the exchange $r_1 \rightleftarrows r_2$, the factor of 3 stems from the degeneracy of the triplet state ξ_S and the factor q^2 stems from orbital angular momentum degeneracy.

IIb. Number- densities and the Saha equation

Consider the ionizing reaction

$$\mathrm{He}(q) \rightleftarrows \mathrm{He}^{+}(b)+e. \tag{8}$$

The notation is such that q and b denote the quantum number of excited states. The equation of the reaction equilibrium [7] for the process (8) is

$$\mu_0 = \mu_i + \mu_e\,, \tag{9}$$

where μ denotes the chemical potential. With $\beta \equiv 1/k_B T$, one obtains for the fugacity $z = e^{\beta\mu}$

$$z_0 = z_i z_e\,. \tag{10}$$

The average value of an occupation number $N(j)$ for the j^{th} state with the degeneracy g_j, for any of the three species in (8), follows naturally from the ground partition function [8]. One obtains

$$N(j) = z g_j \exp(-\beta\varepsilon_j). \tag{11}$$

The energy ε_j may be divided into kinetic and internal energy terms

$$\varepsilon_j = \frac{p_j^2}{2m} + W_j\,. \tag{12}$$

Thus, (11) becomes

$$N_j = z g_j \exp\left[-\beta\left(\frac{p_j^2}{2m}+W_j\right)\right]. \tag{13}$$

Let the reacting plasma be confined to the volume V. Then the number densities are given by

$$n(j) = \frac{1}{V}\int_{p_j} N(j) = \frac{z g_j \exp(-\beta W_j)}{\lambda^3} \tag{14}$$

where $2\pi\lambda$ is the effective de Broglie wavelength

$$\lambda^2 = \frac{2\pi\hbar^2\beta}{m}. \tag{15}$$

With (14) we obtain the three densities

$$n_e = \frac{2z_e}{\lambda_e^3} \tag{16a}$$

$$n_i(b) = \frac{g_{i,b}\, e^{-\beta W_i(b)} z_i}{\lambda_i^3} \tag{16b}$$

$$n_0(q) = \frac{g_{0,q}\, e^{-\beta W_0(q)} z_i z_e}{\lambda_0^3}. \tag{16c}$$

The degeneracy g-factors, as obtained above, are given by

$$g_{0,q} = 6q^2$$
$$g_{i,b} = 2b^2\,. \tag{17}$$

With $n = \Sigma n(j)$ denoting the average number density, one obtains from (16),

$$\frac{n_e \sum_b n_i(b)}{n_0(q)} = \frac{n_e n_i}{n_0(q)} = \frac{\sum_b 2(b/q)^2\, e^{-\beta[W_i(b)-W_0(q)]}}{3\lambda_e^3}. \tag{18}$$

Here we have recalled (10) and have further set $(\lambda_0/\lambda_i)^2 = 1$. Eq. (18) may be rewritten, with (7),

$$\frac{n_e n_i}{n_0(q)} = \frac{\sum_b 2(b/q)^2\, e^{-4\beta R}\, e^{4\beta R\left[\frac{1}{b^2}+\Delta(q)-\frac{1}{4q^2}+\Lambda(q)\right]}}{3\lambda_e^3}. \tag{19}$$

With (5) this equation may be expressed in terms of the difference in ion energies

$$\tilde{W}_{bq} = W_b^{ion} - W_q^{ion} = -4R\left[\frac{1}{b^2}-\frac{1}{4q^2}\right]. \tag{20}$$

There results,

$$\frac{n_e n_i}{n_0(q)} = \frac{\sum_b 2(b/q)^2\, e^{-4\beta R}\, e^{-\beta \tilde{W}_{bq}}\, e^{\beta 4R\Lambda(q)}}{3\lambda_e^3}. \tag{21}$$

The divergence in the summation over b in (19) may be attributed to the fact that we have assumed particles in the plasma to be non-interacting. Collisions of ions with electrons and atoms, as well as with other ions, would provide a cutoff in the b-summation, thereby rendering it finite [9].

The largest term in the b-summation in (19) stems from the ion ground state value, $b = 1$. Assuming that this term represents the dominant contribution we obtain the canonical form

$$\frac{n_e n_i}{n_0(q)} = \frac{2e^{-\beta I_q}}{3\lambda_e^3 q^2}, \tag{22}$$

where,

$$I_q = 4R\left[\frac{1}{4q^2} - \Lambda(q)\right] \tag{23}$$

represents the ionization energy of the Helium atom from the q_{th} excited state, as given by (4a) and for $q = 1$ has the value

$$I_1 = 54.4 - 29.9 = 24.5 \text{ eV}.$$

IIc. The doubly-ionized Helium plasma

At higher temperatures, the Helium ion loses its remaining electron through reactions of the form

$$e + He^+(b) \rightleftarrows \alpha + e + e, \tag{25}$$

where α denotes an alpha particle. The density $n_\alpha(b)$ is given by

$$n_\alpha(b) = \frac{g_\alpha e^{-\beta W_\alpha(b)} z_\alpha}{\lambda_\alpha^3}. \tag{26}$$

With $g_\alpha = 1$, we obtain

$$\frac{n_e \sum_b n_\alpha(b)}{n_i(s)} = \frac{n_e n_\alpha}{n_i(s)} = \frac{e^{-\beta I'_s}}{\lambda_e^3 s^2}, \tag{27}$$

where I'_s is the ionization energy of the Helium ion in the s^{th} excited state,

$$I'_s = \frac{4R}{S^2} \tag{28}$$

of $n_i(s)$ in (27) is summed over s and we encounter a divergence which again may be attributed to the absence of interactions in the analysis. Once more assuming that the dominant contribution is contained in the ground ion-state, $s = 1$, term, we obtain

$$\frac{n_e n_\alpha}{n_i} = \frac{e^{-\beta I'_1}}{\lambda_e^3}. \tag{29}$$

This equation, together with (22) and the equation of charge neutrality

$$n_e = n_i + 2n_\alpha \tag{30}$$

may be employed to obtain equilibrium relations among the four species n_e, n_α, n_i, $n_0(q)$. For example, multiplication of (22) and (29) eliminates n_i and yields

$$\frac{n_e^2 n_\alpha}{n_0(q)} = \frac{2e^{-\beta(I'_1 + I_q)}}{3\lambda_e^6 q^2}, \tag{31}$$

where

$$I'_1 + I_q = 4R\left[1 + \frac{1}{4q^2} - \Lambda(q)\right].$$

This Saha equation is relevant to the process

$$He \rightleftarrows \alpha + 2e. \tag{32}$$

The corresponding fugacity equation is

$$z_0 = z_\alpha z_e^2. \tag{33}$$

Eq. (31) results, providing one assumes that the Helium atom is ionized first through losing an electron in the state (6) and then through losing the remaining electron in the ground state.

Division of (22) and (29) eliminates n_e and gives

$$\frac{n_i^2}{n_0(q) n_\alpha} = \frac{2e^{-\beta(I_q - I'_1)}}{3q^2} \tag{34}$$

where

$$I_q - I'_1 = 4R\left[\frac{1}{Q^2} - 1 - \Lambda(q)\right].$$

Electrostatic interaction

A tractable form for the electrostatic interaction term is obtained in the Bohr limit [5] with $q = l + 1$. It is given by

$$-\Lambda(q) = \frac{1}{(2q-1)^{2q+1}}\left(1 + \frac{2q-1}{2q^2}\right) + \frac{16q^2(2q+3)}{(2q-1)^{2q+4}}.$$

Substituting this form into (22) we obtain

$$\frac{n_e n_i}{n_0(q)} = \frac{2 \exp - 4\beta R\left[\frac{1}{4q^2} - \Lambda(q)\right]}{3\lambda_e^3 q^2}. \tag{35}$$

Assuming $|\Lambda(q)| \ll I_q$ indicates that the ratio $n_e n_i/n_0$ is maximum at the q-quantum value

$$q \simeq \sqrt{\beta R} \equiv \bar{q}.$$

At this value one obtains

$$\left(\frac{n_e n_i}{n_0}\right)_{MAX} = \frac{2}{3\lambda_e^3 \bar{q}^2} \exp\left[-1 + 4\bar{q}^2 \Lambda(\bar{q})\right]. \tag{36}$$

A sketch of the ratio $n_e n_i/n_0$ as a function of q is shown in Fig. 1. A similar expression for the maximum value of the ratio $n_e^2 n_\alpha/n_0$ is obtained from (31) with q replaced by $\bar{q}$.

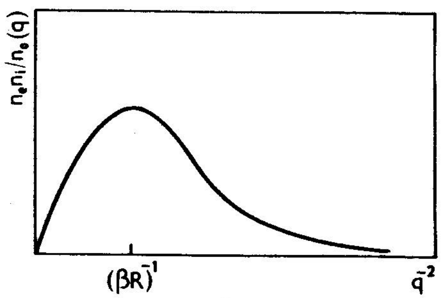

Fig. 1. Sketch of the ratio $n_e n_i/n_0(q)$ vs inverse square quantum number.

III. CONCLUSION

Various forms of the Saha equation have been obtained for a high temperature helium plasma. In evaluating partition function summations it was assumed that the dominant contribution is contained in the ground ion-state for the singly ionized species. Closed forms for the ration $n_e n_i/n_0(q)$, and $n_e^2 n_\alpha/n_0(q)$ including the effects of electrostatic interaction were obtained as explicit functions of the excitation quantum number q of the neutral helium atom. These ratios were found to be maximum at the quantum value $q = R/k_B T$. Equivalently one may say that at this temperature a minimum number of atoms would be found in this quantum state.

, We note finally that the later conclusion does not infer that photons passing through the plasma would suffer coherent amplification. As it is well known, exponential growth of radiation occurs when the probability that a resonant photon stimulates emission outweighs the probability that it is absorbed in the excitation of the atom. For the two states $E(q) > E(q')$ this gives the criterion [10, 11]

$$\frac{n(q)}{g_q} > \frac{n(q')}{g_{q'}}. \tag{37}$$

Typically [see (17)], $g \propto q^2$, so that for the configurations considered (37) is never satisfied.

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