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C. S. Helrich

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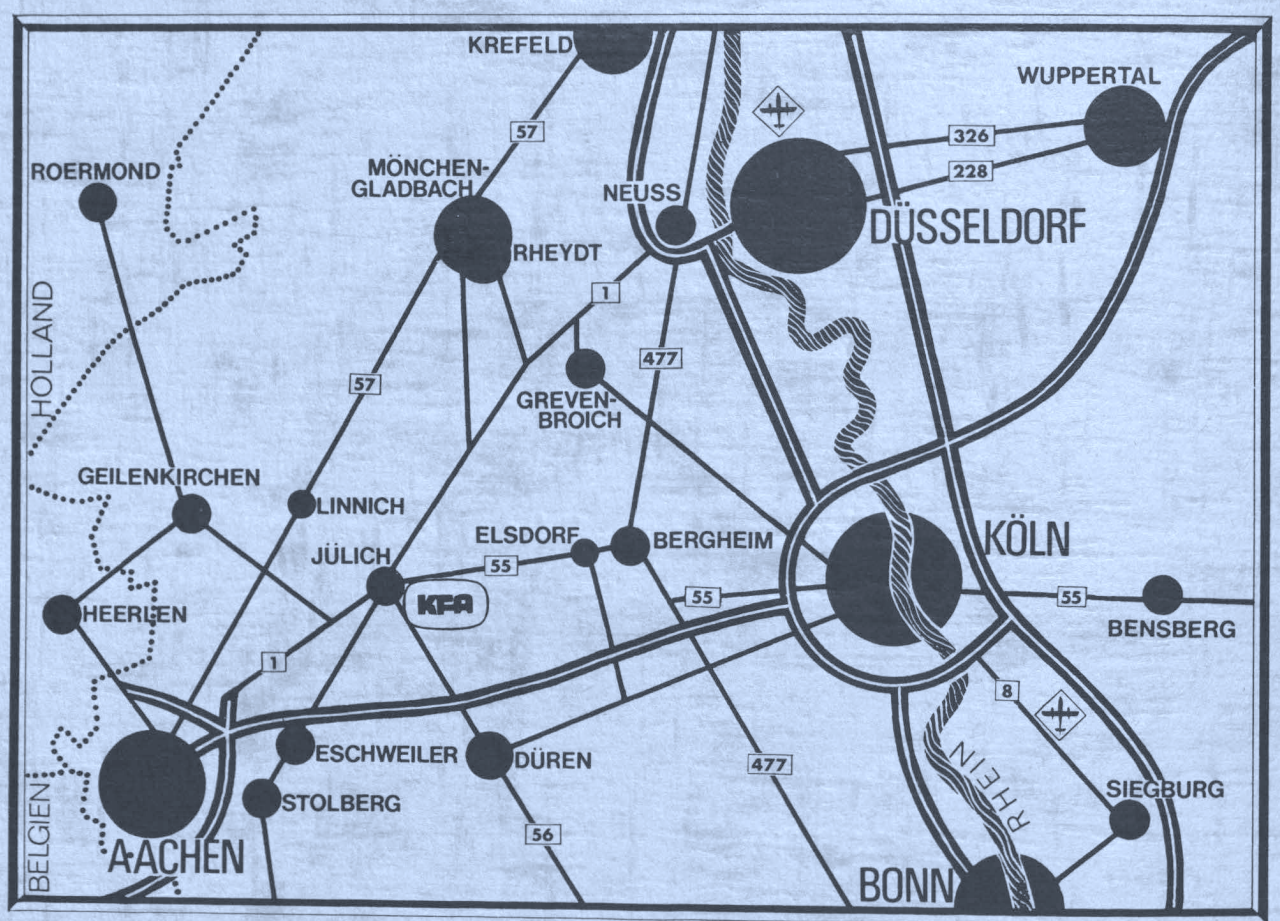

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Effective Level Schemes for the Neutral Component of a Plasma

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C. S. Helrich

The work reported here was performed within the activities of the Sonderforschungsbereich Plasmaphysik Bochum-Jülich.

Abstract

A procedure is presented by which the level scheme of the neutral component of a plasma may be converted into an effective level scheme consisting of a small number of effective levels. Cesium under conditions of technological interest is treated as an example. An effective level scheme consisting of five levels is seen to give results deviating less than 5% from those of Norcross and Stone [5] who considered 53 levels.

I. Introduction

A determination of the internal state of the neutrals is of central importance in any realistic analysis of a three component plasma. Because of the complexity of atomic level schemes, however, the calculation of occupation numbers in a nonequilibrium plasma is not an easy task. This task can be greatly simplified if it is possible to reduce the level scheme to a model scheme containing a small number of equivalent levels.

To produce such a model, we proceed directly from the basic equations for the occupation number densities making use of the observation that even under conditions insufficient for equilibrium of the total level scheme, certain groups of levels may still be in relative equilibrium. As an example of this procedure, a cesium plasma under conditions of technological interest is considered.

II. Specification and Development of the Model

a) The System

We consider a plasma consisting of free electrons, ions only in their ground state, and atoms in any state of excitation. The plasma will be assumed to be spatially homogeneous. Such a condition is realized if the inhomogeneity lengths are large compared to the relaxation lengths of the excited states [1,2]. We shall also assume that the characteristic times associated with the relaxation of atomic states are much smaller than those of the bulk plasma processes under investigation. Because of the temperatures involved, all molecular effects will be ignored. It will be assumed that collisional excitation and ionization arises only from electron-atom collisions. The plasma will be assumed to be optically thin to all but resonance radiation, which is assumed to be totally absorbed.

b) Analytical Formulation

The occupation number densities of the atomic states,

N_p, satisfy the equations [3]

$$\frac{dN_p}{dt} = -N_p\left\{\sum_{q\neq p} N_e K(p,q) + \sum_{q<p} A(p,q) + N_e K(p,c)\right\} + \sum_{q\neq p} N_e N_q K(q,p) + \sum_{q>p} N_q A(q,p) + N_e^3 K(c,p) + N_e^2 \beta(p) \quad (1)$$

and the free electron density, N_e, satisfies [3]

$$\frac{dN_e}{dt} = \sum_p N_e N_p K(p,c) - \sum_p \left[N_e^3 K(c,p) + N_e^2 \beta(p)\right] \quad (2)$$

where

A(p,q)= Einstein spontaneous emission coefficient between levels p and q

K(p,q)= collisional transition coefficient between levels p and q

K(p,c)= collisional ionization coefficent from level p

K(c,p)= three body recombination coefficient to level p

β(p)= radiative recombination coefficient to level p .

The general problem of determining the internal state of the neutrals involves the solving of equations (1) and (2). It is often possible to reduce this set of equations to a finite set of reasonable dimension by collecting certain levels together to form groups. The criterion for this grouping is the transition rate. That is, if each of the transition rates between the levels of a set greatly exceeds those to levels outside the set, the set forms a group, the relative densities of whose levels may be solved for independently. The overall group densities may then be obtained from a separate set of group equations. A computational simplification is obtained when, in addition, the levels within these groups are in relative Saha-Boltzmann equilibrium.

The levels of a group are in relative Saha-Boltzmann equilibrium when the transition rates within the group are collision dominated and the free electron distribution function is Maxwellian in the energy range of importance for the respective transitions. This limitation on the electron distribution function is not as restrictive as it

may appear. For transitions within the group, the low energy electrons are the most important because of the relatively small energy difference between levels within a group and because the density of low energy electrons is so much higher than that of high energy electrons. In this enegy region, the electron distribution is essentially Maxwellian even though it may deviate from Maxwellian for higher energies as a result of inelastic effects [4].

Since the relaxation times of the internal atomic states are assumed small compared to the characteristic times of other plasma processes under investigation, the occupation densities of the excited states may be treated as time independent, although not in equilibrium. We shall call these non-equilibrium, steady-state number densities $\bar{N}_p$ and the corresponding free electron density $\bar{N}_e$. It is this set of densities we wish to determine.

As they stand, a direct comparison of the transition rates in equations (1) is impossible because these rates depend upon the $\bar{N}_p$ and $\bar{N}_e$ which are unknown. If, however,

rather than considering the equations (1) directly, we study equations in linear form for the perturbations around $\bar{N}_p$ and $\bar{N}e$, the transition rates responsible for the relaxation of the perturbations may easily be compared with one another. That the relationships between the transition rates is unaltered whether one considers the set (1) or the perturbation equations follows provided the perturbations are small.

For convenience, the perturbations will be normalized with respect to the Saha-Boltzmann densities. That is

$$\eta_p = (N_p - \bar{N}_p) / \tilde{N}_p \tag{3a}$$

$$\eta_e = (N_e - \bar{N}_e) / \tilde{N}_e \tag{3b}$$

where $\tilde{N}_p$ and $\tilde{N}_e$ are Saha-Boltzmann densities related by

$$\tilde{N}_p = (2L_p + 1)(2\pi\hbar^2/m\,kT)^{3/2}\,\tilde{N}_e^2\,\exp(E_p/kT) \tag{4}$$

in which L_p is the orbital angular momentum quantum number and E_p the ionization potential of level p, T is the electron temperature, and m the electron mass. With equation (3) and the conditions of detail balance, the linearized equations for η_p and η_e are

$$\frac{d\eta_p}{dt} = -\eta_p \left\{ \sum_{p \neq q} \bar{N}_e K(p,q) + \sum_{q<p} A(p,q) + \bar{N}_e K(p,c) \right\}$$
$$+ \sum_{q \neq p} \eta_q (\tilde{N}_q / \tilde{N}_p) \bar{N}_e K(q,p) + \sum_{q>p} \eta_q (\tilde{N}_q / \tilde{N}_p) A(q,p)$$
$$+ \eta_e \left\{ \sum_{q \neq p} [(\bar{N}_q / \tilde{N}_q) - (\bar{N}_p / \tilde{N}_p)] \tilde{N}_e K(p,q) \right.$$
$$+ [3(\bar{N}_e / \tilde{N}_e)^2 - (\bar{N}_p / \tilde{N}_p)] \tilde{N}_e K(p,c)$$
$$\left. + 2 (\bar{N}_e / \tilde{N}_e)(\tilde{N}_e^2 / \tilde{N}_p) \beta(p) \right\} \qquad (5)$$

$$\frac{d\eta_e}{dt} = \sum_p \eta_p (\tilde{N}_p / \tilde{N}_e) \bar{N}_e K(p,c)$$
$$+ \sum_p \eta_e [\bar{N}_p - 3 \bar{N}_e^2 (\tilde{N}_p / \tilde{N}_e^2)] K(p,c)$$
$$- 2 \sum_p \eta_e \bar{N}_e \beta(p) \qquad (6)$$

Quite often it is possible to simplify the set (5) and (6) further. Because the level spacing decreases as one goes higher in the level scheme, above a certain point the levels are in equilibrium with the free electrons [5]. Therefore, we focus our interest on a modeling of the lower levels. Here it is often possible to ignore the ionization and recombination terms compared to the collisional transition and radiative decay terms. That is, the last two terms of equation (5) may often be dropped facilitating an uncoupling of equations (5) and (6). The model may then be established by considering only

$$\frac{d\eta_p}{dt} = -\eta_p \left\{ \sum_{p \neq q} \bar{N}_e K(p,q) + \sum_{q<p} A(p,q) + \bar{N}_e K(p,c) \right\} + \sum_{q \neq p} \eta_q (\tilde{N}_q / \tilde{N}_p) \bar{N}_e K(q,p) + \sum_{q>p} \eta_q (\tilde{N}_q / \tilde{N}_p) A(q,p) \qquad (7)$$

$$= \sum_q B_{pq} \eta_q$$

into which $\bar{N}_e$ is introduced as a parameter.

The general solution of the set of equations (7) is

$$\eta_p = \sum_\ell C_\ell \exp(\lambda_\ell t)$$

in which the λ_ℓ are the eigenvalues of the coefficient matrix appearing in (7). The level p belongs to a set of levels L (= $\{p\}$) if the time response as determined by the λ_ℓ is strongly dependent on the set of coefficients B_{pq} where p and q are contained in L and only weakly dependent on other elements of $\underline{\underline{B}}$. It can be shown that this is the case provided

$$B_{pq}, B_{qp} >> B_{pm}, B_{qm}, B_{mp}, B_{mq}$$

for all levels p and q contained in L and m not contained

in L. That is to say, the model may be established by comparing coefficients in equation (7) directly and invoking the criteria (9). The proof of this straightforward, although cumbersome. One proceeds by studying the effect on the eigenvalues of a $n \times n$ matrix $\{B_{pq}\}$ of the addition of a set of elements $B_{pm}, B_{mp}, \ldots\ldots$ satisfying the conditions (9). If the effect is negligible, the contention is valid. This has been carried out for 3×3 and 4×4 matrixes. The general case could presumably be established by induction.

III. Group Equations and Coefficients

The model established in the preceding section will consist of a set of groups A, B, C, ..., N containing one or more levels each. The corresponding group densities are

$$N(L) = \sum_{p \in L} N_p$$

Upon introducing sums over the levels in the various groups, equations for these group densities follow immediately from equations (1)

$$\frac{dN(L)}{dt} = -\sum_{p\in L}\left\{N_p\left[\sum_{\substack{G=A\\G\neq L}}^{N}\sum_{q\in G} N_e K(p,q) + \sum_{G=A}^{L-1}\sum_{q\in G} A(p,q) + N_e K(p,c)\right]\right\}$$
$$+\sum_{p\in L}\left\{\sum_{\substack{G=A\\G\neq L}}^{N}\sum_{q\in G} N_q N_e K(q,p) + \sum_{G=L+1}^{N}\sum_{q\in G} N_q A(q,p)\right\}$$
$$+\sum_{p\in L}\left\{N_e^3 K(c,p) + N_e^2 \beta(p)\right\} \qquad (8)$$

Defining group coefficients

$$K(L,G) = \frac{\sum_{p\in L}\sum_{q\in G} g_p K(p,q)\exp(E_p/kT)}{\sum_{p\in L} g_p \exp(E_p/kT)} \qquad G\neq L \qquad (9)$$

$$A(L,G) = \frac{\sum_{p\in L}\sum_{q\in G} g_p A(p,q) \exp(E_p/kT)}{\sum_{p\in L} g_p \exp(E_p/kT)} \qquad G<L \qquad (10)$$

$$K(L,C) = \frac{\sum_{p\in L} g_p K(p,c) \exp(E_p/kT)}{\sum_{p\in L} g_p \exp(E_p/kT)} \qquad (11)$$

$$K(C,L) = \sum_{p\in L} K(c,p) \qquad (12)$$

$$\beta(L) = \sum_{p\in L} \beta(p) \ , \qquad (13)$$

equation (8) becomes

$$\frac{dN(L)}{dt} = -N(L)\left\{\sum_{G\neq L} Ne\, K(L,G) + \sum_{G<L} A(L,G) + Ne\, K(L,C)\right\}$$
$$+ \sum_{G\neq L} N(G)\, Ne\, K(G,L) + \sum_{G>L} N(G)\, A(G,L)$$
$$+ N_e^3\, K(C,L) + N_e^2\, \beta(L) \qquad (14)$$

Here g_p is the statistical weight and E_p is the ionization

potential of level p.

IV. Cesium as a Numerical Example

Interest in the thermionic converter has spawned considerable effort directed toward an understanding of cesium plasmas. Consequently, the necessary atomic data are known for cesium and occupation numbers have been calculated (considering 53 levels) for a range of conditions [5]. Cesium is thus an excellent candidate on which to test the results of sections II and III.

The cesium plasma we shall consider is one in which the heavy particles have a temperature of 1000 ^{o}K and a pressure of 1 Torr. Electron temperatures in the range of 2000 ^{o}K to 3000 ^{o}K and densities of 10^{13} and 10^{14} cm^{-3} were considered.

For these studies, Einstein spontaneous emission

coefficients were obtained from reference 5 and radiative recombination coefficients from reference 6 . The collisional transition and ionization coefficients were calculated using classical formulae derived by Gryzinski [7].

Following the procedure outlined in Section III, four models were derived which may be expected to describe the plasma in the ranges considered. These are summarized in the table. Calculations based on these models were compared with the results of Norcross and Stone (reference 5) obtained using 53 levels of which 27 were in equilibrium with the free electrons. Results of these calculations are presented graphically in Figures 1 and 2. Here we have plotted ocuupation number densities, normalized to the corresponding Saha-Boltzmann densities, for the levels 6S, 7S, 7P, 4F, 8P against the electron temperature for electron densities of 10^{13} and 10^{14} cm^{-3}. These levels were chosen because they are the lowest levels of the groups

of the most complete scheme, Scheme IV.

V. Discussion

We have presented a procedure by which the level scheme of the neutral component of a plasma may be converted into an effective level scheme consisting of groups of levels. In the event that the levels within these groups are in relative Saha-Boltzmann equilibrium, a considerable computational simplification is realized, since then only the group densities need be calculated.

A set of levels constitutes a group when the transition rates between levels within the set are much greater than those to levels outside the set. This will provide a time scale characteristic for the relaxation of levels within a group relative to one another which is much shorter than the time associated with the relaxation of the overall group densities relative to one another. That is, the

idea underlying this procedure is that underlying a multiple time scale formalism.

The levels within these groups will be in relative Saha-Boltzmann equilibrium when the transition rates between levels within the group are collision dominated and the low energy portion of the electron distribution function is Maxwellian. This condition may be realized for sufficiently high electron densities at any given temperature.

To test the validity of the ideas presented, we chose a cesium plasma under conditions of technological interest (heavy particle temperature of 1000 ^{o}K and pressure of 1 Torr, electron temperatures in the range 2000 ^{o}K to 3000 ^{o}K, and electron densities of 10^{13} and 10^{14} cm^{-3}). For this plasma we obtained the four effective level schemes presented in the table of the previous section. These were chosen to provide various approximations to the level scheme under the conditions considered. That is, the scheme IV with five effective levels may be expected to

provide a good approximation to much of the scheme over a wide range, whereas scheme I with only two effective levels may be expected to furnish good results only for higher electron densities.

In Figures 1 and 2, where the results of calculations based on the effective level schemes are compared with those of Norcross and Stone who used 53 levels, this is indeed seen to be the case. Scheme IV provides a fairly accurate picture of the actual occupation number densities for all conditions considered. In contrast, Scheme I, in which all levels above 6P are assumed to be in Saha-Boltzmann equilibrium with the free electrons, provides a rather poor estimate (36% error at 3000 ^{o}K) of the density of level 6S at an electron density of 10^{13} cm^{-3}, while at 10^{14} cm^{-3}, the estimate is tolerable (8% error at 3000 ^{o}K).

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Table

Effective Level Schemes for Cesium (2000 - 3000°K)

Scheme	Group Number	Levels
I	1	6S, 6P, 5D
	2	7S, 7P, 6D, ...
II	1	6S, 6P, 5D
	2	7S
	3	7P, 6D, 8S, ...
III	1	6S, 6P, 5D
	2	7S
	3	7P, 6D, 8S
	4	4F, 8P, 7D, ...
IV	1	6S, 6P, 5D
	2	7S
	3	7P, 6D, 8S
	4	4F
	5	8P, 7D, 9S, ...

Figure Captions

Figure 1. Occupation number densities normalized to corresponding Saha-Boltzmann densities as functions of the electron temperature for the levels 1 (6S), 4 (7S), 5 (7P), 8 (4F). Electron density = 10^{13} cm^{-3}.

Legend: Calculation based on

Scheme I ×

Scheme II △

Scheme III □

Scheme IV ○

Norcross and Stone's results ———

Figure 2. Occupation number densities normalized to corresponding Saha-Boltzmann densities as functions of the electron temperature for the levels 1 (6S), 4 (7S), 5 (7P), 8 (4F). Electron density = 10^{14} cm^{-3}.

Legend: Calculation based on

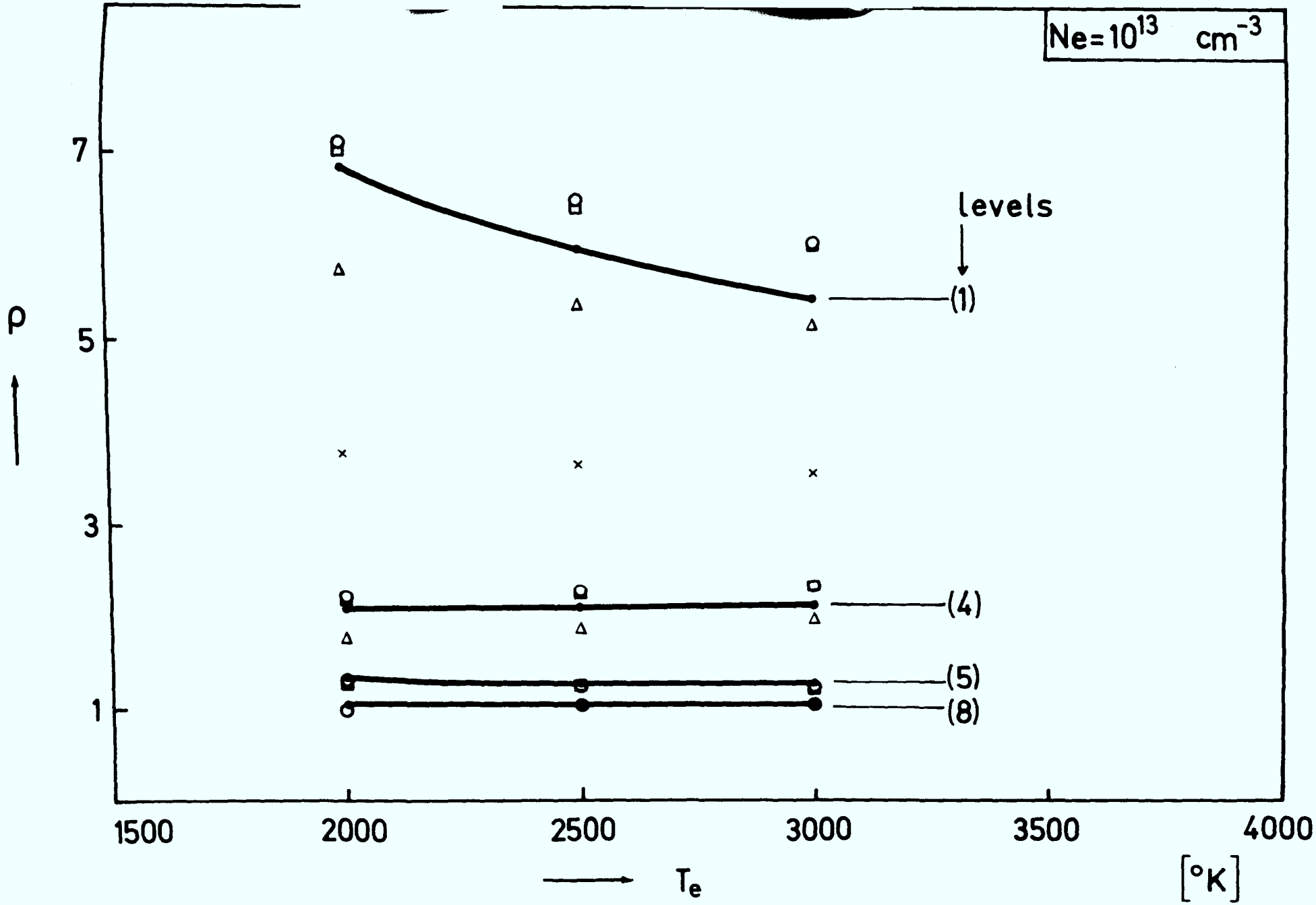
Scheme I ×

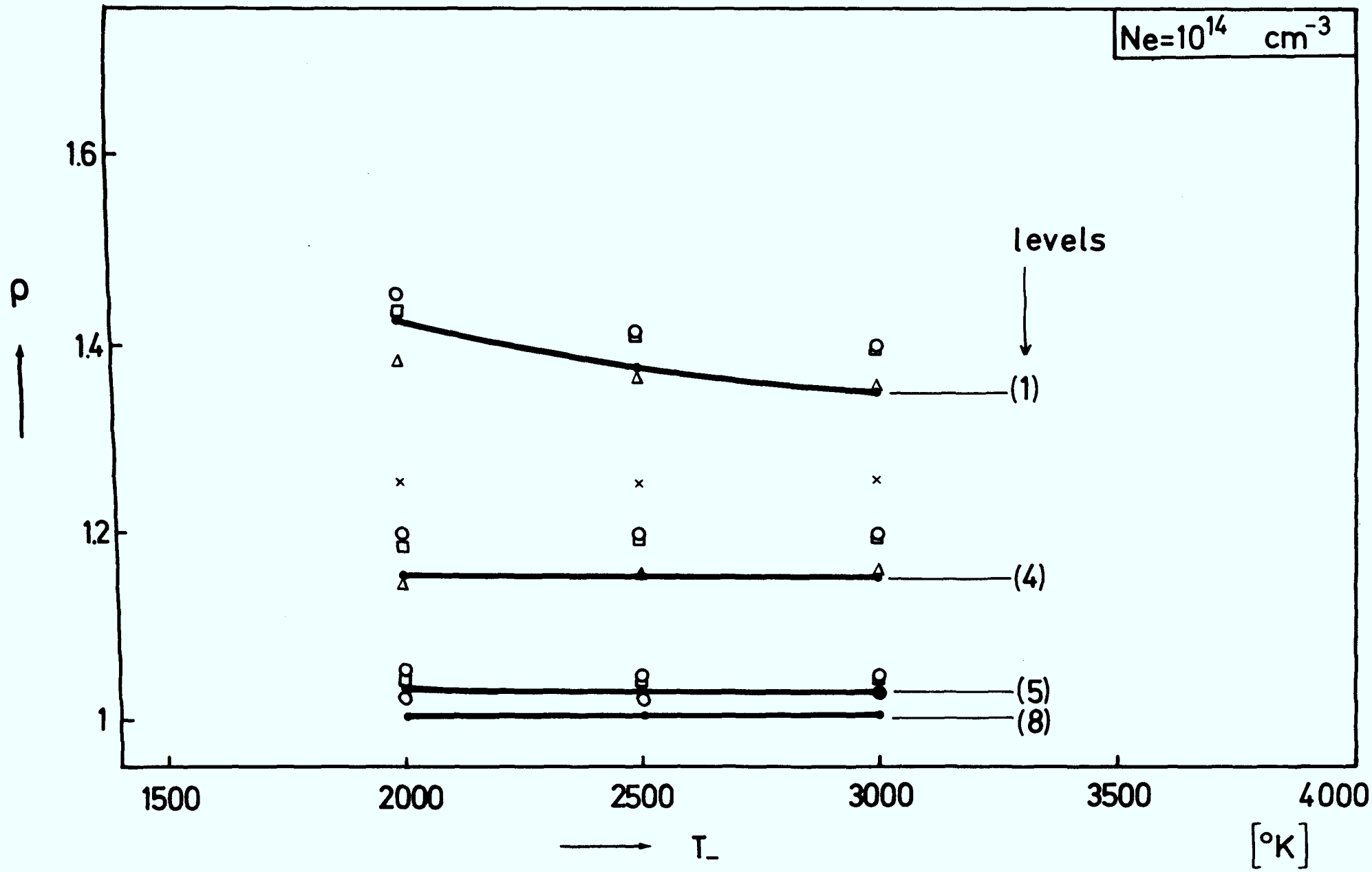
Scheme II △

Scheme III □

Scheme IV ○

Norcross and Stone's results ———


Ne=10^13 cm^-3
levels
(1)
(4)
(5)
(8)
ρ
7
5
3
1
1500
2000
2500
3000
3500
4000
T_e
[°K]


Ne=10^14 cm^-3
levels
ρ
1.6
1.4
1.2
1
(1)
(4)
(5)
(8)
1500
2000
2500
3000
3500
4000
T_
[°K]