

with  $k_i$  and  $k_f$  the initial and final wave numbers in the excitation process.

In a calculation which will be reported later the present calculation will be extended to higher excited states and to higher energy ranges, and exchange of the electrons will be included.

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## Radiative Cascade Theory

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A steady-state cascade theory has been set up for radiative electron transitions. These are assumed to occur between a continuum and various excited states, as well as between any two excited states, of hydrogen-like atoms. The work contains two features which have not previously been fully taken into account: (1) Both spontaneous and induced transition probabilities have been included exactly. (2) In addition to the radiative transitions, the reverse transitions due to absorption of background radiation have also been included. The following graphical results are given: (a) The steady-state occupation probabilities of the excited states as a function of excess electron density. (b) A "sticking probability"  $P_n$  (for an electron from a level  $n$  to reach the ground state without leaving the atom) as a function of the principal quantum number  $n$ . (c) The effect of the cascade on the transition rate into the ground state. The calculation is valid for semiconductors and for the analogous astrophysical problem. Temperature dependences have also been studied. The graphs shown bear out quantitatively the expectation that  $P_n$  decreases as either the temperature or the principal quantum number increases.

### 1. INTRODUCTION

RECOMBINATION-generation processes involving a series of levels (e.g., excited atomic states) lead automatically to cascade problems. In these, electrons can move up and down the energy scale and the transition probabilities between any two levels, together with the assumption of a steady state, leads to a steady non-equilibrium probability distribution for the occupation of the quantum states involved. This will in general differ from the cruder "quasi-Fermi" distribution often hypothesized in solid-state work.

The simplest cascades are those involving a conduction band (a continuum in astrophysics) and the states, labeled by the principal quantum number  $n$ , of hydrogen-like ions. In such cases the results of the calculation may be given in terms of the probabilities  $\Pi_n$  that an electron will reach the ground state from level  $n$  without leaving the atom. This has been called the "sticking probability" in solid-state work, and has proved difficult to calculate. If states lying above  $n=N$  are neglected an approximate probability  $\Pi_{n,N}$  is obtained. Many results of this paper are presented in terms of "reduced" sticking probabilities  $P_{n,N}$ . As far as we

are aware, this is the first time this probability has been investigated systematically for a solid-state problem by a quantum-mechanical method.

The assumptions made in this paper are: the electrons in the band having a Maxwell distribution in the steady state; hydrogen-like wave functions for the discrete and continuum states, modified by an effective mass and a dielectric constant; black-body radiation in the solid; Saha dissociation formula for equilibrium even for the large principal quantum numbers  $n$ ; neglect of term structure for given  $n$ . If the steady state is maintained by pumping electrons back into the continuum a general theory is readily set up [Eq. 4.2(a)]. If it is also assumed that all transitions are radiative, the matrix elements which occur are standard. For the purposes of numerical calculations the problem can be further simplified by supposing that because the lowest level  $n=1$  is the most highly populated of the discrete levels, the pumping action may be neglected for the levels  $n \geq 2$ . This leads to the final set of Eqs. (5.17) whose solutions are readily computed.

The cascade model set up in this way is informative in spite of the limitations implied by the above assumptions. It provides guiding lines for a more complete cascade theory which incorporates also the effect of phonons and of electron collisions, but such a theory is not attempted here.

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The first question is whether the distribution obtained has the correct properties in the limit  $N \rightarrow \infty$  (Sec. 6). The calculations could also apply to steady-state gaseous nebulae and stellar atmospheres. Something equivalent to a pumping rate occurs also in these cases, and in the *numerical* part of earlier work its effect on levels  $n \geq 2$  has been neglected (see Sec. 4). In such cases the cutoff level  $n=N$  can be much higher than in a realistic solid-state problem ( $N \sim 7$ ). One, therefore, wants to know up to what level  $n$  the distribution obtained is reliable for various values of  $N$ . We find that with  $N=55$ , the results are reliable up to  $n \sim 30$ . We, therefore, do not extrapolate to  $N = \infty$  in presenting our later results (Figs. 5 to 10).

Apart from the cutoff value  $N$ , the same figures serve to give results for the solid-state and the astrophysical situation [see Eqs. (5.14) and (5.16)], and the reduced sticking probability is given as a function of  $n$ ,  $N$ , and of temperature in Figs. 5 to 8.

One also wants to know the extent to which the existence of cascade paths enhances the transition rate into level  $n=1$  for a given steady-state electron concentration in the band. This is measured by a cascade ratio  $C$  (Figs. 9 and 10).

The connection with previous work is as follows:

#### (i) Solid-State Work

Phonon cascades in the steady state were considered by Lax<sup>1</sup> and by Ascarelli and Rodriguez<sup>2a,b</sup>. For a systematic account of the radiative transition probabilities for solids, see Lasher and Stern<sup>3</sup> and references given there. None of these authors considered the radiative cascade, though the formal considerations of Nagae<sup>4</sup> should be mentioned.

#### (ii) Astrophysics and Plasmas

Upward electron transitions (absorption) have normally been neglected, and induced emission due to radiation at the electron temperature has been taken into account approximately as negative absorption.<sup>5,6</sup> Both effects have been included exactly here. For a review of earlier work, see Ref. 7. For the case where there is no cascade, adequate discussions of spontaneous emission are available (e.g., Milne,<sup>8</sup> Biberman *et al.*,<sup>9</sup> etc.), but the present paper goes further in the case

<sup>1</sup> M. Lax, Phys. Rev. **119**, 1502 (1960).

<sup>2</sup> G. Ascarelli and S. Rodriguez, (a) Phys. Rev. **124**, 1321 (1961); (b) **127**, 167 (1962).

<sup>3</sup> G. Lasher and F. Stern, Phys. Rev. **133**, A553 (1964).

<sup>4</sup> M. Nagae, J. Phys. Soc. Japan **18**, 207 (1963).

<sup>5</sup> M. J. Seaton, Monthly Notices Roy. Astron. Soc. **119**, 90 (1959).

<sup>6</sup> D. H. Menzel and J. G. Baker, Astrophys. J. **86**, 70 (1937).

<sup>7</sup> R. N. Thomas, in *Physics of the Solar Chromosphere*, edited by R. N. Thomas and R. G. Athay (Interscience Publishers, Inc., New York, 1961), p. 83.

<sup>8</sup> E. A. Milne, Phil. Mag. **47**, 209 (1924).

<sup>9</sup> L. M. Biberman, Y. N. Toropkin, and K. N. Ul'yanov, Zh. Tekhn. Fiz. **32**, 827 (1962) [English transl.: Soviet Phys.—Tech. Phys. **7**, 605 (1963)].

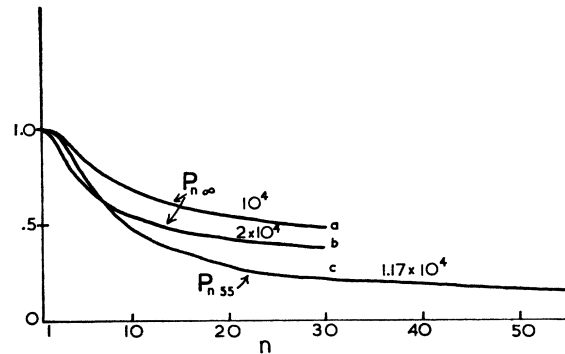


FIG. 1. The effect of induced emission and absorption on the reduced sticking probability  $P_{nN}$ . The effects are neglected in curves a and b (taken from Seaton, Ref. 5). Curves c are based on the present work.  $N$  is the value of the principal quantum number beyond which the excited states are neglected.  $P_{nN}$  is defined in Eq. (5.19). Temperatures are given on the curves.

of the induced and total emission. Thus the usual expression for the negative absorption rate is shown in Sec. 3 to be valid only in equilibrium, and it has been replaced by a more accurate expression in the present work. On the other hand, collisions between electrons have been introduced in astrophysical work (Bates *et al.*<sup>10</sup>) in addition to the radiative effects. In the present paper collisional contributions to the cascade are neglected. That the two physical effects incorporated here can be of importance is illustrated in Figs. 1 and 2. The fact that curve  $c$  lies below the other curves shows that on balance these two effects make ionizing transitions out of the discrete levels more probable. Thus the effect of absorption on the occupation probabilities is more important than the effect of induced emissions. A simple demonstration that both effects can become important, and that absorption tends to be more important, where higher excited states are involved is given at the end of Sec. 5.

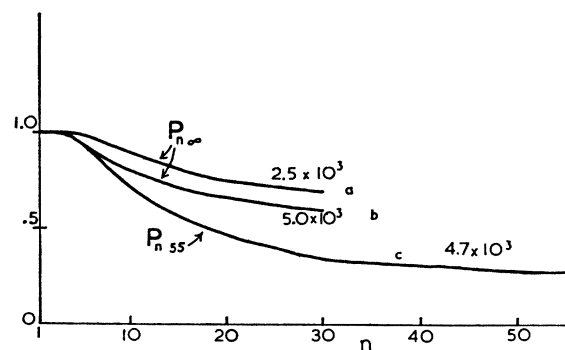


FIG. 2. The effect of induced emission and absorption on the reduced sticking probability  $P_{nN}$ . The effects are neglected in curves a and b (taken from Seaton, Ref. 5). Curves c are based on the present work.  $N$  is the value of the principal quantum number beyond which the excited states are neglected.  $P_{nN}$  is defined in Eq. (5.19). Temperatures are given on the curves.

<sup>10</sup> D. R. Bates, A. E. Kingston, and R. W. P. McWhirter, Proc. Roy. Soc. (London) **A267**, 297 (1962).

## 2. BOUND-BOUND TRANSITIONS

Let  $N_n$  be the concentration of electrons in the atomic levels having principal quantum number  $n$ . Then the radiative transition rate per unit volume out of levels  $n'$  is

$$R_{n'n} = N_{n'} [A_{n'n}^E + B_{n'n}^E I_\nu] - N_n B_{nn'}^E I_\nu \quad (n' > n). \quad (2.1)$$

Here  $A^E$  and  $B^E$  are the Einstein coefficients, and the terms on the right represent in turn: spontaneous emission, induced emission and absorption.  $I_\nu$  is the energy emitted normally by a black body per unit time, per unit frequency range, per unit area, per unit solid angle:

$$I_\nu = (2h\nu^3\mu^2/c^2) [\exp h\nu/kT - 1]^{-1} \quad (2.2)$$

and  $\nu \equiv \nu_{n'n}$  is the frequency corresponding to a transition between levels  $n'$  and  $n$ . Here  $\mu$  is the refractive index of the solid, and may be replaced by unity in some astrophysical applications. If  $g_n$  be the number of atomic states with quantum number  $n$  one has in thermodynamic equilibrium at temperature  $T$ , denoted by an additional suffix 0,

$$N_{n'0}/N_{n0} = (g_{n'}/g_n) e^{-h\nu_{n'n}/kT}, \quad (2.3)$$

Einstein's argument applied to these equations enables one to infer

$$g_{n'} A_{n'n}^E / g_n B_{nn'}^E = 2h\nu^3\mu^2/c^2, \quad (2.4)$$

$$g_{n'} B_{n'n}^E = g_n B_{nn'}^E. \quad (2.5)$$

Substituting (2.2), (2.4), (2.5) into (2.1), one finds

$$R_{n'n} = N_{n'} A_{n'n}^E (1 - N_n N_{n'0} / N_{n0} N_{n'}) \quad (n' > n), \quad (2.6)$$

where

$$A_{n'n} = [1 - e^{-h\nu/kT}]^{-1} A_{n'n}^E. \quad (2.7)$$

It appears that in astrophysical work (Seaton,<sup>5</sup> Menzel and Pekeris<sup>11</sup>), induced emission can normally be neglected. This enabled one to use the Einstein  $A^E$  coefficient in (2.6) instead of the coefficient (2.7).

## 3. BOUND-FREE TRANSITIONS

The radiative transition rate per unit volume from the continuum to states with principal quantum number  $n$  is

$$d(R_{cn}) = N_i N_e f(v) dv [\sigma_{cn} v + (4\pi/h\nu) \alpha_{cn} I_\nu] - (4\pi/h\nu) \alpha_{nc} N_n I_\nu dv \quad (3.1)$$

for electrons with velocities in the range  $(v, v+dv)$ .  $N_i$  and  $N_e$  are the concentrations of ions and of conduction electrons, respectively.  $f(v)dv$  is the probability of finding a conduction electron in the velocity range  $(v, v+dv)$ .  $\sigma_{cn}$  is the cross section for spontaneous emission, and  $\alpha_{nc}$  is the cross section per atom for radiative absorption.  $\alpha_{cn}$  has dimensions  $[L^5 T^{-1}]$ , and since it is a coefficient describing induced emission, this term is proportional to  $N_i$  and  $N_e$ . The relation between  $v$  and  $\nu$  is given by energy conservation

$$\frac{1}{2} m^* v^2 + I_n = h\nu, \quad dv/dv = m^* v/h, \quad (3.2)$$

where  $I_n$  is the ionization energy for the levels  $n$ . The effective mass  $m^*$  may be replaced by the electron mass in astrophysical applications.

As in the Einstein argument quoted in Sec. 2, one may first consider thermodynamic equilibrium. Then (3.1, 3.2) yield

$$I_\nu = \frac{v h \nu}{4\pi [m^* v / f(v) h]} \frac{\sigma_{cn} / \alpha_{cn}}{(N_{n0} / N_{i0} N_{e0}) (\alpha_{nc} / \alpha_{cn}) - 1}. \quad (3.3)$$

For black-body radiation (2.2) one now finds

$$\sigma_{cn} / \alpha_{cn} = 8\pi\nu^2\mu^2 / v c^2, \quad (3.4)$$

$$\frac{N_{n0}}{N_{i0} N_{e0}} = \frac{f(v) h \alpha_{cn}}{m^* v \alpha_{nc}} e^{h\nu/kT} \quad (n = 1, 2, \dots). \quad (3.5)$$

Introduce next the mass-action constant for the reaction ion + electron = neutral atom, which is given by the Saha dissociation formula

$$\frac{N_{n0}}{N_{i0} N_{e0}} = \frac{g_n}{g_i g_e} \frac{h^3}{(2\pi m^* kT)^{3/2}} e^{I_n/kT} \quad (n = 1, 2, \dots), \quad (3.6)$$

where  $g_i$  is the degeneracy factor for the state of the ion, and  $g_e = 2$ . For equilibrium the Maxwell distribution

$$f(v) = 4\pi (m^*/2\pi kT)^{3/2} v^2 e^{-m^* v^2/2kT} \quad (3.7)$$

may be used. Putting (3.6), (3.7) into (3.5), one finds, in analogy with (2.5)

$$g_n \alpha_{nc} = g_c \alpha_{cn}, \quad g_c \equiv 4\pi m^* v h^{-2} g_i g_e. \quad (3.8)$$

The analog of (2.4) is obtained from (3.4) and (3.8), and is

$$\frac{\sigma_{cn}}{\alpha_{nc}} = \frac{g_n}{g_i g_e} \frac{2\nu^2 h^2 \mu^2}{m^* v^2 c^2}. \quad (3.9)$$

This relation is due to Milne,<sup>3</sup> and the above equations

<sup>11</sup> D. H. Menzel and C. L. Pekeris, Monthly Notices Roy. Astron. Soc. **96**, 77 (1935).

are well known in astrophysics (Aller,<sup>12</sup>), except for (3.1), (3.8) which may be new.

One can now substitute (3.2) to (3.9) into (3.1) in order to obtain expressions for the nonequilibrium steady state. All rates will be expressed in terms of  $\alpha_{nc}$ . Hence,

$$N_i N_e \frac{g_n}{g_i g_e} \frac{2\mu^2}{c^2} \left(\frac{2}{\pi}\right)^{1/2} (m^* k T)^{-3/2} \times (h\nu)^2 \alpha_{nc} e^{(I_n - h\nu)/kT} d(h\nu), \quad (3.10)$$

$$N_i N_e \frac{g_n}{g_i g_e} \frac{2\mu^2}{c^2} \left(\frac{2}{\pi}\right)^{1/2} (m^* k T)^{-3/2} \times \frac{(h\nu)^2 \alpha_{nc}}{e^{h\nu/kT} - 1} e^{(I_n - h\nu)/kT} d(h\nu), \quad (3.11)$$

$$\frac{8\pi\nu^2 \mu^2}{hc^2} \frac{\alpha_{nc} N_n}{e^{h\nu/kT} - 1} d(h\nu) = \frac{N_n N_{i0} N_{e0}}{N_{n0}} \frac{g_n}{g_i g_e} \times \frac{2\mu^2}{c^2} \left(\frac{2}{\pi}\right)^{1/2} (m^* k T)^{-3/2} \frac{(h\nu)^2 \alpha_{nc}}{e^{h\nu/kT} - 1} e^{I_n/kT} d(h\nu), \quad (3.12)$$

are, respectively, spontaneous emission, induced emission and absorption rates per unit volume, due to electrons in the velocity range  $(v, v+dv)$ . (3.6) has been used in (3.12). Combining these rates, (3.1) becomes

$$d(R_{cn}) = N_i N_e \frac{g_n}{g_i g_e} \frac{2\mu^2}{c^2} \left(\frac{2}{\pi}\right)^{1/2} (m^* k T)^{-3/2} \times \frac{(h\nu)^2 \alpha_{nc}}{e^{h\nu/kT} - 1} e^{I_n/kT} (1 - b_n) d(h\nu), \quad (3.13)$$

$$b_n = \frac{N_n/N_{n0}}{(N_i/N_{i0})(N_e/N_{e0})}. \quad (3.14)$$

The factor  $1 - b_n$  measures the extent by which the steady state departs from the equilibrium state. (3.13) implies the assumption that the Maxwell distribution and the black-body radiation formula hold also in the

steady state. The integrated form of (3.13) is

$$R_{cn} = N_i N_e B_{cn} (1 - b_n) \quad (n = 1, 2, \dots) \quad (3.15)$$

$$B_{cn} \equiv \frac{g_n}{g_i g_e} \frac{2}{c^2} \left(\frac{2}{\pi}\right)^{1/2} (m^* k T)^{-3/2} \times e^{I_n/kT} \int_{I_n}^{\infty} \frac{\mu^2 (h\nu)^2 \alpha_{nc}}{e^{h\nu/kT} - 1} d(h\nu). \quad (3.16)$$

In astrophysical problems  $N_i$  is usually the concentration of ionized hydrogen atoms. In semiconductors  $N_i$  may be interpreted from

$$N_i = N_A + N_e, \quad (3.17)$$

where  $N_A$  is the concentration of acceptors.

In astrophysical work, the induced emissions, represented by the second term in (3.1), have been taken into account as negative absorptions (Aller<sup>12</sup>). To explain this idea, consider the last two terms in (3.1) as negative and positive absorptions, respectively. The absorption rate per unit volume becomes then

$$\frac{4\pi}{h\nu} \left[ 1 - \frac{N_i N_e}{N_n} \frac{\alpha_{cn}}{\alpha_{nc}} \frac{dv}{d\nu} \right] \alpha_{nc} N_n I_\nu d\nu. \quad (3.18)$$

By (3.2) and (3.8) this becomes in the case of thermodynamic equilibrium

$$(4\pi/h\nu)(1 - e^{-h\nu/kT}) \alpha_{nc} N_n I_\nu d\nu. \quad (3.19)$$

The negative term in (3.19) is due to induced emissions and gives the volume rate of negative absorption. (3.19) has been used extensively also away from equilibrium. The above argument shows that this is an approximation, and the present theory, which is based on (3.1) is more accurate.

#### 4. THE STEADY-STATE CONDITION

Suppose that  $G_n$  is the transition rate per unit volume out of the levels  $n$  due to some external pumping action into the conduction band. Then the condition for a steady population of levels  $n$  is by (2.6) and (3.15)

$$G_n = N_i N_e B_{cn} (1 - b_n) + \sum_{n' > n} N_{n'} A_{n'n} (1 - N_n N_{n'0} / N_{n'} N_{n0}) - \sum_{n''=1}^{n-1} N_{n''} A_{nn''} (1 - N_{n''} N_{n0} / N_n N_{n''0}) \quad (n = 1, 2, \dots). \quad (4.1)$$

It will eventually be supposed that the external pumping acts predominantly on electrons in levels  $n=1$ , i.e.,  $G_n = G_1 \delta_{n1}$ . This is in agreement with the usual approximations in astrophysics (Seaton<sup>5</sup>, Baker and Menzel<sup>6</sup>). The condition for a steady population in the conduction band is then

$$G_1 = N_i N_e \sum_{n=1}^{\infty} B_{cn} (1 - N_n N_{e0} V_{i0} / N_e N_{n0} V_i). \quad (4.2)$$

<sup>12</sup> L. H. Aller, *Astrophysics* (Ronald Press Company, New York, 1953), p. 148.

This is not an independent condition, since it may be obtained by summing (4.1) over all  $n$ . As a result the steady-state occupation number must be specified for one set of levels  $n$ , since one is otherwise one equation short. It will be convenient to take  $b_1$  as given, and determine the other  $b$ 's in terms of it. For the formal part of the theory, all  $G$ 's will be kept, as this does not cause any difficulties.

Using (3.6), (4.1) becomes with  $x_n \equiv I_n/kT$ ,

$$\frac{G_n}{N_i N_e} = B_{cn}(1-b_n) + \frac{h^3}{g_i g_e} (2\pi m^* kT)^{-3/2} \left\{ \sum_{n' > n} (b_{n'} - b_n) g_{n'} A_{n'n} e^{x_{n'}} - \sum_{n''=1}^{n-1} (b_n - b_{n''}) g_n A_{nn''} e^{x_n} \right\} \quad (n=2, 3, \dots). \quad (4.2a)$$

In virtue of (3.2) and (3.16) this may be written

$$\frac{g_i g_e}{h^3} (2\pi m^* kT)^{3/2} G_n - z_n = \sum_{n'=1}^{\infty} D_{nn'} b_{n'} \quad (n=2, 3, \dots), \quad (4.3)$$

where

$$z_n \equiv \frac{8\pi I_n^3 g_n}{c^2 h^3} e^{x_n} \int_0^{\infty} \frac{(1+u)^2 \alpha_{nc} \mu^2 du}{e^{x_n(1+u)} - 1} \quad (4.4)$$

and

$$\begin{aligned} D_{nn'} &= g_{n'} A_{n'n} e^{x_{n'}} \quad (n < n') \\ &= -z_n - \sum_{n' > n} g_{n'} A_{n'n} e^{x_{n'}} - g_n e^{x_n} \sum_{n''=1}^{n-1} A_{nn''} \quad (n = n') \\ &= g_n A_{nn'} e^{x_n} \quad (n > n'). \end{aligned} \quad (4.5)$$

(4.3) are the cascade equations.

By treating the term  $n''=1$  in (4.2a) separately, one can obtain this equation in the form

$$\frac{G_n}{N_i N_e (1-b_1)} + \frac{h^3 g_n A_{n1} e^{x_n}}{g_i g_e (2\pi m^* kT)^{3/2}} = f \left[ \frac{1-b_2}{1-b_1}, \frac{1-b_3}{1-b_1}, \dots \right], \quad (n=2, 3, \dots),$$

where  $f$  denotes an appropriate function. This shows that in the present case when  $G_n=0$  for  $n=2, 3, \dots$ , values of  $b_n$  need be obtained for only one value of  $b_1$ . The values of the  $b_n$  ( $b_n'$  say) can be deduced from them for other values of  $b_1$  ( $b_1'$  say) by the relation

$$P_n \equiv \frac{1-b_n}{1-b_1} = \frac{1-b_n'}{1-b_1'}. \quad (4.6)$$

$P_n$  is a reduced sticking probability (Sec. 7). Hence it was thought useful to show the sticking probability rather than  $b_n$  in most figures given in this paper.

Seaton's results, given in Figs. 1 and 2, and originally calculated for  $b_1=0$ , can also be adapted so as to be applicable to general  $b_1$ .

## 5. DERIVATION OF FINAL FORM OF CASCADE EQUATION

The  $A$ 's and the absorption cross sections can be related to the oscillator strengths<sup>13</sup>  $f_{n'n}$

$$A_{n'n} = \frac{g_n}{g_{n'}} \frac{8\pi^2 e^2 \mu^2}{m^* c^3} \nu_{n'n}^2 f_{n'n} [1 - e^{-h\nu/kT}]^{-1}, \quad (n' > n) \quad (5.1)$$

$$\alpha_{nc} = \frac{\pi e^2 \kappa^3}{mc 2R} f_{nc}. \quad (5.2)$$

<sup>13</sup> See Ref. 12, pp. 131, 146.

Here  $R$  is the modified Rydberg constant

$$R = (2\pi^2 m e^4 / h^2) (m^* / m \epsilon^2) Z^2, \quad (5.3)$$

where  $\epsilon$  is the static dielectric constant of the material and may be replaced by unity in some astrophysical applications.  $Ze$  is the nuclear charge of the hydrogen-like atoms.  $\kappa$  is introduced in order to enable one to put the energy in the conduction band in a form analogous to that appropriate to discrete levels in a hydrogen-like atom:

$$I_n = R/n^2, \quad \frac{1}{2} m v^2 \equiv R/\kappa^2. \quad (5.4, 5.5)$$

Provided (5.4) is not used as an identification of  $I_n$  in (4.4), the results (4.3), (5.1), and (5.2) are general in the sense that the wave functions for the various electron states  $n$  enter only into the oscillator strengths, and have not yet been specified.

Using now Coulomb functions for the continuum and for the discrete states, one finds with  $g_n = 2n^2$  (Menzel and Pekeris<sup>11</sup>)

$$f_{n'n} = \frac{2^5}{3\sqrt{3}\pi n^5 n'^3} \left( \frac{1}{n^2} - \frac{1}{n'^2} \right)^{-3} g_{\text{I}}, \quad (5.6)$$

$$f_{nc} = \frac{2^5}{3\sqrt{3}\pi n^5 \kappa^3} \left( \frac{1}{n^2} + \frac{1}{\kappa^2} \right)^{-3} g_{\text{II}}. \quad (5.7)$$

Here  $g_I$  and  $g_{II}$  are Gaunt factors and are of order unity. They are complicated expressions, and will therefore be replaced by unity in subsequent numerical work.

The above results enable one to give simple expressions for the quantity  $z$  of (4.4) and for the modified  $A$  coefficients of (2.7)

$$z_n = \frac{\beta}{n^3} e^{-x_n} \int_0^\infty \frac{g_I du}{[e^{x_n(1+u)} - 1][1+u]}, \quad (5.8)$$

$$A_{n'n} = \frac{\beta g_I}{nn'^3(n'^2 - n^2)}, \quad (5.9)$$

where

$$\beta \equiv (2^{10}\pi^5/3\sqrt{3})(e^{10}m^*\mu^2Z^4/\epsilon^4c^3h^6). \quad (5.10)$$

Although normally  $g_i = 1$  and  $g_e = 2$ , one may put

$$N_e \equiv g_i g_e (2\pi m^* kT)^{3/2} / h^3 \quad (5.11)$$

and note that the quantity  $B_{cn}$  occurring in (3.15) satisfies

$$B_{cn} = z_n / N_e. \quad (5.12)$$

To write the set of Eqs. (4.3) for the  $b_n$  in final form, note that one of the equations must be omitted, since it is not independent, as already observed with (4.2). Since  $G_n = G_I \delta_{n1}$  by hypothesis, it is convenient to omit the equation for  $n=1$ . All remaining terms in the set (4.3) are proportional to  $\beta$  in virtue of (5.8), (5.9), and this quantity cancels out of (4.3).

In order to solve the equations (4.3) the excited energy levels must be cut off at some value  $n=N$ . This leaves  $N-1$  independent equations, and implies neglect of the discrete energy levels for which  $E_n > E_N$ . We shall, therefore, write  $b_{nN}$  instead of  $b_n$ . The only parameters left in (4.3) are then  $b_{1N}$ ,  $x_n$ , and  $N$ . These determine the cascade completely. The refractive index  $\mu$  cancels out.

By (5.3), (5.4),

$$x_n \equiv I_n / kT = R / n^2 kT. \quad (5.13)$$

The cascade problem will be considered for the case of germanium

$$\begin{aligned} Z &= 1, \quad m^* = 0.22m, \quad \epsilon = 16, \\ T &= 4^\circ\text{K (semiconductors)} \end{aligned} \quad (5.14)$$

so that

$$x_n = 33.944 / n^2. \quad (5.15)$$

Our calculations remain valid, however, for any set of values (5.14) which lead to (5.15). The same numerical values for  $x_n$  arise in the astrophysical problem specified by

$$\begin{aligned} Z &= 1, \quad m^* = m, \quad \epsilon = 1, \\ T &= 4650^\circ\text{K (astrophysics)}. \end{aligned} \quad (5.16)$$

This is in the range of interest in astrophysics.

The equations to be solved are now given by (4.3) with  $z_n$  and  $A_{n'n}$  given by (5.8), (5.9)

$$\begin{aligned} 0 &= \frac{1}{2n^3} \int_0^\infty \frac{e^{x_n}}{e^{x_n(1+u)} - 1} \frac{du}{1+u} + b_{1N} \frac{e^{x_n}}{n(n^2 - 1)} \\ &+ \sum_{n''=2}^{n-1} \frac{e^{x_{n''}}}{e^{x_{n''}n} - 1} \frac{b_{n''N}}{nn''(n^2 - n''^2)} + \sum_{n'=n+1}^N \frac{e^{x_n}}{e^{x_{nn'}} - 1} \frac{b_{n'N}}{nn'(n'^2 - n^2)} - b_{nN} \left\{ \frac{1}{2n^3} \int_0^\infty \frac{e^{x_n}}{e^{x_n(1+u)} - 1} \frac{du}{1+u} \right. \\ &\left. + \sum_{n''=1}^{n-1} \frac{e^{x_{n''}}}{e^{x_{n''}n} - 1} \frac{1}{nn''(n^2 - n''^2)} + \sum_{n'=n+1}^N \frac{e^{x_n}}{e^{x_{nn'}} - 1} \frac{1}{nn'(n'^2 - n^2)} \right\}, \quad (n=2, 3, \dots, N) \end{aligned} \quad (5.17)$$

where

$$x_{nn'} = \frac{R}{kT} \left( \frac{1}{n^2} - \frac{1}{n'^2} \right) \quad (n' > n). \quad (5.18)$$

Here  $b_{1N}$  must be assigned a numerical value appropriate to the steady state under consideration. (5.17) may then be used to obtain the other  $b_{nN}$ 's. This was done on a digital computer for values up to  $N=55$ .

If now a different value of  $b_{1N}$  ( $b_{1N}'$ , say) is chosen, the resulting new values,  $b_{nN}'$  say, of  $b_{nN}$  need not be worked out again, since the argument leading to (4.6) is valid even if the levels considered are cut off at  $n=N$

$$P_{nN} \equiv \frac{1 - b_{nN}}{1 - b_{1N}} = \frac{1 - b_{nN}'}{1 - b_{1N}'}, \quad b_{nN} \equiv \left\{ \frac{N_n / N_{n0}}{(N_i / N_{i0})(N_e / N_{e0})} \right\}_{\text{for cutoff at } n=N}. \quad (5.19)$$

A simple estimate of the effects of stimulated emission and of absorption can be obtained as follows. Let

$$s_{n'n} \text{ (or } a_{nn'}) \equiv \frac{\text{Rate of stimulated emission } n' \rightarrow n \text{ (or of absorption } n \rightarrow n')}{\text{Rate of spontaneous emission } n' - n}. \quad (5.20)$$

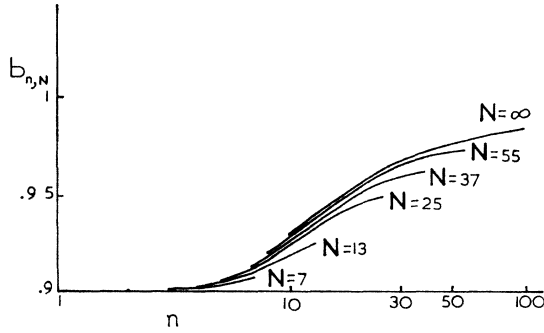


FIG. 3. The steady-state concentration, as measured by  $b_{nN}$  [see Eq. (5.19)], obtained by solving the cascade equations (5.17) with  $x_n$  given by (5.15).

The definition can be made to include transitions which involve the continuum, if the latter is identified by  $n = \infty$ . For bound-bound transitions the two ratios (5.20) can be obtained from (2.1), (2.2), (2.4), (2.5). For bound free transitions, they are obtainable from (3.10), (3.11), (3.12). The four results can be summarized thus ( $b_\infty \equiv 1$ )

$$s_{n'n} = [e^{x_{nn'}} - 1]^{-1}, \quad \frac{b_{n'}}{b_n} a_{nn'} = e^{x_{nn'}} s_{n'n}. \quad (5.21), (5.22)$$

Adopting the numerical value (5.15), i.e.,

$$\frac{R}{kT} = \frac{2\pi^2 m e^4 m^* Z^2}{h^2 k T m e^2} = 33.944,$$

one finds the results given in Table I.

It will be seen that, given  $n' > n$ , both effects can be appreciable as  $n$  increases. In particular (5.22) shows that the effect of absorption tends to be a more important correction than the effect of stimulated emission.

## 6. EXTRAPOLATION TO AN INFINITE NUMBER OF EXCITED STATES

Equations (5.17) describe a steady-state radiative cascade in which the total electron concentration  $N_e + \sum_{n=1}^N N_n$  is constant for given  $N$ . Consider now the concentration  $N_n$ , as measured by  $b_{nN}$  [Eq. (3.14)] for fixed  $n$ , and fixed  $b_{1N}$ , as  $N$  increases. This introduces additional excited states, and the total number of electrons increases. Since, however, for the levels already present the equilibrium concentration  $N_{n0}$  remains

TABLE I. Ratios of rates of stimulated to spontaneous emission and absorption.

$(n', n)$	(10,1)	(3,2)	(6,5)	(10,9)	$(\infty, 1)$	$(\infty, 2)$	$(\infty, 5)$	$(\infty, 9)$
$s_{n'n}$	$10^{-14}$	$10^{-2}$	2.0	12	$10^{-14}$	$2 \times 10^{-14}$	0.34	2.0
$\frac{b_{n'}}{b_n} a_{nn'}$	1	1	3.1	13	1	1	1.3	2.9

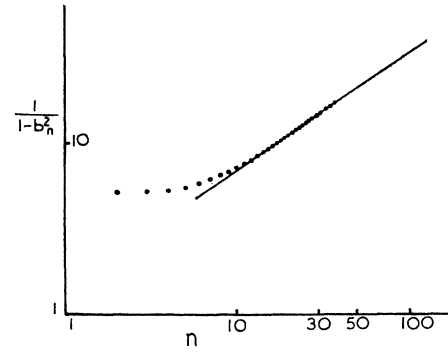


FIG. 4. For  $N \rightarrow \infty$ ,  $b_{1n} = 0.9$  and  $x_n$  given by (5.15)  $b_{nN}$  [see Eq. (5.19)] follows the asymptotic law (6.3).

fixed by (3.6), one would expect the value of  $b_{nN}$  for given  $n$  to increase as  $N$  increases. This is borne out by the calculation (Fig. 3). Next consider  $b_{nN}$  for given  $N$  as  $n$  increases. The equilibrium concentrations  $N_{n0}$  decrease as  $n$  goes up, but the steady-state concentrations  $N_n$  decrease less rapidly, so  $b_{nN}$  increases. For large  $n$  the occupation probability entering into  $N_n$  must tend towards that entering into  $N_e$ . The same is true for  $N_{n0}$  and  $N_{e0}$ . Hence one would expect

$$\lim_{n \rightarrow \infty} \{ \lim_{N \rightarrow \infty} b_{nN} \} = 1. \quad (6.1)$$

An extrapolation procedure was used to check (6.1). From values of  $b_{nN}$  for fixed  $n$  and  $N = 37, 40, 43, 46, 49, 52, 55$  the constants  $c_j$  in the formula

$$b_{nN} = b_n + \sum_{j=1}^6 c_j e^{-jN/6}$$

were identified. Hence

$$b_n \equiv \lim_{N \rightarrow \infty} b_{nN} \quad (6.2)$$

was found. The quantities (6.2) are also shown in Fig. 3. The extrapolated values were found to obey the law

$$b_n^2 = 1 - (6/11n)^{2/3} \quad (n \text{ large}) \quad (6.3)$$

as shown in Fig. 4. This confirms (6.1).

In the semiconductor case only values of  $N$  up to about  $N = 12$  will in general be of interest.

If the values for  $b_{n55}$  are compared with those of  $b_n$ , one can estimate the error caused by the neglect of levels with  $n > 55$ . The results are given in Table II. Thus no great error is incurred up to  $n = 35$  by a cutoff

TABLE II. Percentage errors in distribution parameters caused by neglect of levels with  $n > 55$ .

$n$	5	10	15	20	25	30	35
Error in $b_{n55}$ for $b_{155} = 0.9$	0.004	0.032	0.061	0.087	0.11	0.13	0.15
Error in $P_{n55}$ (for all values of $b_{155}$ )	0.04	0.4	1.0	1.8	2.6	3.6	4.6

at  $N=55$ . In the results to be presented below there has therefore been no extrapolation to  $N=\infty$ .

### 7. THE STICKING PROBABILITY: THEORY

The steady-state cascade equation (5.17) which has been solved here arose from (4.2a) which holds for more general cascade processes, for instance, phonon cascades or photon-phonon cascades in solids. In the solid-state work the concept of sticking probability has been used in order to take approximate account of the effect of reverse transitions into the continuum (Lax,<sup>1</sup> Ascarelli and Rodriguez,<sup>2a</sup> and Hamann and McWhorter<sup>14</sup>). In the case of the photon cascade the reverse transitions appear to have been neglected (Baker and Menzel,<sup>6</sup> Seaton<sup>5</sup>), but the concept of sticking probability can be applied also in this case as will be seen below. In the present work the reverse transitions are taken into account exactly, and in the form of Eq. (4.2a) the theory applies to photon and phonon cascades. The connection between this equation and a theory using sticking probabilities will be discussed in this section.

In the absence of reverse transitions the first two  $b_n$ 's on the right-hand side of (4.2a) and  $b_{n'}$  all become zero. Insofar as return transitions to the continuum are concerned, therefore, the present theory replaces  $B_{cn}$  by  $B_{cn}(1-b_n)$ . This may also be seen from (3.15) which can be written

$$R_{cn} = W_{cn}\Pi_n, \quad W_{cn} \equiv N_i N_e B_{cn}.$$

Thus the net transition rate from the continuum to levels  $n$  may be thought of as the difference between the downward ( $c \rightarrow n$ ) transition rate  $W_{cn}$  in the absence of all return transitions and an upward ( $n \rightarrow c$ ) reverse rate  $W_{cn}(1-\Pi_n)$  due to all cascade paths.  $\Pi_n$  is therefore a probability that an electron in level  $n$  will not make a transition into the continuum by any cascade path (excepting a transition via level 1 when it can be aided by the pumping to the continuum from level 1). Alternatively,  $\Pi_n$  is the probability that an electron will reach the ground state from level  $n$  without leaving the atom. Thus  $\Pi_n$  is a "sticking probability," and  $\Pi_n/(1-b_1)$  is by (4.6) the "reduced" sticking probability  $P_n$ . It is determined by the assumed parameters of the

cascade process. An explicit expression for  $b_n$  will now be derived from (4.2a).

The following symbols are useful

$$H_n \equiv (B_{cn} - G_n/N_i N_e)N_e \quad (7.1)$$

$$N_e \equiv (g_i g_e / h^3) (2\pi m^* kT)^{3/2} \quad (7.2)$$

$$\begin{aligned} G_{mn} &\equiv g_m e^{z_m} A_{mn} \quad (m > n) \\ &\equiv B_{cn} N_e + \sum_{n' > n} g_{n'} A_{n'n} e^{z_{n'}} \\ &\quad + \sum_{n'=1}^{n-1} g_n A_{nn'} e^{z_n} \quad (m=n) \\ &\equiv g_n e^{z_n} A_{nm} \quad (m < n). \end{aligned} \quad (7.3)$$

The cascade equation (4.2a) is (the case  $n=1$  is again included),

$$\begin{aligned} b_n G_{nn} = H_n + \sum_{n'=n+1}^{\infty} b_{n'} G_{n'n} \\ + \sum_{n'=1}^{n-1} b_{n'} G_{n'n} \quad (n=1, 2, 3, \dots). \end{aligned} \quad (7.4)$$

By examining these equations for  $n=1, 2, 3$ , etc., the last sum can be eliminated and one finds by a procedure similar to Gaussian elimination methods (Newman<sup>5b</sup>)

$$b_n G_{nn} n^{-1} = H_n n^{-1} + \sum_{n'=n+1}^{\infty} b_{n'} G_{n'n} n^{-1}. \quad (7.5)$$

Here

$$H_n^m \equiv H_n^{m-1} + H_m^{m-1} G_{mn}^{m-1} / G_{mm}^{m-1} \quad (7.6)$$

$$\begin{aligned} G_{kn}^m &\equiv G_{kn}^{m-1} + G_{km}^{m-1} G_{mn}^{m-1} / G_{mm}^{m-1} \quad (k \neq n) \\ &\equiv G_{kn}^{m-1} - G_{nm}^{m-1} G_{mn}^{m-1} / G_{mm}^{m-1} \quad (k = n), \end{aligned} \quad (7.7)$$

where

$$H_n^0 \equiv H_n, \quad G_{kn}^0 \equiv G_{kn}. \quad (7.8)$$

Equation (7.5) is a generalization of Eq. (2) of Baker and Menzel and Eq. (5) of Seaton. Using this procedure it may be solved for the  $b_m$ 's in terms of the quantities

$$P_{km} \equiv G_{km}^{m-1} / G_{kk}^{k-1} \quad (k > m). \quad (7.9)$$

One finds

$$\begin{aligned} b_n G_{nn} n^{-1} = H_n n^{-1} + \sum_{n_1=n+1}^{\infty} H_{n_1}^{n_1-1} P_{n_1 n} + \sum_{n_2=n+2}^{\infty} \sum_{n_1=n+1}^{n_2-1} H_{n_2}^{n_2-1} P_{n_2 n_1} P_{n_1 n} \\ + \sum_{n_3=n+3}^{\infty} \sum_{n_2=n+2}^{n_3-1} \sum_{n_1=n+1}^{n_2-1} H_{n_3}^{n_3-1} P_{n_3 n_2} P_{n_2 n_1} P_{n_1 n} + \dots \end{aligned} \quad (7.10)$$

This is the required expression for  $b_n$ .

To interpret these results, suppose first that the return transitions from the lower levels into level  $n$  are

<sup>14</sup> D. R. Haman and A. L. McWhorter, Phys. Rev. 134, A250 (1964).

negligible. Then the last sum in (7.4) disappears, and (7.4) and (7.5) are identical. The terms  $H_n$  in the solution (7.4) for  $b_n$  represent the transition rate into

<sup>15</sup> M. Newman, in *Surveys of Numerical Analysis*, edited by J. Todd (McGraw-Hill Book Company, New York, 1962), p. 222.



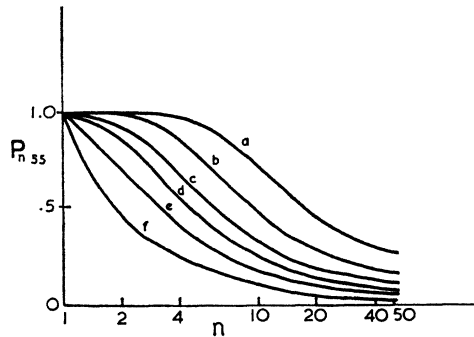


FIG. 5. The reduced sticking probability as a function of principal quantum number  $n$  and temperature  $T$  if the levels are cut off at  $n=N=55$ . The temperatures are as follows [see Eq. (5.14), (5.16)]:

	a	b	c	d	e	f
Semiconductor case ( $^{\circ}\text{K}$ )	4	10	20	30	50	100
Astrophysical case ( $10^8$ $^{\circ}\text{K}$ )	4.65	11.65	23.30	34.95	58.25	116.5

the level  $n$  from the conduction band.  $G_{mn}$  represents the transition rates from the discrete levels  $m$  into levels  $n$  ( $m \neq n$ ) for unit concentration in the continuum.  $G_{nn}$  is the total transition rate out of levels  $n$  for unit concentration  $N_n$ . The quantities (7.9) have now no superfluous and are analogous to conditional probabilities.  $P_{km}$  is the transition rate  $k \rightarrow m$  given a unit transition rate out of levels  $k$ . (7.10) states that the rate out of levels  $n$  is equal to the rate into levels  $n$ . If the last term in (7.4) is not negligible, the generalized expressions, characterized by superfluous are needed. These terms take into account the possibility of transitions

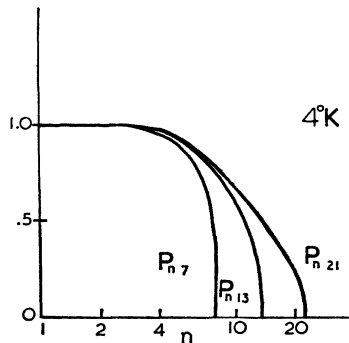


FIG. 6. The reduced sticking probability if the continuum is assumed to start at the level  $n=N+1$ . The temperature stated is for the semiconductor case. For the astrophysical case the corresponding temperatures of Fig. 5 should be used.

into the levels  $n$  via levels lying below  $n$ . For example from Eq. (7.6)  $H_3^1$  takes into account the direct transition from the continuum into levels three already included in  $H_3$ , as well as direct transitions into levels one, which are followed by transitions from levels one to levels three.  $H_3^2$  takes account of the transitions included in  $H_3^1$  as well as of transitions via levels one and two.

It is therefore seen from (7.10) that the sticking probability  $1-b_n$  may be thought of as composed of separate contributions from many different transitions. This agrees with the analogous, but more ap-

proximate, series given earlier (Seaton<sup>5</sup> and Ascarelli and Rodriguez).<sup>2a</sup> The quantities (4.6) and (5.19) are "reduced" sticking probabilities.

## 8. STICKING PROBABILITY AND CASCADE RATIO; NUMERICAL RESULTS

Figure 5 illustrates the expected drop in the sticking probability as the continuum is approached. As the temperature is raised the increased background radiation causes more upward transitions, and the sticking probability is therefore again decreased. This is in contrast with the sticking probability obtained by Ascarelli

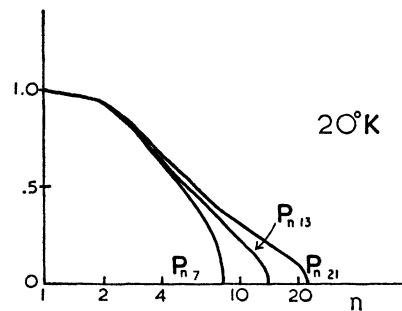


FIG. 7. The reduced sticking probability if the continuum is assumed to start at the level  $n=N+1$ . The temperature stated is for the semiconductor case. For the astrophysical case the corresponding temperatures of Fig. 5 should be used.

and Rodriguez<sup>2a</sup> for their phonon cascade, which becomes zero abruptly at  $n=4$ .

In the semiconductor case it may sometimes be a better approximation to regard the discrete levels  $n > N$  as merged with the continuum, than to neglect them altogether. An approximate way of taking this effect into account is to bring down the bottom of the conduction band to the level  $n=N+1$ . In this case  $x_n$  in (5.17) is replaced by  $x_{n N+1}$  [see Eq. (5.18)]. The sticking probability for this situation is illustrated in Figs. 6, 7, 8, which should be compared with Fig. 5. The lowering of

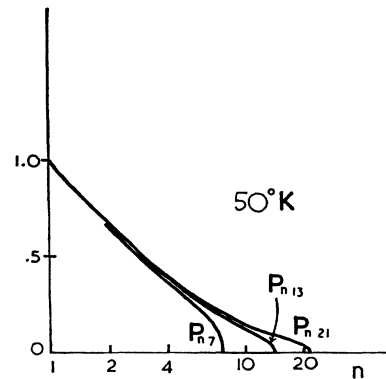


FIG. 8. The reduced sticking probability if the continuum is assumed to start at the level  $n=N+1$ . The temperature stated is for the semiconductor case. For the astrophysical case the corresponding temperatures of Fig. 5 should be used.

the continuum, even down to the level  $n=8$ , has no marked effects on the sticking probabilities up to  $n=4$ . Above this value there is a more rapid drop to zero than is found in Fig. 5.

In order to have a parameter which gives information about the effect of the cascade paths on the recombination traffic in the absence of the cascade, it is convenient to define a cascade ratio

$$C \equiv \frac{\text{Transition rate into level 1 due to all cascade paths}}{\text{Transition rate into level 1 directly from the conduction band}}$$

calculated for fixed temperature and other parameters. For a steady state the numerator is, by [4.2(a)],

As the temperature is increased, it has been seen in Fig. 5 that the sticking probability goes down. Hence

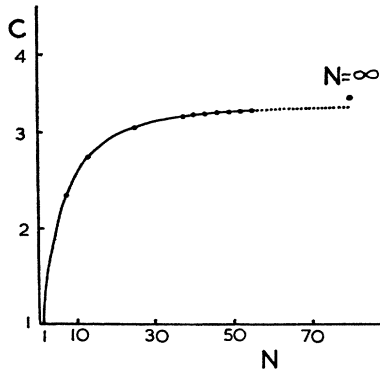


FIG. 9. The cascade ratio  $C$  at  $4^\circ\text{K}$  in the semiconductor case and at  $4650^\circ\text{K}$  in the astrophysical case.

simply  $\sum_{n=1}^N B_{cn}(1-b_{nN})$  and the denominator is  $B_{c1}(1-b_1)$ . Hence

$$B_{c1}C = \sum_{n=1}^N B_{cn}P_{nN}. \quad (8.2)$$

Figure 9 shows how the cascade ratio increases as the number of excited states increases. The change is seen to be slight for  $N > 30$ . An extrapolation procedure analogous to that leading to Eq. (6.2) was used to find the value for  $N = \infty$ . The curve can be fitted by the equation

$$C = 3.35 - 2.35N^{-1/3}e^{-(N-1)/30}. \quad (8.3)$$

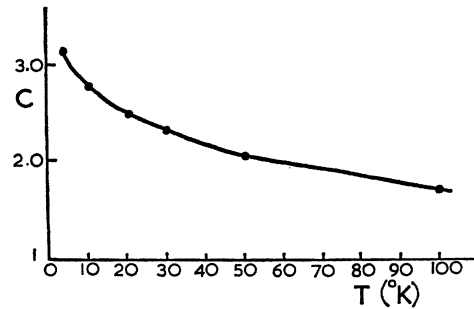


FIG. 10. The cascade ratio as a function of temperature for  $N=55$ . The temperature axis is labeled for the semiconductor case.

from (8.2) one would expect the cascade ratio also to decrease. This is illustrated in Fig. 10.

**ACKNOWLEDGMENTS**

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