THE ASTROPHYSICAL JOURNAL, Vol. 156, June 1969

THE GENERAL SOLUTION OF THE b_n PROBLEM FOR GASEOUS NEBULAE

T. J. SEJNOWSKI*
Department of Physics, Case Western Reserve University, Cleveland, Ohio
AND
ROBERT M. HJELLMING
National Radio Astronomy Observatory,† Green Bank, West Virginia
Received October 11, 1968; revised November 8, 1968

ABSTRACT

The departures of the populations of the excited states of hydrogen from those found under conditions of thermodynamic equilibrium are calculated using a general iterative method. Calculations of b_n and $d(\ln b_n)/dn$ are carried out for conditions found in gaseous nebulae, and the sensitivity of the solution to certain assumptions is discussed.

I. PROLOGUE

The observed intensities of the radio recombination lines of hydrogen emitted by gaseous nebulae are difficult to interpret because the excited atoms emitting the radiation are not in thermodynamic equilibrium (TE). Goldberg (1966) has shown that this type of radio line emission is extremely sensitive to $d(\ln b_n)/dn$, where b_n is a measure of the departure of the concentration of atoms in the energy level with quantum number n from TE as defined by

$$b_n = N_n/(N_n)_{\mathrm{TE}} . \tag{1}$$

The purpose of this paper is to use a general iterative technique to obtain solutions for the b_n's and the associated $d(\ln b_n)/dn$'s for conditions valid in gaseous nebulae.

For a typical radio recombination line produced by $(n \rightarrow m)$-transitions, the absorption coefficient in the line is

$$\kappa_\nu{}^L = \frac{b_m[1 - (b_n/b_m)\ \exp\ (-h\nu/kT_e)](\kappa_\nu{}^L)_{\mathrm{TE}}}{[1 - \exp\ (-h\nu/kT_e)]} , \tag{2}$$

where T_e is the electron temperature, ν is the frequency, h is Planck's constant, k is the Boltzmann constant, and $(\kappa_\nu{}^L)_{\mathrm{TE}}$ is the TE absorption coefficient in the line. As pointed out by Goldberg (1966), the factors b_n/b_m and $\exp\ (-h\nu/kT_e)$ are very close to unity, so that, after making the appropriate expansion of each to first order, one obtains

$$\kappa_\nu{}^L = b_n\{1 - (m - n)(kT_e/h\nu)[d(\ln b_n)/dn]\}(\kappa_\nu{}^L)_{\mathrm{TE}} . \tag{3}$$

For physical conditions in gaseous nebulae, as first pointed out by Goldberg (1966), the second term in the braces in equation (3) is usually large compared with unity, so that $\kappa_\nu{}^L < 0$, which implies that the observed radio recombination line is predominantly produced by stimulated emission.

The key factor in the use of equation (3) to interpret data on radio recombination lines is the accurate theoretical prediction of $d(\ln b_n)/dn$ and, to a lesser extent, b_n. Early

* Present address: Department of Physics, Princeton University.

† Operated by Associated Universities, Inc., under contract with the National Science Foundation.

calculations of the b_n's have been carried out in the context of this problem by Hayler (1967), Dyson (1967*a*, *b*, 1968), and McCarroll and Binh (1968). These papers, with the exception of Hayler (1967), have mainly extended the computational methods developed by Seaton (1964). In the following sections of this paper we develop and utilize a more general and independent method of solution in which all radiative and collisional transitions affecting the b_n's are considered.

II. FORMULATION OF THE b_n PROBLEM

The time scales for changes in conditions in gaseous nebulae are assumed to be long enough so that we equate the rates of population and depopulation of an atomic-energy level of hydrogen. We express this equation of statistical equilibrium (see Aller 1956; Menzel 1962) as

$$N_n P_n = N_c P_{cn} + \sum_{m=1}^{\infty} N_m P_{mn} , \tag{4}$$

where the right-hand side of equation (4) represents the rate of population. We use the subscript c to refer to the continuum, and P_{mn} is the probability per unit time of a transition from a level denoted by m to a level denoted by n. The left-hand side of equation (4) is the depopulation rate, where

$$P_n = \sum_{m=1}^{\infty} P_{nm} . \tag{5}$$

The P_{mn}'s involve both radiative and collisional processes which will be distinguished by the superscripts R and C, respectively; the calculation of the P_{mn}'s will be discussed in § III.

The equation of statistical equilibrium can be most conveniently expressed in terms of the b_n's. By using the Saha-Boltzmann equation, which determines $(N_n)_{\mathrm{TE}}$, in conjunction with equation (1), one can substitute

$$N_n = b_n N_c N_e \frac{h^3}{(2\pi m k T_e)^{3/2}} n^2 \exp (x_n) , \tag{6}$$

where N_e = electron concentration, m = electron mass, $x_n = I_n/kT_e$, and I_n is the energy needed to ionize an atom in level n, into equation (4) to obtain

$$b_n = T_n + \sum_{m=1}^{\infty} b_m S_{mn} , \tag{7}$$

where

$$T_n = \frac{(2\pi m k T_e)^{3/2}}{N_e h^3} \frac{P_{cn}}{n^2 P_n \exp (x_n)} \tag{8}$$

and

$$S_{mn} = \frac{P_{mn}}{P_n} \frac{m^2}{n^2} \exp (x_m - x_n) . \tag{9}$$

In general, equation (7) represents an infinite number of equations to be solved for an equally infinite number of unknowns—the b_n's. If all upward transitions are ignored ($P_{mn} = 0$ for $m < n$), a nearly analytic solution is possible (Seaton 1959); however, this leads to serious errors for $n > 50$ as shown by Seaton (1964) in a paper where, by making certain simplifying assumptions, he reduces equation (7) to a second-order differential equation which can be solved to determine the b_n's. In § IV we will discuss a more general iterative process for solving equation (7).

III. TRANSITION PROBABILITIES

a) Formulae

Once the transition probabilities in equations (7)–(9) are specified, the solution for the b_n's is determined, subject only to errors involved in the method of solution.

The radiative-transition probabilities are well understood (cf. Seaton 1959), and we will only summarize the results:

$$P_{mn}{}^{R} = A_{mn}(1 + c^2 J_\nu / 2h\nu^3) \qquad m > n \,, \tag{10}$$

$$P_{nm}{}^{R} = A_{mn} \frac{g_m}{g_n} \frac{c^2}{2h\nu^3} J_\nu \qquad m > n \,, \tag{11}$$

$$P_{nc}{}^{R} = \int_0^\infty \frac{4\pi J_\nu}{h\nu} a_n(\nu) d\nu \,, \tag{12}$$

and

$$P_{cn}{}^{R} = N_e \int_0^\infty \sigma_n(v)(1 + c^2 J_\nu / 2h\nu^3) v f(v) dv \,, \tag{13}$$

where $g_n = 2n^2$ is the statistical weight of the nth level, A_{mn} is the Einstein coefficient for spontaneous emission (using accurate Gaunt factors), J_ν is the average intensity of the radiation field at frequency ν, $a_n(\nu)$ is the cross-section for photo-ionization from the level n by a photon of frequency ν, v is the speed of a free electron, $\sigma_n(v)$ is the cross-section for electrons of speed v to recombine to the level n (related to $a_n(\nu)$ by the Milne relation), and $f(v)$ is the Maxwellian velocity-distribution function for the free electrons.

Collisional-transition probabilities are much more poorly known, especially for large n, and this provides one of the major sources of uncertainty in the solution for b_n. Keeping in mind that one would be optimistic in trusting a collisional cross-section to a factor of 2, we will discuss results for two combinations of cross-sections denoted by Class I and Class II. For Class I cross-sections we will use the dipole approximation as formulated by Seaton (1962*b*) and utilized by Zel'dovich and Raizer (1966) to obtain the ionization and excitation transition probabilities:

$$P_{nc}{}^{C}\,(\text{Class I}) = 4\pi a_0^2 \left(\frac{8kT_e}{m}\right)^{1/2} \left(\frac{I_1}{kT_e}\right)^2 \left[\frac{\exp(-x_n)}{x_n} - E_1(x_n)\right] N_e \,, \tag{14}$$

and

$$P_{nm}{}^{C}\,(\text{Class I}) = 4\pi a_0^2 \left(\frac{8kT_e}{m}\right)^{1/2} \left(\frac{I_1}{kT_e}\right)^2 \left[\frac{\exp(-x_{nm})}{x_{nm}} - E_1(x_n)\right] (3f_{nm}) N_e \,, \tag{15}$$

where $\pi a_0^2 = 8.797 \times 10^{-17}$ cm^2, I_1 is the ionization potential of the ground state of hydrogen, f_{nm} is the f-value for the transition $n \rightarrow m$ (Menzel and Pekeris 1935), E_1 indicates the exponential integral of order 1, and $x_{nm} = (I_m - I_n)/kT_e$.

As Class II cross-sections, we will use an ionization formula given by Jeffries (1968) based on a semi-empirical dipole-approximation formula discussed by Seaton (1962*b*), i.e.,

$$P_{nc}{}^{C}\,(\text{Class II}) = 7.8 \times 10^{-11}\, T_e^{1/2}\, n^3 \exp(-x_n) N_e \text{ cgs units} \,, \tag{16}$$

and the following interpolation formula approximating the results of an impact-parameter treatment developed by Seaton (1962*a*) and Saraph (1964) and discussed by Jeffries (1968):

$$P_{nm}{}^{C}\,(\text{Class II}) = 1.2 \times 10^{-7} f_{nm} \exp(-x_{nm}) \left(\frac{I_m - I_n}{I_1}\right)^{-1.1856} N_e \text{ cgs units} \,. \tag{17}$$

The approximation formula given in equation (17) was found to represent the more detailed impact-parameter calculations (even over the temperature range 6000°–12000° K) with an average error of about 10 per cent and an extreme error of about 25 per cent for important transitions in the range $50 < n < 250$. Because of the great uncertainty in the cross-sections, the approximation formula given by equation (17) should be adequate. Saraph (1964) and Seaton (1965) have argued that the impact-parameter results should be the best for the problem under consideration; hence, if a choice is necessary, the Class II results are probably to be preferred.

Once the probabilities of collisional ionization and excitation are specified by equations (14)–(15) or (16)–(17), one can utilize the equations of detailed balancing:

$$n^2 \exp(x_n) P_{nm}{}^C = m^2 \exp(x_m) P_{mn}{}^C , \tag{18}$$

and

$$P_{cn}{}^C = \frac{N_e h^3}{(2\pi m k T_e)^{3/2}} n^2 \exp(x_n) P_{nc}{}^C , \tag{19}$$

which are assumed to be valid for collisional processes, to determine the probabilities of de-excitation and three-body recombination.

For both the Class I and Class II bound-bound transition probabilities, the contributions are the largest when $\Delta n = m - n$ is the smallest; therefore, under most conditions, as has been discussed by Dyson (1968), most of the collisional population and depopulation rates are due to transitions with $\Delta n \lesssim 5$. However, for different values of N_e and T_e, the largest Δn that need be considered varies; thus in utilizing the method discussed in this paper Δn was taken to be 20, and the remaining transitions were treated approximately.

b) Parameters of the Solution

Since the parameters which must be specified to determine the b_n's are the parameters of the transition probabilities, let us now discuss them. If we exclude the parameters of the procedure of numerical calculation, it is clear from equations (7)–(19) that the solution can depend only on the specification of N_e, T_e, and J_ν.

Initially an attempt was made to specify J_ν as a functional parameter; however, it became clear that the values of J_ν specified do not affect the values of b_n for $n \geq 3$ for gaseous nebulae containing sufficient matter to be observable. For large n the collisional processes are so dominant over the radiative processes that the b_n's are not changed by changing J_ν over any range in equations (10)–(13). For intermediate n, the small populations (of the order of 10^{-14} of N_1) and the weak non-Lyman radiation field insure that radiative processes not involving the ($n = 1$)-level will not affect the b_n's. Even radiative depopulation of the ground state does not affect the b_n's for $n \geq 3$. It is indeed impossible to avoid specifying the Lyman-continuum radiation field if one wishes to calculate b_1, but the value of b_1 does not affect the b_n's for $n > 3$. The latter is clear from the following argument (see Aller 1956; Menzel 1962, the latter of which contains many of the relevant early papers). The coupling between upper levels and the ground state is primarily through Lyman-line absorption; and, as has been known for a long time, observable nebulae like H II regions should be optically thick to Lyman-line radiation. Under these circumstances one can show that, for each Lyman line,

$$J_\nu = \frac{2h\nu^3}{c^2} \left[\frac{b_1}{b_n} \exp\left(\frac{I_1 - I_n}{kT_e} \right) - 1 \right]^{-1} , \tag{20}$$

and this insures that

$$N_1 P_{1n} = N_n P_{n1} . \tag{21}$$

Using equation (21), N_1P_{1n} can be eliminated from the equations of the problem. For all of the above reasons we will deal exclusively with the classical Case B situation (cf. Aller 1956; Menzel 1962); and the b_n solutions we will discuss will depend only on N_e, T_e, and assumptions concerning cross-sections and the techniques of calculation.

IV. SOLUTION BY ITERATION

a) Iterative Procedure

Equation (7) can be used to define the iterative procedure of Jacobi (cf. Varga 1962) as follows:

$$b_n^{\text{new}} = T_n + \sum_{m=1}^{\infty} b_m^{\text{old}} S_{mn} , \tag{22}$$

where initially all b_n's are set equal to unity. The T_n's and S_{mn}'s depend only on N_e and T_e (cf. § III). In actual practice the convergence of equation (22) is very slow for large n because, typically, $(T_n + \Sigma S_{mn} - 1)$ is of the order of 10^{-6} and thus each iterative step will improve b_n by only about this amount; and the larger the value of n, the smaller this quantity becomes and the more iterations are needed for convergence. Standard techniques for accelerating convergence are not useful because the system is ill conditioned and becomes unstable when overrelaxed. One successful technique for improving convergence is to solve equation (7) for b_{n+1} and define the new iteration scheme:

$$b_{n+1}^{\text{new}} = \left(b_n^{\text{old}} - T_n - \sum_{m \neq n+1} b_m^{\text{old}} S_{mn} \right) \Big/ S_{n+1,n} . \tag{23}$$

Alternate iterations using equations (22) and (23) have been found to give good convergence properties.

Because of the finite memory capacity of computers, actual calculations using equations (22) and (23) must involve truncating the summation at some $n = N$. The spurious effects of truncation can be minimized by analytically continuing b_n beyond N. This is a reliable procedure because (1) b_n is very close to unity for large n and is changing slowly and (2) the transition-probability matrix is highly peaked around the diagonal. In most cases b_n and $d(\ln b_n)/dn$ are insensitive to N for $N - n > 10$, as long as $n > 100$.

b) Comparison with Differential Equation Method

The method developed by Seaton (1964) and used by Dyson (1967*a*) and McCarroll and Binh (1968) to treat cases where $\Delta n = 1$ for collisional transitions is based on reducing equation (7) to a second-order differential equation. The boundary conditions imposed on the solution are (1) $b_n \rightarrow 1$ as $n \rightarrow \infty$ and (2) b_n merges with a solution neglecting all collisional processes at small n. The computational problem is greatly simplified if one uses the approximation that the b_n's are set equal to unity in the so-called cascade term; therefore, Seaton (1964), Dyson (1967*a*), and McCarroll and Binh (1968) used this approximation. Unfortunately, it can be shown that this can cause an error of up to a factor of 2 in $d(\ln b_n)/d_n$ for certain ranges of n. In Figure 1, *a* and *b*, plots of b_n and of $d(\ln b_n)/dn$, respectively, as functions of n are presented for the case where one uses the approximation in the cascade term (solution by differential-equation method) and for the case where one does not use this approximation (solution by the iterative method). For the solution in Figure 1, the Class I cross-sections are used, $T_e = 10000°$ K, $\Delta n = 1$, and $N_e = 10$, 10^2, and 10^4 cm^{-3}. The pure-radiative solutions obtained both with and without the approximation are also plotted in Figure 1. It is clear that the error induced by the approximation arises from the fact that the "correct" radiative solution for small n is dependent on the b_n's in the transition region between the radiative solution and the

collision-dominated solution. The effects of the erroneous assumption in the cascade term are seen from Figure 1 to be largest for the smallest N_e, hence it will typically cause more error for normal H II regions than for normal planetary nebulae.

Because the usefulness of the differential-equation method is greatly decreased if the b_n's must be included in the cascade term and if Δn in excess of unity is used, the general iterative method of solution should be preferable in computing b_n's for large n.

c) *General Solutions*

Figures 2, 3, and 4 show results of computations of b_n and $d(\ln b_n)/dn$ for $T_e = 10000°$, $7500°$, and $5000°$, respectively, where results for both Class I and Class II cross-sections are given and $N_e = 10$, 10^2, 10^3, and 10^4 cm^{-3}. The general iterative method was used to obtain the solutions, and truncation at $N = 240$ was used with analytic

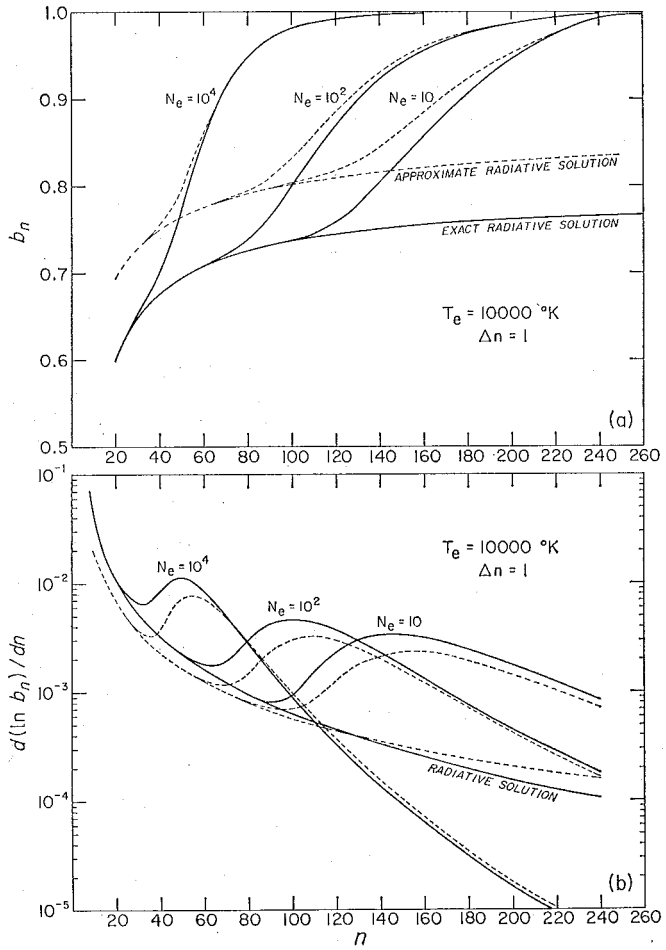

FIG. 1.—Solution for (*a*) b_n and (*b*) $d(\ln b_n)/dn$ as functions of n, plotted for both the case where the exact cascade term is used (*solid lines*) and the case where the approximate cascade term is used (*dashed lines*). The radiative solutions in both approximations are also plotted. For all cases $T_e = 10^4$ ° K, $N_e = 10^4$ cm^{-3}, $\Delta n = 1$, and Class I cross-sections are used.

continuation for larger n. The iteration was carried through fifteen cycles, with each cycle consisting of five iterations using equation (22) and five iterations using equation (23). Accuracy to better than three significant figures in $d(\ln b_n)/dn$ was achieved in all cases.

It is clear from Figures 2, 3, and 4 that the solution depends strongly upon N_e and T_e and that the effects of different collisional cross-sections are also very dependent on N_e and T_e. The results presented in Figures 2, 3, and 4 should be quite general and subject to change only upon a change in collisional cross-sections or abandonment of the conditions which make the Case B solution the only reasonable possibility.

By using the data contained in Figures 2, 3, and 4, the ratio $\kappa_\nu{}^L/(\kappa_\nu{}^L)_{\rm TE}$ has been calculated (assuming Class II cross-sections) for a variety of radio recombination lines which have been observed: 94α, 109α, 126α, 158α, 137β, and 225γ. The results are shown in

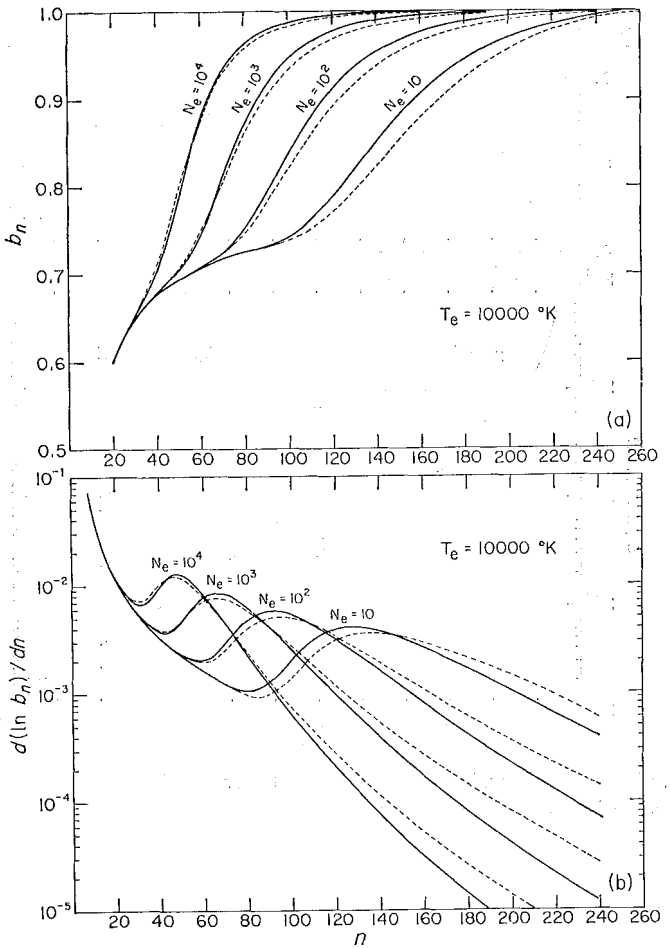

FIG. 2.—Solutions for (*a*) b_n and (*b*) $d(\ln b_n)/dn$ as functions of n, shown for both Class I (*dashed lines*) and Class II (*solid lines*) collisional cross-sections. The general iterative method of solution is used, assuming $T_e = 10000°$ K, $N_e = 10$, 10^2, 10^3, 10^4 cm^{-3}, and truncation of the solution at $n = 240$.

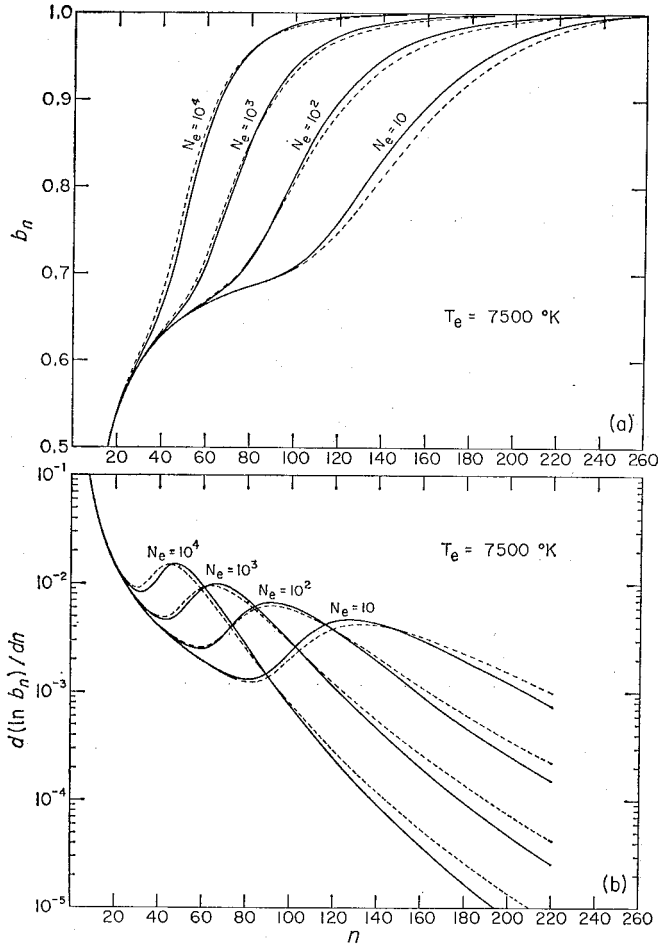

FIG. 3.—Solutions for (*a*) b_n and (*b*) $d(\ln b_n)/dn$, plotted as functions of n, assuming $T_e = 7500°$ K, the other assumptions being as listed in Fig. 2.

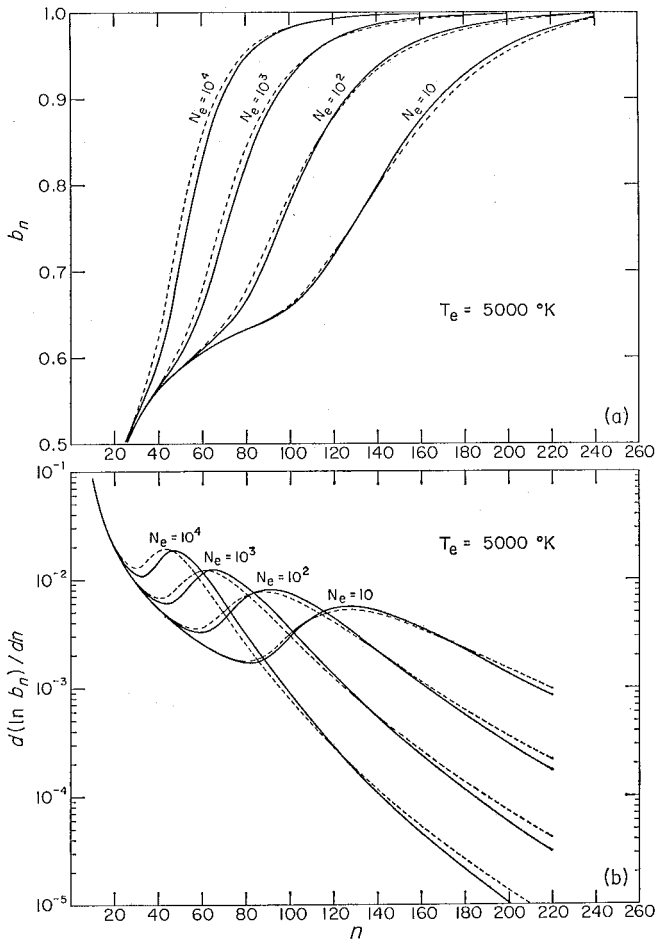

FIG. 4.—Solutions for (*a*) b_n and (*b*) $d(\ln b_n)/dn$, plotted as functions of n, assuming $T_e = 5000°$ K, the other assumptions being as listed in Fig. 2.

Table 1, taking $T_e = 10000°$, 7500°, and 5000° K and $N_e = 10$, 10^2, 10^3, and 10^4 cm^{-3}. It is seen that $(\kappa_\nu{}^L)/(\kappa_\nu{}^L)T_e$ is very dependent on both N_e and T_e.

V. CONCLUDING REMARKS

The general iterative method for solving the b_n problem discussed in this paper provides basic data needed in discussion of radio recombination lines. The next step to be taken is the combination of realistic models of H II regions, such as those computed by Hjellming (1966) and Rubin (1968), with the solution of the radiative-transfer problem for selected radio recombination lines using the b_n computations discussed in this paper. We will present the results of such calculations in a forthcoming paper. It is unfortunately clear that whenever deviations from TE are relevant, the interpretation of data on radio recombination lines will be very questionable except when coupled with realistic model-building in which temperature and ionization structure are calculated (assuming a particular density structure).

TABLE 1

THE DEVIATION OF $\kappa_\nu{}^L$ FROM TE

LINE	ν	T_e(° K)	$\kappa_\nu{}^L/(\kappa_\nu{}^L)_{TE}$			
			$N_e=10$	$N_e=10^2$	$N_e=10^3$	$N_e=10^4$
94α.....	7797.2 MHz	12500	− 30.06	−134.96	−90.57	−25.19
		10000	− 27.51	−131.16	−81.80	−23.00
		7500	− 23.88	−102.23	−70.48	−20.03
		5000	− 18.84	− 79.17	−55.48	−15.95
		3000	− 13.39	− 55.64	−39.68	−11.46
109α.....	5009.02	12500	−101.45	−175.74	−70.13	−15.72
		10000	− 90.68	−157.41	−63.64	−14.41
		7500	− 77.01	−134.29	−55.11	−12.60
		5000	− 59.57	−104.72	−43.73	−10.07
		3000	− 41.77	− 74.21	−31.99	− 7.21
126α.....	3248.9	12500	−228.00	−170.03	−48.64	− 9.27
		10000	−203.00	−152.94	−44.36	− 8.53
		7500	−171.99	−131.20	−38.63	− 7.47
		5000	−132.99	−103.04	−30.86	− 5.96
		3000	− 93.45	− 73.59	−22.36	− 4.22
158α.....	1651.59	12500	−344.28	−114.37	−23.78	− 3.51
		10000	−307.29	−103.60	−21.85	− 3.23
		7500	−261.45	− 89.63	−19.19	− 2.81
		5000	−203.57	− 71.17	−15.46	− 2.18
		3000	−144.28	− 51.40	−11.25	− 1.43
137β.....	5004.75	12500	−296.99	−154.16	−38.38	− 6.70
		10000	−264.56	−139.03	−35.10	− 6.18
		7500	−224.42	−119.64	−30.67	− 5.42
		5000	−173.92	− 94.36	−24.59	− 4.30
		3000	−122.58	− 67.68	−17.87	− 3.00
225γ	1697.95	12500	−225.42	− 42.02	− 6.14	−0.113
		10000	−201.25	− 38.18	− 5.62	−0.048
		7500	−177.61	− 33.16	− 4.89	+0.052
		5000	−134.15	− 26.44	− 3.84	+0.204
		3000	− 95.54	− 19.11	− 2.63	+0.389

The work of one of the authors (T. J. S.) was begun as a senior honors research problem at Case Western Reserve University and was completed while he was a participant in the summer student program at the National Radio Astronomy Observatory. During the early phases the project was sponsored by the Warner and Swasey Observatory under National Science Foundation grant GP 6207.

REFERENCES

Aller, L. H. 1956, *Gaseous Nebulae* (New York: John Wiley & Sons), chap. iv.
Dyson, J. E. 1967*a*, *Ap. J.* (*Letters*), **150**, L45.
———. 1967*b*, *A.J.*, **73**, 511.
———. 1968, *Interstellar Ionized Hydrogen: Proceedings of NRAO-AIO* H II *Region Symposium*, ed. Y. Terzian (New York: Benjamin Press).
Goldberg, L. 1966, *Ap. J.*, **144**, 1225.
Hayler, D. 1967, *A.J.*, **73**, 518.
Hjellming, R. M. 1966, *Ap. J.*, **143**, 420.
Jeffries, J. T. 1968, *Spectral Line Formation* (Waltham, Mass.: Blaisdell Publishing Co.), chap. vi.
McCarroll, R., and Binh, D. H. 1968, *Ann. d'ap.*, **31**, 123.
Menzel, D. H. 1962, *Selected Papers on Physical Processes in Ionized Plasmas* (New York: Dover Publications).
Menzel, D. H., and Pekeris, C. L. 1935, *M.N.R.A.S.*, **96**, 77.
Rubin, R. H. 1968, *Ap. J.*, **153**, 761.
Saraph, H. E. 1964, *Proc. Phys. Soc.*, **83**, 763.
Seaton, M. J. 1959, *M.N.R.A.S.*, **119**, 90.
———. 1962*a*, *Proc. Phys. Soc.*, **79**, 1105.
———. 1962*b*, *Atomic and Molecular Processes*, ed. D. R. Bates (New York: Academic Press), chap. xi.
———. 1964, *M.N.R.A.S.*, **127**, 177.
———. 1965, in *Proc. 2d Harvard-Smithsonian Conf. Stellar Atm., Smithsonian Ap. Obs.* Spec. Rept. 174, pp. 33-45.
Varga, R. S. 1962, *Matrix Iterative Analysis* (Englewood Cliffs N.J.: Prentice-Hall, Inc.), chap. iii.
Zel'dovich, Y. B., and Raizer, Y. P. 1966, *Physics of Shock Waves and High Temperature Hydrodynamic Phenomena* (New York: Academic Press), chap. vi.