CALCULATION OF THE OPACITY OF STARS WITH ACCOUNT TAKEN OF LIGHT ABSORPTION IN SPECTRAL LINES

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Abstract

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CALCULATION OF THE OPACITY OF STARS WITH ACCOUNT TAKEN OF LIGHT ABSORPTION IN SPECTRAL LINES

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In constructing models of stars it is necessary to have data on the opacity of stellar matter. Until recently, in calculations of opacity, among the processes of light absorption only photoionization and bremsstrahlung absorption were taken into account (^{1}). However, in the range of temperatures and densities of the Rosseland mean that is of interest to astrophysicists, as the first calculations (^{2}) have shown, the path length may decrease by a factor of 3-5 owing to absorption in lines. Such an influence of discrete-discrete transitions on the opacity of stars is explained by the presence in them of elements with comparatively large atomic numbers, for which, at high temperatures, there is a large number of atomic states with various degrees of ionization and excitation, as well as by the broadening of spectral lines.

We have carried out calculations of the Rosseland mean free path for a number of astrophysical mixtures, taking into account the absorption of photons in spectral lines.

To calculate the effective cross sections for absorption and scattering of photons under given physical conditions, it is necessary to find: 1) the wave functions of electrons of the discrete and continuous spectra and the energy levels of bound electrons; 2) the mean occupation numbers of electron states and the mean degree of ionization of the substance; 3) the probability distribution for different occupation numbers of electron states; 4) the probability distribution for different values of the electric field produced by ions; 5) the shape and position of spectral lines.

Since at high temperatures the Thomas-Fermi statistical model is sufficiently accurate and practically convenient for a given temperature and density (^{3}-^{4}), in finding the electron wave functions the Schrödinger equation with the Thomas-Fermi potential was used as the initial approximation. The subsequent calculation was carried out according to the method set forth in (^{5}).

Depending on the value of the electron energy, one can classify the electron states within the atomic cell as states of the discrete spectrum, of the continuous spectrum, and of a so-called intermediate group. The results of the calculations and the analysis carried out showed that, under the conditions considered, the number of electrons occupying states of the intermediate group is small, and they can be effectively taken into account by assigning them to the electrons of the continuous spectrum.

To find the discrete energy levels and the corresponding wave functions, a phase method was proposed (^{6}), based on a generalization of the Bohr–Sommerfeld quasiclassical conditions. At sufficiently high temperatures a more economical trial-potential method was applied (^{7}). With the aid of this method, the possibility of using hydrogen-like wave functions was analyzed. Tests of the method on many problems gave good agreement with results obtained by direct numerical solution of the Schrödinger equation by the phase method.

In finding the wave functions of the continuous spectrum, it was possible to avoid numerical integration of the Schrödinger equation. It turned out that the quasiclassical approximation for a centrally symmetric field, using Airy functions, gives quite satisfactory accuracy, including near the turning points.

The mean occupation numbers for electrons of the discrete spectrum were determined from Fermi–Dirac statistics. In choosing the probability distribution for different occupation numbers, the binomial distribution was used. This distribution, as well as the Saha distribution, can be obtained from the Gibbs distribution for a subsystem with a variable number of particles, for small deviations of the occupation numbers from their mean values, if an atomic cell is considered as the subsystem.

In determining the positions of spectral lines, relativistic effects and the shift of lines due to fluctuations of the occupation numbers were taken into account. Effects associated with the deviation of the self-consistent field from a centrally symmetric one were neglected.

The effective cross sections of photon-absorption processes were calculated in the nonrelativistic dipole approximation. Owing to the fact that the formulae for photoionization cross sections can be derived by means of the corresponding limiting transition from the expressions for line-absorption cross sections, it proved possible to take discrete–discrete transitions into account effectively only for comparatively small values of the principal quantum number n. Since Stark splitting falls off sharply with decreasing n, in a number of cases it was possible to disregard the Stark effect. In view of the fact that the line shape has only a weak influence on the opacity, a Lorentz line shape was used. The line widths were calculated with the aid of the electron wave functions. Line broadening due to collisions of the ion under consideration with free electrons, natural broadening, and Doppler broadening were taken into account. The analysis showed that autoionization broadening, as a rule, may be neglected in calculations of Rosseland mean free paths.

The effective photon-scattering cross sections were calculated in the same way as in ([11]).

Calculations of opacity with allowance for absorption in lines were carried out by A. Cox and co-workers ([2,8]) and, very recently, by T. Carson et al. ([9,10]). Since the results of Rosseland mean-free-path calculations performed by these authors sometimes differ considerably (by factors of 2-3), it is natural to analyze each of the calculation methods and compare them with the methods used by us.

In their physical formulation of the problem and in their allowance for the various effects that influence the opacity of matter, works ([2,8–10]) differ little from the present work. The main difference lies in the methods used to determine the electron wave functions of the discrete and continuous spectra, the energy levels, and the chemical potential of the electrons.

In his calculations A. Cox uses a model of constant density of free electrons, and as wave functions takes the wave functions of a hydrogen-like atom, determined with the aid of semiempirical screening constants of the Slater type. One of the principal shortcomings of these calculations consists in the use of screening constants, which strongly affect the occupation numbers of electron shells but themselves cannot be determined with sufficient reliability.

The results of T. Carson’ s calculations, which use the self-consistent Thomas-Fermi potential to find the electron wave functions, contain a number of errors. In thermodynamic equilibrium the chemical potentials of the electrons for each of the components of the mixture must be equal. The validity of this requirement is confirmed, in particular, by the fact that at the boundaries of atomic cells, where Coulomb forces do not act on the electrons, the density of free electrons, when the chemical···

···chemical potentials for each component of the mixture will be the same. T. Carson, however, takes as the equilibrium condition the equality of the total pressures at the boundary of the atomic cells created by the electrons and nuclei of each element. This leads to the density of free electrons at the boundaries of the atomic cells being discontinuous. As a result, in T. Carson’ s calculations the partial densities of substances with large atomic numbers may differ almost by a factor of two from those used by us.

The incorrectness of equating the total pressure at the boundaries of the cells also follows from the fact that the thermodynamic equilibrium of the electrons, owing to their greater velocity compared with the nuclei, is established over such time intervals during which the nuclei remain practically immobile, and one may speak of thermodynamic equilibrium of the electrons at fixed positions of the nuclei. In our calculations the motion of the nuclei is taken into account in the quasistatic approximation when considering the shift of energy levels due to the Stark effect caused by the electric fields of neighboring ions.

The computational methods used in (9, 10) are comparatively cumbersome, and errors of a computational nature occur in the calculations.

We present the results of calculations of the opacity for astrophysical mixture I from (9), showing the influence of different approaches in computing the Rosseland mean free path.

T	ρ	k_1	k_2	k_3
0.1	0.2017	79.86	225.7	86.34
0.3162	0.0626	1.779	5.180	2.126
0.3162	0.6288	8.378	11.86	8.463
0.3162	6.310	21.25	18.56	20.15
1.0	1.977	0.533	0.6461	0.5900

Here T is the temperature of the mixture in keV, ρ is the mean density of the mixture in g/cm^3; k_1, k_2, k_3 are the opacities of the mixture in cm^2/g, computed by us, by T. Carson (9), and by A. Cox (8), respectively ($k = 1/l\rho$, l is the Rosseland mean free path). Analogous results were obtained for opacities calculated without allowance for absorption in lines.

Thus, in computing the Rosseland mean free path in astrophysical mixtures, our results sometimes differ from T. Carson' s results by more than a factor of two and, as a rule, are close to A. Cox' s results.

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