HIGHLY EXCITED HYDROGEN LINES IN STELLAR SPECTRA. I

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Abstract. The solutions of the hydrogenic Schrödinger equation are given with two boundary conditions imposed on the wave function, for distances of the order of magnitude of one hundred times the Bohr radius from the central nucleus. Thus the shifts and splitting of the $H_7$-$H_{18}$ lines are given which arise from the non-vacant environment. The Inglis-Telter limit is revised since from the shifts it follows that it gives a correct charged particle density only in the case of extremely high electron and ion densities. The gas density is derived from the number of the visible Balmer lines, and usually the widths and the contours but not the coalescence include information on the charged particle density.

1. Introduction

In an earlier paper of the author (Barcza (1970), hereafter referred to as Paper I) a quantum-mechanical cellular method is described for investigating the behaviour of materials under pressure. The half empirical boundary condition

$$\frac{d\psi}{dr} \bigg|_{r=r_s} = 0$$

is applied to the Schrödinger equation of hydrogen where $r_s$ is the radius of the sphere $s$, the spherical volume occupied by an atom, and $\varphi = \varphi^* \varphi$ where $\varphi$ is the wave function, and the shift and the splitting of the levels – the equivalent of the Balmer formula – are derived. Boundary condition (1) involves the two extreme cases of the compression because (1) may be fulfilled by $\varphi(r_s)=0$ or $(d\varphi/dr)|_{r=r_s}=0$, the former is the hardest compression – i.e. made by an infinitely high potential barrier – while the latter suggests an image of a cool metal. Strictly speaking it may only be stated that the real shifts of the levels (lines) must inevitably be less than the shifts derived from $\varphi(r_s)=0$.

Boundary condition (1) is extended to dilute atomic hydrogen too and by this the density of a hydrogen plasma can be measured from its spectrum. The theoretical foundation of (1) and the detailed description of the advantages of (1) can be found in Paper I. In the present paper some possibilities of astrophysical utilization of Equation (1) will be discussed.

It is well known from quantum mechanics (e.g. Messiah, 1961) that in the class of potentials characterized in the asymptotic region by

$$\lim_{r=\infty} r^2 V(r) = -\infty,$$

there are an infinite number of bound levels approaching the ionization limit, the zero value of the energy eigenvalue; and of course having an infinite number of bound levels it is obvious that the (Bohr) radius of the atom tends to infinity too. But this is
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never realised because after reaching the range \( r \) where the wave functions of the neighbouring atoms begin overlapping each other considerably the potential \( V(r) \) is drastically perturbed by the environment; the perturbation with increasing \( r \) becomes larger than the original \( V(r) \). Certainly, the term system obtained from \( V(r) \) will be modified too if the effect of the environment is taken into account. Otherwise an infinite number of bound levels would cause divergency in the partition function, to avoid it one must take into consideration the environment of the atom. The method described in detail in Paper I solves these problems adequately.

The essence of the method outlined in this paper is to use the multiplets consisting originally \((r_s = \infty)\) of an infinite number of levels determining the averaged volume belonging to these kinds of atoms; consequently the atom number density of the stellar atmosphere may be 'guessedimated' only from a look at a spectrum obtained with moderate or slight dispersion. Observing the levels which are still in their normal place one can get some crude information about the radius of the last level. If this conception is appropriate then the shifted – or sometimes splitted – lines should be found in the spectrum too.

The two extreme shifts between which the lines must fall are hoped to be derived from boundary condition (1) because it involves the two extreme possibilities of the compression. This method is applied in detail for hydrogen because here the original \( V(r) \) of (2) gives the Balmer formula, this and the deviations from it can easily be studied. Nevertheless, the solutions are of much more general importance because the single excited states of a lot of elements are hydrogen-like. Thus the method may be applied to other species as well, but the calculations are sometimes more complicated and less accurate. Considerable success can be expected if the unperturbed level scheme \((r_s = \infty \text{ in (1)})\) can be calculated with high accuracy: the wave function which stood the test at \( r_s = \infty \) must be applied with boundary condition. If the multiplet is a single excited one (and in astrophysical cases predominantly it is) then for larger \( r_s \) values \( \psi(r) \) will practically depend only on the coordinates of one electron, if it is doubly excited then \( \psi(r) \) depends on the coordinates of two electrons and so on. (Large \( r_s \) means that \( r_s \) is greater than, let us say, decuple of the atomic radius in the ground state.)

In the curve of growth and line contour calculations one must solve the problem of the chemical composition iteratively because both the chemical composition and the structure of the stellar atmosphere are unknown. Applying the method described in the following part of this paper one is able to get direct information about the density of stellar atmospheres and sometimes the partial density of a few elements may be estimated as well.

2. Solution of the Schrödinger Equation of Hydrogen with Boundary Condition (1)

The solution described in Paper I has rather unfavourable convergency properties even at \( r_s = 60-70a_0 \) \((a_0 \text{ is the first Bohr radius})\) therefore another solution is given here (Bethe and Salpeter, 1957). This solution applies only for negative energy eigenvalues.