ON THE NEGATIVE HYDROGEN ION AND ITS ABSORPTION COEFFICIENT

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ABSTRACT

The continuous absorption coefficient of the negative hydrogen ion is discussed from the point of view of the sum rules, and it is shown that the absorption coefficient to the red of 5000 A is predominantly governed by the wave-function of the ground state of H^- at distances of the order of five times the Bohr radius from the center. It appears that the wave-functions for H^- now in use are not sufficiently accurate at these distances to provide reliable values for the absorption coefficient beyond 5000 A. Further, some objective criteria are stated which should enable the reliability of a given absorption curve to be tested.

1. It is now generally recognized that the negative hydrogen ion provides the principal source of opacity in stellar atmospheres. Consequently, some effort has been spent to evaluate its continuous absorption coefficient. The most recent of such attempts is that of R. E. Williamson,[1] who derived for this purpose a "sixth-order" wave-function to describe the ground state of H^- similar in form to Hylleraas' wave-function for the ground state of helium. However, when Williamson derived the theoretical color-effective temperature relations on the basis of his absorption coefficient, he found that significant discordances between the predictions of the theory and the results of observations still remained.[2] These remaining discordances all appear to result from the single fact that, contrary to what can be inferred from the observations, the theoretical continuous absorption coefficient decreases in the spectral region from 5000 to 7000 A. Moreover, it is clear that, if we could in some way shift the maximum of the absorption coefficient from its present position at 5000 A to somewhere in the region of 7000 A, we should probably be able to remove all the principal discrepancies which now exist between theory and observation. In view of this, we have for some time past been wondering if certain objective criteria could not be established which would enable one to specify the extent to which a computed continuous absorption coefficient of H^- can be relied upon. We have now found that such criteria can be given in terms of the so-called "sum rules."[3] And, moreover, an examination of Williamson's absorption coefficient on the basis of the criteria established discloses certain other features which throw doubt on his values for the absorption coefficient.

2. First consider his formula for the matrix element μ_z (W, eq. [50]) which enters in the expression for the atomic absorption coefficient k_ν (W, eq. [11]). It will be noticed that in this formula there occurs a term, namely, $(4\rho_3 k \cos 5\xi_1 - \sin 4\xi_1)$ which has $(\gamma + \epsilon + \zeta)$ as a factor. On evaluating the matrix element μ_z for the wave lengths of $\lambda = 5000, 6000,$ and 10,000 A, it was found that the term involving $(\gamma + \epsilon + \zeta)$ alone contributed as much as 84, 87, and 93 per cent, respectively, toward its entire value. This fact has an important interpretation. It is that the absorption coefficient of H^- at these wave lengths depends dominantly on the value of the wave-function of the ground state of H^- at relatively large distances from the center of the ion. This becomes evident when it is noted that $(\gamma + \epsilon + \zeta)$ occurs precisely as the coefficient of the term r^6 in the charge

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[1] *Ap. J.*, **96**, 438, 1943. This paper will be referred to as "W."

[2] *Ap. J.*, **97**, 51, 1943; see particularly Fig. 6 in this paper.

[3] Cf. H. Bethe, *Handb. d. Phys.*, XXIV, Part I, 434–439, Berlin, 1933.

distribution of H^-, which for the wave-function used by Williamson has the form (Cf. W, Appen., eq. [3'])

$$-\frac{dZ}{dr} = \sum_{i=1}^{6} a_i r^i e^{-2ar} + \sum_{j=1}^{4} b_j r^j e^{-4ar}. \tag{1}$$

This raises at once the question as to how reliable Williamson's wave-function for the ground state of H^- is at distances of the order of four or five times the Bohr radius from the center of the ion.[4] It appears that we can settle this question in the following manner:

For any quantum mechanical system we have

$$\sum_j |(i|\boldsymbol{R}|j)|^2 = (i||\boldsymbol{R}|^2|i) \tag{2}$$

for any initial state i and where the summation over the j's is extended over all the final states. Further,

$$\boldsymbol{R} = \sum_{l=1}^{n} \boldsymbol{r}_l \tag{3}$$

for an n-electron system. In the case of H^- we have a two-electron system with most probably only a single discrete state.[5] Consequently, the summation on the left-hand side reduces in this case to an integral over the continuous absorption coefficient (due allowance being made for the passage from a discrete to a continuous spectrum). In this manner we find that

$$(1|r_1^2 + r_2^2|1) = 3Ry a^2 \frac{mc}{\pi e^2} \int_{\nu_0}^{\infty} \frac{k_\nu}{\nu} d\nu, \tag{4}$$

where a stands for the radius of the first Bohr orbit for the hydrogen atom, Ry for the Rydberg frequency, ν_0 denotes the frequency of the absorption limit, and the rest of the symbols have their usual meanings. (In eq. [4] we have used "1" to denote the ground state of H^-.) The matrix element which occurs on the left-hand side of equation (4) can properly be regarded as defining the mean-square radius of the negative hydrogen ion; and we shall, accordingly, denote it by $\overline{r^2}$. After some transformations we find that equation (4) can be expressed in the form

$$\overline{r^2} = 3.716 a^2 \int_0^{17.2} \frac{a_x}{x} dx, \tag{5}$$

where a_x denotes the atomic absorption coefficient in units of 10^{-17} cm² and x the wave length expressed in units of 1000 A.

The mean-square radius $\overline{r^2}$ can be readily evaluated from the formula for the charge distribution given by Williamson (W, Appen., eq. [4']). On evaluating this quantity it was found that the term in r^6 (cf. eq. [1]) contributed over 50 per cent to the total value. More particularly, while it was found that

$$\overline{r^2} = 19.21 a^2, \tag{6}$$

[4] That we are concerned with the value of the wave-function at these distances is evident from eq. (6) below.

[5] It is extremely unlikely that H^- has an excited state which is discrete. For discussions on these and related matters we are greatly indebted to Dr. E. Teller.

the term in r^6 alone contributed as much as 11.02 a^2. This again confirms our earlier indications that, while Williamson's wave-function for H^- is probably sufficiently accurate to determine the energy of the ground state, it does not provide the necessary accuracy at distances of the order of four to five times the Bohr radius and, consequently, is inadequate to determine the absorption coefficient, particularly beyond 5000 Å, to an accuracy demanded by astrophysical theory.

We may also note in this connection that a direct numerical evaluation of the right-hand side of equation (5), using Williamson's absorption coefficient, gave 17.1 a^2. The closeness of the agreement of this value with 19.2 a^2 should not, however, be allowed to mislead one's judgment, for the absorption coefficient beyond 5000 A contributes less than 50 per cent to the integral and, moreover, is divided in these regions by factors exceeding 5.

3. There is another sum rule—namely, the more familiar f-rule—which can also be used to test the reliability of a computed absorption curve for H^-. Assuming again that H^- has no discrete excited states, the f-rule reduces to

$$\frac{m\,c}{\pi e^2}\int_{\nu_0}^{\infty} k_\nu d\nu = 2 \;,\tag{7}$$

or, somewhat differently, to

$$1.1303\int_0^{17.2} \frac{a_x}{x^2}\,dx = 2 \;,\tag{8}$$

where a_x and x have the same meanings as in equation (5). A numerical integration over Williamson's absorption coefficient gave for the left-hand side of equation (8) the value of 1.70; and this has to be compared to the value to be expected theoretically, namely, 2. This discrepancy to the extent of 15 per cent is again somewhat serious, since the dominant contribution to the integral on the left-hand side of equation (8) comes from the spectral regions to the violet of 5000 A, while over 50 per cent comes from regions with wave lengths less than 3000 A. All this amounts to simply this: Williamson's absorption coefficient cannot be relied upon in the spectral regions to the red of 4500 A; and, more particularly, the dependence on the wave length in these regions can be seriously in error.

4. While our discussion in the earlier paragraphs has largely been of a destructive nature, we may be allowed to draw attention to the objective criteria which have been disclosed, first, for establishing whether a given wave-function for the ground state of H^- has the necessary accuracy to yield reliable absorption coefficients in the visual and the red regions of the spectrum and, second, for estimating the over-all accuracy of the computed absorption coefficients. Regarding the first, it may be stated that the absorption coefficient due to H^- in the region beyond (i.e., to the red of) 5000 A depends decisively on the value of the wave-function of the ground state of H^- at distances of the order of five times the Bohr radius from the center. The reliability of the wave-function at these distances can be measured by the contribution to the value of $\overline{r^2}$ by the term involving the highest power of r in the charge distribution and verifying that the term in the matrix element μ_z which occurs with the same coefficient as the highest power of r in the charge distribution does not make a significant contribution to its value in the spectral region of astrophysical interest. Once these conditions have been met, the over-all accuracy of the computed absorption coefficient can be readily estimated from the extent to which the relations (5) and (8) are satisfied.

5. So far we have concerned ourselves only with the wave-function representing the ground state of the negative hydrogen ion. However, in computing the matrix element

μ_z a further approximation is generally introduced, namely, that the state after the absorption of the light quantum is described by a wave-function of the form[6]

$$\frac{1}{\sqrt{2\pi}}\left(e^{-r_2+i\,p\cdot r_1}+e^{-r_1+i\,p\cdot r_2}\right),\qquad(9)$$

where p denotes the momentum of the free electron. In other words, we ignore the distortion of the plane wave-functions caused by the presence of the hydrogen atom. It seems to us that this approximation cannot introduce any serious error in the computed absorption coefficients. For, in addition to the arguments advanced by Massey and Bates in favor of this approximation, the following circumstance appears to us as relevant to the problem: As we have seen, in the spectral region which is of particular astrophysical interest, the controlling factor, as far as the initial state is concerned, is the value of the wave-function of H^- at distances of the order of five times the Bohr radius from the center of the ion. But it is clear that at such distances from the center of a hydrogen atom in the ground state the distortion of the plane wave-functions representing the free electrons cannot be very significant. And, in any event, the extent to which the relations (5) and (8) are satisfied will enable us to estimate the over-all accuracy of the computed absorption coefficient.

[6] Cf. Massey and Bates, *Ap. J.*, **91**, 202, 1940; also Williamson, *loc. cit.*