THE 1s 2s STATES OF NEGATIVE HYDROGEN

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(Received 7 July, 1969)

Abstract. Term values for the 1s 2s states of H⁻ are calculated with the use of simple eigenfunction approximations constructed on the basis of available Hartree-type functions for the 1s⁰ and 2s⁰ states of the ion. The results seem to support a tentative identification of the interstellar diffuse absorption bands at λ 4890 and λ 6 as due to negative hydrogen.

Hartree-Fock type eigenfunctions for the ground 1s² and the doubly excited 2s² and 2p² states of negative hydrogen have been found by one of the authors (Ingemann-Hilberg, 1970) in an investigation of H⁻ states. The feasibility of solving the equations for this type of eigenfunctions seems to be due to the identity of the two radial functions in these cases.

For the purpose of calculating the position of the energy levels of the singly excited 1s 2s states we shall use the following approximation to the eigenfunctions for these states

\[ P(r_1, r_2) = \frac{1}{\sqrt{2}} (P_{1s}(r_1) P_{2s}(r_2) \pm P_{2s}(r_1) P_{1s}(r_2)), \]  

(1)

where \( P_{2s}(r) \) is a linear combination of the functions \( P_{1s}(r) \) and \( P_{2s}(r) \), which enter the Hartree-type approximations

\[ P_{1s}(r_1) P_{1s}(r_2) \quad \text{and} \quad P_{2s}(r_1) P_{2s}(r_2) \]

(2)

to the eigenfunctions for the 1s² and 2s² singlet S states. The distances of the electrons from the proton are denoted by \( r_1 \) and \( r_2 \). The reason for using the ground state function \( P_{1s}(r) \) as one of the functions entering the Expression (1) is that the orthogonality condition

\[ \int_0^\infty P_{1s}(r) P_{2s}(r) \, dr = 0, \]

(3)

which is necessary for the use of (1) for the triplet case, automatically makes the eigenfunction approximation orthogonal to that for the ground state, such as it has to be in the singlet case. The orthogonality condition, in combination with the usual normalization of the radial functions, determines \( P_{2s}(r) \) uniquely. We find

\[ P_{2s}(r) = (1 - A^2)^{-1/2} \left( P_{2s}(r) - A P_{1s}(r) \right), \]

(4)

where
\[ A = \int_0^\infty P_{1s}(r) P_{2s}(r) \, dr. \] (5)

The eigenfunction approximations to all three singlet S states here considered become mutually orthogonal if we take
\[ P_2(r_1) P_2(r_2) \] (6)
as the function for the 2s^2 state instead of the Hartree-Fock approximation. The use of the Expression (6) makes the calculated energy of the ion in that state correspond closely to the position found by Holøien (1958) for the 2s^2 level (Ingemann-Hilberg, 1970).

Then an alternative argument for introducing the function \( P_2(r) \) as given by (4) and (5) into the approximation to the 1s 2s eigenfunction is that (1) is the only expression based on the available spherically symmetric one-electron s functions, which has the correct symmetry and which is orthogonal to the eigenfunctions used for the two other singlet S states considered.

An inclusion of terms belonging to eigenfunction approximations for other states of the ion might be considered. However, as the functions in question may be expected to correspond to electron configurations with low densities in the central part of the ion, such higher approximations will be less important for the energy calculations than for the calculation of transition probabilities.

A reason for the use of functions that belong to states of negative hydrogen, instead of for instance neutral hydrogen eigenfunctions, is that the H^- functions may be expected to behave in a more correct way for large values of \( r \). We may also expect, with the use of eigenfunction approximations of the same general type for all the states considered, instead of a combination of Hartree-type functions for the excited states with a more advanced approximation to the ground-state function, that errors in the expressions for the energy may cancel to some degree in the term differences in which we are in fact more interested than in absolute energy values.

We calculate the energy of the states described by the eigenfunction approximation (1) as the corresponding mean value of the Hamilton operator
\[ H = -\frac{1}{2}(A_1 + A_2) - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}}. \] (7)

This is, in our case, equal to
\[ \int_0^\infty \int_0^\infty PHP \, dr_1 \, dr_2, \] (8)
because our function \( P(r_1, r_2) \) is real.

This procedure is based on the usual argument that any reasonably good approxima-