wert. Diese Abweichung ist darauf zurückzuführen, daß einmal mit diesem Verfahren die Dissoziationsprodukte nicht berechnet werden können, zum anderen dürfte dadurch auch die Korrelationsenergie in stärkerem Maße vom Kernabstand abhängen.

Zur Interpretation der Formel (1) kann folgendes gesagt werden. In der Regel erhält man mit dem SCF-Verfahren dann gute Bindungsenergiewerte, wenn auch die Dissoziationsprodukte mit dem gleichen Verfahren berechnet werden können, was soviel bedeutet, daß die rechnerische Genauigkeit beim Molekül sowie bei den Dissoziationsprodukten ziemlich gleich ist und bei der Bildung der Bindungsenergie die beiden Fehler sich nahezu kompensieren. Das gleiche ist auch in (1) geschehen, denn die methodischen Fehler bei $\varepsilon(F_2)$ und $\varepsilon(F^-) - J_{\exp}(F^-)$ sind ebenfalls von gleicher Größenordnung, indem von der Energie des F^- der experimentelle Wert der Ionisierungsenergie abgezogen wird. Mit anderen Worten, nach (1) ist an Stelle von $\varepsilon(F)$ eine Energie eingesetzt worden, die in der Güte einer SCF-Energie des Fluoratoms entspricht, indem die Größe

$$2\,\varepsilon(F^-) - 2\,J_{\exp}(F^-) \qquad (2)$$

für die Dissoziationsprodukte eingesetzt wurde.

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An Analytical Formula for Continuous Absorption Coefficient for Negative Hydrogen Ion

T. TIETZ

Department of Theoretical Physics, University of Łódź, Łódź-Poland

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The paper deduces an analytical expression for the continuous absorption coefficient of H^-. As known H^- absorption plays an important role in many stellar atmospheres. The coefficient has been calculated by several authors [1–13] the most accurate numerical calculations being of CHANDRASEKHAR [10] and JOHN [12].

The previous theoretical calculations have been carried out with many parameter ground states wave functions e. g. CHANDRASEKHAR and ELBERT used a HART and HERZBERG 20-parameter ground state wave function and a Hartree approximation for the continuum wave function.

A very simple expression for the coefficient has also been given by the author [13]. In order to derive an analytical expression for the continuous absorption coefficient of H^- we use the following ansatz for the 2-electron wave function which destribes the bound state of H^- ion, namely:

$$\Psi_b(r, r') = \varphi_0(r)\ \varphi_1(r') \qquad (1)$$

where

$$\varphi_1(r') = \frac{1}{\sqrt{\pi}}\, e^{-r'} \qquad (2)$$

is the 1s-function of neutral hydrogen. Exchange is neglected. The choice of ansatz (1) with φ_1 given by Eq. (2) leads to the following differential equation for φ_0:

$$[\nabla^2 - 2\,V(r) + 2\,E_0]\ \varphi_0 = 0\,. \qquad (3)$$

This equation is written in atomic units and $2\,|E| = k_0^2$; E_0 is the bound state having an energy equal in magnitude to the acepted electron affinity of hydrogen atom. The potential appearing in the last equation is known and given by:

$$V(r) = -e^{-2r}(1 + 1/r)\,. \qquad (4)$$

Since Eq. (3) cannot be solved exactly if $V(r)$ is given by the last equation we adopt for $V(r)$ the following approximate potential:

$$V(r) = -\frac{b\,e^{-ar}(1 + d\,e^{-ar})}{(1 - e^{-ar})\,(1 + c\,e^{-ar})} \qquad (5)$$

where a, b, c and d are constants. Our approximate potential $V(r)$ has the advantage that with it one can solve exactly the Schrödinger Eq. (3) and obtain the ground state wave function

$$\varphi_0(r) = \frac{N_0}{2\sqrt{\pi}}\,\frac{e^{-k_0 r}(1 - a^{-ar})\,(1 + c\,e^{-ar})}{r} \qquad (6)$$

where

$$b = \frac{a}{2}\,(1 - c)\,(2\,k_0 + a) \quad \text{and} \quad d = \frac{4\,c\,(k_0 + a)}{(1 - c)\,(2\,k_0 + a)} \qquad (7)$$

and N_0 is the radial normalization constant given by

$$N_0^2 = \left[\frac{2\,(k_0 + a)}{a^2}\right] \cdot \left[\frac{k_0\,(2\,k_0 + a)\,(2\,k_0 + 3\,a)\,(k_0 + 2\,a)}{2\,k_0 + 3\,a)\,(k_0 + 2\,a) + 4\,c\,k_0\,(k_0 + 2\,a) + c^2\,k_0\,(2\,k_0 + a)}\right]. \qquad (8)$$

[1] C. K. JEN, Phys. Rev. **43**, 540 [1935].
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The best values for the electron affinity of the hydrogen atom are given by JOHN [12] and PEKERIS [14].

In order to obtain the numerical values of the constants a and c appearing in φ_0 given by Eq. (6) we require that our approximate potential given by Eq. (5) together with Eq. (7) is as close as possible to the exact potential.

In Table 1 we have compared the approximate potential given by Eq. (5) with the exact Hartree potential of the hydrogen atom given by Eq. (4) for two sets of parameters: $a=8\,k_0$, $c=-0.125$ where $k_0=0.2356$ is taken from PEKERIS [14], and $a=2.40$, $c=-0.15$.

r	$-V(r)$ [Eq. (4)]	$-V(r)$ [Eq. (5)]	
		$a=8\,k_0$ $c=-0.125$	$a=2.40$ $c=-0.15$
0.00			
0.01	99.00	90.89	101.75
0.02	49.00	45.44	51.10
0.03	32.33	30.28	34.27
0.04	24.00	22.70	25.72
0.05	19.00	18.14	20.62
0.06	15.67	15.09	17.21
0.08	11.50	11.28	12.92
0.09	10.12	10.02	11.48
0.10	9.01	8.98	10.32
0.20	4.02	4.33	4.99
0.30	2.38	2.73	3.11
0.40	1.57	1.92	2.13
1.00	0.27	0.33	0.38
2.00	0.028	0.053	0.033
	0.000	0.000	0.000

Table 1. A comparison of the approximate potential $V(r)$ given by Eq. (5) with the exact one given by Eq. (4).

Table 1 shows that the approximate potential $V(r)$ given by Eq. (5) in case $a=2.40$, $c=-0.15$ fits the exact potential $V(r)$ given by Eq. (4) better for small and larger values of r than the approximate potential in case $a=8\,k_0$ and $c=-0.125$ which approximates better the exact $V(r)$ for intermediate values of $0\leqq r<2$. The simple analytical form of $\varphi_0(r)$ may be used to calculate the total absorption coefficient $\varkappa_\nu$ which can be written in the form [8]

$$\varkappa_\nu=\frac{32\,\pi^2}{3}\,\alpha_0\,a_0^2\left(\frac{k_0+k^2}{k}\right)\left|\int_0^\infty\varphi_0(r)\,x_1(r)\,r^2\,\mathrm{d}r\right|^2 \qquad (9)$$

where a_0 is the Bohr radius, α is the fine structure constant $k^2=2\,E_k$ where E_k is the continuum state energy.

Between the frequency ν, E_0 and E_k there exists the well known relation $E_0-E_k=h\,\nu$. The partial wave x_1 in the last equation is the wave which contributes to the dipole matrix element in the p-wave. Since 1p-phase shifts δ are small so we do not make a great error if we adopt for x_1 the solution of the Schrödinger equation for $V=0$, which is known and can be written in the following form

$$x_1=\frac{\sin k\,r}{k\,r}-\cos k\,r\,. \qquad (10)$$

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Substituting $\varphi_0(r)$ given by Eq. (6) and $x_1(r)$ given by the last formula in Eq. (10) for $\varkappa_\nu$ we obtain the following expression

$$\varkappa_\nu=\frac{32\,\pi\,\alpha_0\,a_0^2}{3}\left(\frac{k}{k_0+k^2}\right)^3 N_0^2\left\{1\left(\frac{k_0^2+k^2}{(k_0+a)^2+k^2}\right)^2+c\left(\frac{k_0+k^2}{(k_0+a)^2+k^2}\right)^2\left[1-\left(\frac{(k_0+a)^2+k^2}{(k_0+2\,a)^2+k^2}\right)^2\right]\right\}. \qquad (11)$$

In Table 2 we have compared our numerical values of $\varkappa_\nu$ (10^{-17} cm^2) calculated from the last Eq. as a function of k^2 for $a=8\,k_0$, $c=-0.125$, and $a=2.40$ and $c=-0.15$ with the coresponding results of CHANDRASEKHAR and ELBERT's [10].

k^2	$\varkappa_\nu$ (10^{-7} cm^2) Eq. (11)			CHANDRASEKHAR and ELBERT
	$a=8\,k_0$ $c=-0.125$	$a=2.40$ $c=-0.15$		
0	0	0	0	
0.010	1.64	1.54	—	
0.020	3.04	2.84	2.83	
0.030	3.84	3.52	—	
0.035	4.08	3.61	4.03	
0.045	4.34	4.06	4.37	
0.050	4.40	4.11	4.45	
0.055	4.42	4.12	4.49	
0.060	4.41	4.11	—	
0.070	4.33	4.04	4.41	
0.080	4.20	3.92	—	
0.090	4.04	3.79	4.09	
0.100	3.88	3.63	3.90	
0.125	3.46	3.24	3.41	
0.175	2.75	2.66	2.30	
0.250	2.00	1.89	1.83	
0.500	0.93	0.88	0.75	
0.800	0.50	0.48	0.34	

Table 2. A comparison of the numerical values of $\varkappa_\nu$ in our and CHANDRASEKHAR and ELBERT's results [10].

Table 2 shows that our approximate values of $\varkappa_\nu$ calculated from Eq. (11) if $a=8\,k_0$, $c=-0.125$ give quite good results in comparison with Chandrasekhar and Elbert. The numericial values of $\varkappa_\nu$ for $a=2.40$, $c=-0.15$ are lower than the ones for $a=8\,k_0$ and $c=-0.125$. Since the results of SMITH and BURCH [11] for $\varkappa_\nu$ are lower than the corresponding results of CHANDRASEKHAR and ELBERT our numerical values of $\varkappa_\nu$ for $a=2.40$ and $c=-0.15$ agree better with these results than the corresponding results $a=8\,k_0$ and $c=-0.125$.

The simple analytical form for $\varphi_0(r)$ may be used for practical calculations concerning some physical problems connected with H^-, e. g. for caculation of the total cross-section, detachment from the negative hydrogen ion by electron or positron impact [15] and other problems.

The derivation of the analytical approximate formula for $\varkappa_\nu$ given by Eq. (10) did not respect the exchange. The use of the experimental energy for E_0 in Eq. (3) makes up for this short-coming to some extent.

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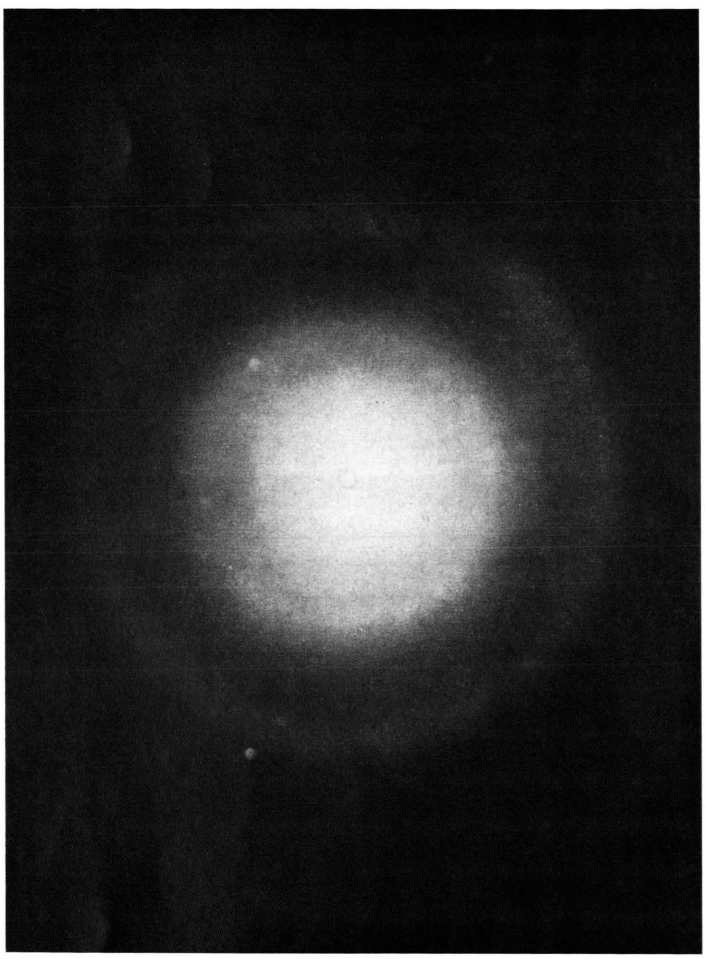

Abb. 1. Beugungsbild der [111]-Zone des kubisch-flächenzentrierten Gitters eines β-Barium-Einkristalles, zusammen mit schwachen Debye-Scherrer-Ringen kleinerer, regellos orientierter Kristalle ($E=80$ keV; $\lambda_E=0{,}0418$ Å; elektronenoptische effektive Beugungslänge $l=587$ mm).