being indeed singular, as shown by Eq. (75)]. On the other hand k_0 must not be too small. We get superlattice reflections only if $2k_0 > \tau_s$. Both requirements may be satisfied if $\tau_s < 2Mc/\hbar$. Expressing J in terms of the Néel temperature of the pure material by the approximate relation $4|J|S(S+1)=k_BT_N$ we find that this condition may be written

$$\rho=\frac{k_BT_NMa^2}{(S+1)\hbar^2}>\frac{\pi}{2}. \tag{78}$$

Taking $a=3$ A, $T_N=80$°K and $S=\frac{5}{2}$ we get $\rho=7$, so that the inequality (78) seems easy to satisfy. In our example, the experiment is feasible with neutron wavelengths $2\pi/k_0$ between 1.5 and 3 A.

Our formula (71) was restricted to cases where the deflection $\epsilon=\epsilon_1=-\epsilon_2$ on the perturbed sites was small. In practice this is not the case, and (71) does not apply. However, it is always a good approximation to assume that all deflections other than ϵ_1 and ϵ_2 are indeed small. It may then be shown that the simple solution (71) is still acceptable provided that we replace ϵ by $\sin\epsilon$. With this slight modification all the later formulas also retain their validity.

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Electron-Hydrogen Scattering at Low Energies

TAKASHI OHMURA* AND HARUKO OHMURA†
Division of Pure Physics, National Research Council, Ottawa, Canada

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The effective range in the singlet electron-hydrogen system has been evaluated as 2.646±0.004 atomic units by using the asymptotic amplitude of the 202-parameter H$^-$ wave function of Pekeris. This value of the effective range, together with the value of the electron affinity of H$^-$, determines the scattering length in the singlet system as 6.167 atomic units. The effective range in the triplet system is calculated to be 1.219 atomic units by a Hartree-Fock approximation. It is shown that the effective-range approximation is very good for all energies at which only elastic scattering is allowed. The photo-ionization of H$^-$ is briefly discussed on the basis of the effective-range theory.

I. INTRODUCTION

THE low-energy scattering of an electron by a hydrogen atom is described by four parameters, the scattering lengths a_+ and a_- and the effective ranges r_{0+} and r_{0-}. $+$ refers to the singlet system and $-$ the triplet system. The s phase shift is given, in the so-called effective range approximation, by

$$k\cot\eta_\pm=-(1/a_\pm)+(r_{0\pm}/2)k^2+O(k^4). \tag{1a}$$

The s scattering in the singlet system is also described by the electron affinity $(\gamma^2/2)$ of H$^-$ and by the effective range ρ at the ion state.

$$k\cot\eta_+=-\gamma+\tfrac{1}{2}\rho(\gamma^2+k^2)+O[(\gamma^2+k^2)^2]. \tag{1b}$$

Detailed variational calculations for the phase shifts have been carried out by Massey and Moiseiwitsch[1] among others[2] by taking into account the effect of the polarization. It has been found[3] recently that Massey-Moiseiwitsch's results are well reproduced by the effective range approximation (1a) and (1b) even for quite high energies, ($k^2\lesssim 1$). The most reliable values hitherto obtained for the low-energy parameters may be summarized as follows:

$a_+=6$—7,[3,4] $a_-=2.33$—2.34,[4,5]

$\rho=2.4_4$—2.6,[3] $r_{0-}=0.8$—1.3.[6,5]

The atomic units are used throughout this paper.

The effective range ρ of the singlet system will be evaluated in II by using the asymptotic amplitude of the Pekeris wave function for the negative hydrogen ion state with 202 adjustable parameters. In III the triplet effective range will be computed in the so-called exchange approximation. In IV a discussion is given of the comparison with Massey and Moiseiwitsch's result and the experimental data, and of the bound-free transition of the negative hydrogen ion.

II. EVALUATION OF ρ BY THE PEKERIS WAVE FUNCTION

Recently Pekeris[7] has succeeded in obtaining very accurate wave functions for the ground states of two-

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[*] National Research Council Postdoctorate Fellow on leave of absence from Department of Physics, University of Tokyo, Tokyo, Japan.

[†] National Research Council Guest Worker on leave of absence from Department of Physics, University of Tokyo, Tokyo, Japan.

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TABLE I. Values of $\psi(r)$, $\rho(r)$, and related functions. $(-n)$ means $\times 10^{-n}$.

r	6	8	10	12	14	16	20
$\psi^{203}(r)$	4.93681(−3)	2.36321(−3)	1.18833(−3)	6.19715(−4)	3.32182(−4)	1.81348(−4)	5.66142(−5)
$\psi^{161}(r)$	4.93809(−3)	2.36265(−3)	1.18903(−3)	6.19846(−4)	3.31666(−4)	1.81325(−4)	5.68303(−5)
$\rho^{203}(r)$	2.5360	2.6101	2.6323	2.6402	2.6458	2.6440	2.6483
$\rho^{161}(r)$	2.5369	2.6093	2.6342	2.6409	2.6408	2.6436	2.6604
$\dfrac{\psi^{161}(r)-\psi^{203}(r)}{\psi^{203}(r)}$	2.60 (−4)	−2.39 (−4)	5.93 (−4)	2.13 (−4)	−15.53 (−4)	−1.26 (−4)	38.17 (−4)
$\dfrac{\psi^{203}(r+2)}{\psi^{203}(r)}-\dfrac{\varphi(r+2)}{\varphi(r)}$[a]	104.9 (−4)	34.3 (−4)	12.80 (−4)	9.38 (−4)	−3.05 (−4)	4.18 (−4)[b]	
$\dfrac{\psi^{161}(r+2)}{\psi^{161}(r)}-\dfrac{\varphi(r+2)}{\varphi(r)}$	102.5 (−4)	38.5 (−4)	10.82 (−4)	−0.08 (−4)	4.75 (−4)	16.49 (−4)[b]	
$0.125874\varphi(r)$	5.10385(−3)	2.38963(−3)	1.19341(−3)	6.20840(−4)	3.32203(−4)	1.81461(−4)	5.65736(−5)

[a] $\varphi(r)=e^{-\gamma r}/r$.
[b] $[\psi(20)/\psi(16)]-\varphi(20)/\varphi(16)$.

electron atoms. The effective range[3] ρ of electron-hydrogen scattering derived from the asymptotic amplitude of Hart and Herzberg's function,[8] 2.4_4—2.6, will be revised in the present section by using the Pekeris wave function of the negative hydrogen ion H⁻.

Let $\psi(\mathbf{r}_1,\mathbf{r}_2)$ be the normalized wave function of H⁻. If we define $C(r)$

$$\psi(\mathbf{r}_1=0,\ |\mathbf{r}_2|=r)=\psi(|\mathbf{r}_1|=r,\ \mathbf{r}_2=0)$$
$$\equiv\psi(r)=C(r)e^{-\gamma r}/r,$$

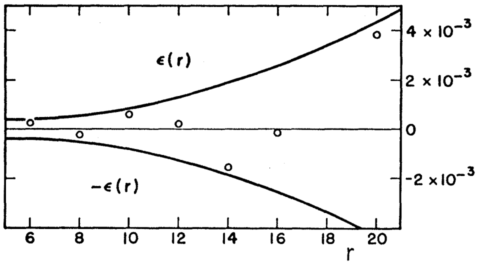

FIG. 1. $[\psi^{161}(r)-\psi^{203}(r)]/\psi^{203}(r)$ is indicated by open circle. An estimated limit of (error of ψ^{161})/ψ^{161} is shown by $\pm\epsilon(r)$.

it has been shown[5] that $C(r)$ converges to a constant value, $C(\infty)$, at large distances. $\gamma^2/2$ is the electron affinity. According to the variational calculation[7] by Pekeris with 202 adjustable parameters, we have

$$\gamma=0.2355883. \tag{2}$$

The effective range is then expressed by,[5]

$$\rho=(1/\gamma)-1/4\pi^2C^2(\infty).$$

For convenience in the later discussions, we introduce the function $\rho(r)$ by

$$\rho(r)=(1/\gamma)-1/4\pi^2C^2(r). \tag{3}$$

$\psi(r)$ is evaluated for the 161-term and 203-term wave functions of Pekeris. The values are tabulated in the first and the second rows of Table I. The values of $[\psi^{161}(r)-\psi^{203}(r)]/\psi^{203}(r)$ in the fifth row may give us a rough idea of the accuracy of $\psi^{161}(r)$. An estimated limit of error of $\psi^{161}(r)$ is given in Fig. 1 by $\epsilon(r)$, which means that

$$|\Delta\psi^{161}(r)/\psi^{161}(r)|\lesssim\epsilon(r).$$

The sixth and seventh rows indicate that $\psi(r)$ approaches very closely its asymptotic form $C(\infty)\varphi(r)=C(\infty)e^{-\gamma r}/r$ at $r=10\sim12$, but the discrepancy between two values for ψ^{161} and ψ^{203} at $r\geqq12$ may be attributed to the inaccuracies of the variational wave functions for $r\geqq12$. This may be seen from Fig. 2 more clearly. The values of $\rho(r)$ calculated by (3) are tabulated in the third and fourth rows of Table I, and also plotted in Fig. 3. The bar indicates the limit of error of ρ^{161} corresponding to $|\Delta\psi^{161}/\psi^{161}|=\epsilon(r)$, namely,

$$\Delta\rho^{161}(r)\sim3.2\epsilon(r).$$

The error in ψ^{203} may be smaller than that in ψ^{161}. Assuming that ψ approaches its asymptotic form practically at $r=14$—16, we may safely set,

$$\rho=\rho(\infty)=2.646\pm0.004. \tag{4}$$

The corresponding $C(\infty)$ is 0.125874. The asymptotic function is shown in the last row. The scattering length of the singlet system can be obtained from (4), (2), and (1b), if the third term in the right side of (1b) can

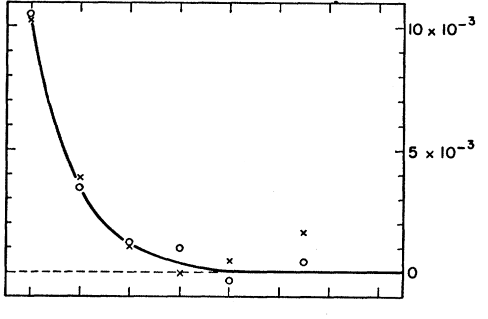

FIG. 2. The open circles represent $[\psi^{203}(r+2)/\psi^{203}(r)]-\varphi(r+2)/\varphi(r)$, and the crosses represent the corresponding ones for ψ^{161}. It can be seen that ψ approaches to its asymptotic form practically at $r=14$.

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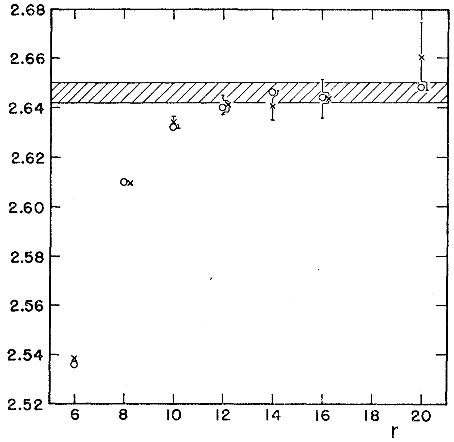

FIG. 3. $\rho^{203}(r)$ is indicated by open circles, and $\rho^{161}(r)$ by the crosses. An error limit of $\rho^{161}(r)$ is shown by the vertical bar. The effective range ρ is estimated to be between 2.642 and 2.650.

be neglected. The calculated value is

$$a_+=6.167. \quad (5)$$

III. EXCHANGE APPROXIMATION

The s phase shift in the singlet system has been expressed by two parameters, $\gamma=0.2355883$, $\rho=2.646$, in the low-energy region. On the other hand, the triplet s scattering is described by (1a)

$$k\cot\eta_-=-(1/a_-)+(r_{0-}/2)k^2+O(k^4).$$

The scattering length a_- is estimated as 2.33 [4] and 2.34 [5] by extrapolating the Massey and Moiseiwitsch result to the zero energy limit assuming linear and quadratic formulas for $k\cot\eta_-$, respectively. The effective range r_{0-} has been calculated as 0.808 by a variational method with an energy-dependent approximate function,[6] and as 1.29 with an approximate zero energy function by the formula,[5]

$$r_{0-}=\frac{1}{4\pi}\int_0^\infty (u_0^2-\psi_0^2)d\tau_1 d\tau_2+8\left(1-\frac{2}{a_-}\right)^2, \quad (6)$$

where

$$u_0=\frac{e^{-r_1}}{\sqrt{\pi}}\left(\frac{1}{r_2}-\frac{1}{a_-}\right)-\frac{e^{-r_2}}{\sqrt{\pi}}\left(\frac{1}{r_1}-\frac{1}{a_-}\right),^{9}$$

and the zero energy wave function ψ_0 must be normalized according to

$$\psi_0\to\frac{e^{-r_1}}{\sqrt{\pi}}\left(\frac{1}{r_2}-\frac{1}{a_-}\right); \qquad (r_2\to\infty)$$

$$\to\frac{e^{-r_2}}{\sqrt{\pi}}\left(\frac{1}{r_1}-\frac{1}{a_-}\right); \qquad (r_1\to\infty).$$

In both calculations of r_{0-} the polarization effect has not been taken into account. The best wave function may satisfy a Hartree-Fock type equation so far as the polarization effect is discarded. The zero energy solution of such an equation (so called exchange approximation equation) has been integrated by Seaton[4] numerically. If we substitute his solution into (6), we get

$$r_{0-}=1.219. \quad (7)$$

This value for the effective range may not be inaccurate. because the polarization effect is not important in the triplet system. The corresponding value for the singlet system, $r_{0+}=3.019$, is not reliable. The value is really 14% larger than the accurate one, (4).

IV. COMPARISON WITH MASSEY-MOISEIWITSCH RESULTS, WITH EXPERIMENT, AND BOUND-FREE TRANSITION OF H⁻

In Fig. 4 the open circles show the values of $k\cot\eta$ calculated by Massey and Moiseiwitsch using three adjustable parameters, with the relative coordinate of the two electrons in one of the terms in the wave function. The straight lines represent the effective range approximation. Four parameters used to draw the lines are given in (2), (4), (7) and $a_-=2.33$. The straight lines are seen to fit the open circles very closely up to $k^2=1$. It is quite remarkable that the straight lines determined by the zero energy solution (or by the negative hydrogen state) represent the actual phase shifts for all energies at which only elastic scattering is allowed, namely, $0\leq k^2<0.75$. The agreement also suggests the accuracy of (5), and (7). It is thus estab-

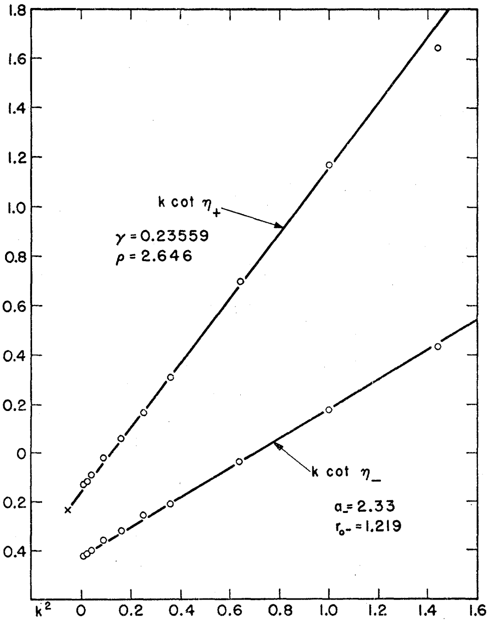

FIG. 4. Full lines represent $k\cot\eta$ in the effective range approximation. The adopted values of the low-energy parameters are given by (2), (4), (7) and $a_-=2.33$. Open circles shows the Massey and Moiseiwitsch values.

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[9] There was a slight error on this notation in reference 5.

lished especially in the low-energy region that the s phase shifts are reproduced quite accurately by the effective range approximation. The small deviations of the Massey and Moiseiwitsch values from the straight lines for $k^2<0.3$ can be attributed to inaccuracies in their trial function. The various theories including those of Massey and Moiseiwitsch and the present work are in accord with the experimental data,[10] within the experimental error, up to 10 ev.

Bethe and Longmire[11] have discussed the photo-disintegration of the deuteron on the basis of the effective range theory. Their arguments can be applied to the photo-ionization (that is, bound-free transition) of the negative hydrogen ion. Their approximate method is essentially based on the loosely bound nature of the deuteron. If a similar approximation is made on the loosely bound electron in H$^-$, the following bound-free coefficient of continuous absorption for photon frequency ν is derived

$$\kappa_\nu=\frac{6.8475\times10^{-18}\gamma k^3}{(1-\gamma\rho)(\gamma^2+k^2)^3}\ \mathrm{cm}^2, \qquad (8)$$

where k is the wave number of the ejected electron in atomic units. The result obtained from (8) is shown in Fig. 5, together with those obtained by Chandrasekhar[12] with the 20-parameter wave function of H$^-$ of Hart and Herzberg.[8] The "loosely bound" approximation (8) may be quite accurate for long wavelengths, but the good agreement with experimental data[13] suggests that it may be valid even for relatively high-energy photons, say $\lambda=6000$ A.

It has been shown[14] that the free-free transition matrix element of the negative hydrogen ion can be expressed, within an accuracy of the order of one percent, in terms of the s phase shifts of the electron-hydrogen atom scattering. Hence the continuous absorption coefficient due to the free-free transition including the exchange and the correlation effects in the s states can be calculated from a knowledge of the s phase shifts alone, which include the exchange and the correlation effects. Since we are interested in the low-energy region (e.g., $k^2=0$—0.2), the effective range approximation will provide accurate phase shifts.

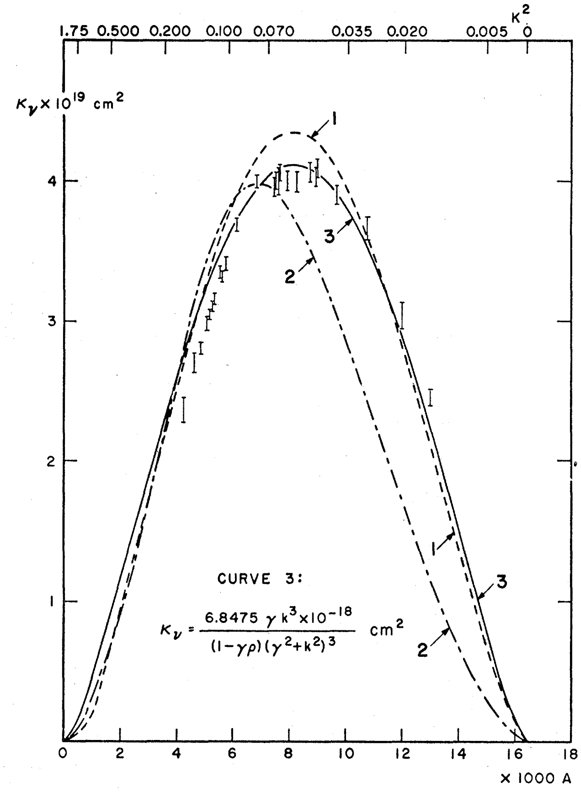

FIG. 5. Theoretical curves for the continuous absorption coefficient due to the bound-free transition of the negative hydrogen ion by (1) dipole velocity formula, (reference 12), (2) dipole length formula (reference 12) using Hart and Herzberg's 20-parameter wave function for H$^-$, and (3) the loosely bound approximation (8). Data from the laboratory experiment (reference 13) are shown by vertical lines.

The free-free transition will be discussed in a separate paper, together with the bound-free transition.

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