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Electron Capture by Alpha Particles Incident on Atomic Hydrogen

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A calculation of capture probability and the total capture cross section of the electron in the system $He^{++}+H \rightarrow He^{+}+H^{+}$ has been made taking into account the couplings of the initial state with the $1s$, $2s$, $2p_0$, and $2p_{\pm1}$ states of He^{+} ion. In the low-energy region, the numerical results for the capture probability agree partly with the experiments of Keever and Everhart. The nature of decrease of calculated total capture cross section with decreasing energy agrees well with the experimental findings of Fite, Smith, and Stebbings.

I. INTRODUCTION

The recent measurement of the capture probability of electron in the collision process $(He^3)^{++}+H \rightarrow He^{+}+H^{+}$ (in the energy range 2–200 keV) by Keever and Everhart[1] is of special interest, because of the possibility of accidental resonance in the capture process due to the equality of energy in $H(1s)$ and He^{+} ($2s$ or $2p$) states (neglecting the very small difference in the reduced masses). The measurement of total capture cross section for this process has been made earlier by Fite, Smith, and Stebbings,[2] who have covered an energy range of 0.1–36 keV. Bates and Lynn[3] in their theoretical work have indicated a qualitative difference between the cases of the accidental resonance and symmetrical resonance; the cross section of capture in the former case falls to zero in the zero-velocity limit, whereas in the latter case it approaches infinity in the same limit. The previous theoretical treatment of electron capture by α particles from the hydrogen atom by McCarroll and McElroy[4] employs a two-state approximation which includes only the initial state and the capture in the ground state of He^{+} ion. McElroy[5] has further extended the work to include with the ground state of the hydrogen atom any one of the $2s$ and $2p$ excited states of the He^{+} ion. He affirms the reliability of the results only above 100 keV and his estimation of the total cross section near 30 keV (where the experimental peak is observed) is too high. Schiff[6] has made similar calculations in the Born approximation in the energy region 100 keV–1 MeV, in which range there are no experimental data for comparison.

The availability of precise experimental findings in the low-energy region and the absence of a theoretical treatment which gives satisfactory agreement with experiment have prompted us to make a fresh theoretical approach to this problem. In the present paper we have investigated the collision process in which the electron is initially in the ground state of the target atomic hydrogen and after impact it either remains as such or is captured by the incoming α particle to form the ionized helium atom in the ground state or in any of the excited states $2s$, $2p_0$ or $2p_{\pm1}$. The electron state at any instant is given by the solution Ψ of the time-dependent Schrödinger equation. A trial wave function Ψ_T, formed as a linear combination of all possible states with coefficients as function of time only, is assumed as an approximate solution of the time-dependent Schrödinger equation. The translatory motion of the electron is neglected; this neglect is justified when the incident velocity of the α particle is small compared to the orbital velocity of the electron. Now, using a variational method proposed by Sil[7] and followed by several authors,[8–10] we minimize the variation integral and obtain a set of coupled differential equations. The solution of this set is equivalent to the solution of the Schrödinger equation.

We follow Everhart *et al.*[11] for the calculation of the impact parameter P at a fixed scattering angle and choose the mass number of α particle as 3, which allows direct comparison of our results with those of Keever and Everhart.[1]

II. THEORY

Let the α particle and the proton move with uniform velocities, with their center of mass (c.m.) at rest. Let $\mathbf{R}$ be the position vector of the α particle relative to the proton and let $\mathbf{r}_A$, $\mathbf{r}_B$, and $\mathbf{r}$ be the position vectors of the electron relative to the α particle, proton, and the c.m., respectively. Initially, the electron is bound to the proton in its ground state, $t=0$ being the time when the α particle and the proton are closest. The Hamiltonian for the motion of the electron in atomic units is given by

$$H=-\tfrac{1}{2}\nabla^2-1/r_A-2/r_B\,, \tag{1}$$

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and the variation integral which leads to the Schrödinger equation $H\Psi=i\partial\Psi/\partial t$ is given by

$$I=-\tfrac{1}{2}\int[\bar{\Psi}H\Psi+\Psi H\bar{\Psi}-i\bar{\Psi}\partial\Psi/\partial t+i\Psi\partial\bar{\Psi}/\partial t]dVdt. \quad (2)$$

We approximate Ψ by a trial wave function

$$\Psi_T=A_1(t)\psi_1+\sum_{n=1}^{5}B_n(t)\psi_n',$$

where ψ_1 represents the 1*s* state of hydrogen atom, ψ_1', ψ_2', and ψ_3' represent, respectively, the 1*s*, 2*s*, and $2p_0$ states, and ψ_4' and ψ_5' the normalized linear combination of $2p_{+1}$ and $2p_{-1}$ states (proportional to $\cos\phi$ and $\sin\phi$) of the He$^+$ ion. Substituting Ψ_T for Ψ in Eq. (2) and minimizing the variation integral for small variations of $\bar{A}_1$ and $\bar{B}_n$, we get the following set of coupled differential equations:

$$g\dot{A}=iFA, \quad (3)$$

where

$$g=\begin{pmatrix} 1 & g_{11} & g_{12} & g_{13} & g_{14} & g_{15} \\ g_{11}' & 1 & 0 & 0 & 0 & 0 \\ g_{21}' & 0 & 1 & 0 & 0 & 0 \\ g_{31}' & 0 & 0 & 1 & 0 & 0 \\ g_{41}' & 0 & 0 & 0 & 1 & 0 \\ g_{51}' & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

$$F=\begin{pmatrix} F_{11} & G_{11}+\frac{1}{2}i\dot{g}_{11} & G_{12}+\frac{1}{2}i\dot{g}_{12} & G_{13}+\frac{1}{2}i\dot{g}_{13} & G_{14}+\frac{1}{2}i\dot{g}_{14} & G_{15}+\frac{1}{2}i\dot{g}_{15} \\ G_{11}'+\frac{1}{2}i\dot{g}_{11}' & F_{11}' & F_{12}' & F_{13}' & F_{14}' & F_{15}' \\ G_{21}'+\frac{1}{2}i\dot{g}_{21}' & F_{21}' & F_{22}' & F_{23}' & F_{24}' & F_{25}' \\ G_{31}'+\frac{1}{2}i\dot{g}_{31}' & F_{31}' & F_{32}' & F_{33}' & F_{34}' & F_{35}' \\ G_{41}'+\frac{1}{2}i\dot{g}_{41}' & F_{41}' & F_{42}' & F_{43}' & F_{44}' & F_{45}' \\ G_{51}'+\frac{1}{2}i\dot{g}_{51}' & F_{51}' & F_{52}' & F_{53}' & F_{54}' & F_{55}' \end{pmatrix},$$

$$A=(A_1 \quad B_1 \quad B_2 \quad B_3 \quad B_4 \quad B_5),$$

(column vector)

in which

$$F_{mn}=\int\bar{\psi}_m\frac{2}{r_B}\psi_n dV=\bar{F}_{nm},$$

$$F_{mn}'=\int\bar{\psi}_m'\frac{1}{r_A}\psi_n'dV=\bar{F}_{nm}',$$

$$G_{mn}=\tfrac{1}{2}\int\bar{\psi}_m(1/r_A+2/r_B)\psi_n'dV=\bar{G}_{nm}',$$

$$g_{mn}=\int\bar{\psi}_m\psi_n'dV=\bar{g}_{nm}'.$$

These matrix elements have been calculated analytically after neglecting the momentum-transfer term and their final values are given below

$$F_{11}=2\left[\frac{1}{R}-\left(\frac{1}{R}+1\right)\exp(-2R)\right],\quad F_{11}'=\frac{1}{R}-\left(\frac{1}{R}+2\right)\exp(-4R),$$

$$F_{22}'=1/R-(1/R+\tfrac{3}{2}+R+R^2)\exp(-2R),$$

$$F_{33}'=F_2'+v^2t^2F_1',\quad F_{44}'=F_3'+\tfrac{1}{2}(P^2-v^2t^2)F_1',\quad F_{34}'=PvtF_1',$$

where

$$F_1'=\frac{9}{2R^5}-\left(\frac{9}{2R^5}+\frac{9}{R^4}+\frac{9}{R^3}+\frac{6}{R^2}+\frac{3}{R}+1\right)\exp(-2R),$$

$$F_2'=\frac{1}{R}-\frac{3}{2R^3}+\left(\frac{3}{2R^3}+\frac{3}{R^2}+\frac{2}{R}+\frac{1}{2}\right)\exp(-2R),$$

$$F_3'=\frac{1}{R}+\frac{3}{4R^3}-\left(\frac{3}{4R^3}+\frac{3}{2R^2}+\frac{5}{2R}+\frac{5}{2}+\frac{3R}{2}+\frac{R^2}{2}\right)\exp(-2R),$$

$$F_{12}'=\sqrt{2}\left(\frac{8}{27}+\frac{8R}{9}\right)\exp(-3R-i\epsilon t),$$

$$F_{13}'=\frac{64\sqrt{2}}{9}vt\left[\frac{1}{27R^3}-\left(\frac{1}{27R^3}+\frac{1}{9R^2}+\frac{1}{6R}+\frac{1}{8}\right)\exp(-3R-i\epsilon t)\right],$$

$$F_{23}'=vt\left[-\frac{3}{2R^3}+\left(\frac{3}{2R^3}+\frac{3}{R^2}+\frac{3}{R}+2+R\right)\exp(-2R)\right],$$

$$F_{14}'=\frac{P}{vt}F_{13}',\quad F_{24}'=\frac{P}{vt}F_{23}',\quad F_{15}'=F_{25}'=F_{35}'=F_{45}'=0,$$

$$G_{11}=\frac{4\sqrt{2}}{3}\exp(i\epsilon t)[2\exp(-R)-\exp(-2R)],\quad G_{12}=-\tfrac{2}{3}R^2\exp(-R),$$

$$G_{13}=vt(\tfrac{2}{3}+\tfrac{2}{3}R)\exp(-R),\quad G_{14}=(P/vt)G_{13},\quad G_{15}=0,$$

$$g_{11}=\frac{16\sqrt{2}}{9}\exp(i\epsilon t)\left[\left(-\frac{8}{3R}+2\right)\exp(-R)+\left(\frac{8}{3R}+1\right)\exp(-2R)\right],$$

$$g_{12}=-(\tfrac{1}{2}+\tfrac{1}{2}R+\tfrac{1}{3}R^2+\tfrac{1}{6}R^3)\exp(-R),$$

$$g_{13}=vt(\tfrac{1}{2}+\tfrac{1}{2}R+\tfrac{1}{6}R^2)\exp(-R),\quad g_{14}=(P/vt)g_{13},\quad g_{15}=0.$$

Here ϵ is the difference in the binding energies of the ground state and the excited states ($n=2$) of the He$^+$ ion and v is the velocity of the α particle relative to the hydrogen atom. Finally, the squares of the absolute values of the coefficients A_1 and B_n's at infinite time give the probabilities of scattering and capture in different states of the He$^+$ ion.

The last of Eqs. (3) together with the initial condition give $B_5=0$, and $|B_4|^2$ at $t=\infty$ determines twice the capture probability in either of $2p_{\pm1}$ states. The matrix g can be easily inverted and (3) is written in the form

$$\dot{A}=iHA,\quad H=g^{-1}F.$$

TABLE I. Calculated values of capture probability in the 1s, 2s, 2p_0, and 2$p_{\pm1}$ states of the He$^+$ ion are given for incident energy E in the range 2–100 keV and at a fixed laboratory scattering angle θ of 1.2°.

E (keV)	Capture probability 1s	2s	2p_0	2$p_{\pm1}$[a]	Total	Probability of scattering
2	9.5×10^{-8}	0.0237	0.0749	0.5966	0.6952	0.3048
3	5.3×10^{-7}	0.2758	0.0074	0.7036	0.9868	0.0132
4	6.8×10^{-6}	0.1416	0.2258	0.6302	0.9976	0.0024
5	3.97×10^{-5}	0.1736	0.2668	0.4736	0.9140	0.0860
7	6.12×10^{-4}	0.4948	0.0106	0.3119	0.8179	0.1821
9	0.0006	0.1246	0.0895	0.2351	0.4498	0.5502
12	0.0005	0.0401	0.5281	0.1171	0.6858	0.3142
15	0.0020	0.1244	0.6456	0.0609	0.8329	0.1671
20	0.0160	0.0917	0.2651	0.0314	0.4042	0.5958
30	0.1066	0.1530	0.0453	0.0137	0.3186	0.6814
40	0.2113	0.2041	0.2159	0.0064	0.6377	0.3623
50	0.2626	0.1885	0.3082	0.0035	0.7629	0.2371
60	0.2519	0.1688	0.3402	0.0019	0.7628	0.2372
70	0.2034	0.1598	0.3378	0.0011	0.7021	0.2979
80	0.1431	0.1580	0.3130	0.0007	0.6148	0.3852
90	0.0886	0.1591	0.2743	0.0005	0.5225	0.4775
100	0.0472	0.1609	0.2299	0.0003	0.4383	0.5617

[a] Sum of equal probabilities in 2p_{+1} and 2p_{-1} states.

TABLE II. The same as for Table I except that θ is 1.7°.

E (keV)	Capture probability 1s	2s	2p_0	2$p_{\pm1}$[a]	Total	Probability of scattering
2	3.6×10^{-8}	0.1024	0.0829	0.7052	0.8905	0.1095
3	1.6×10^{-7}	0.2875	0.0531	0.6130	0.9536	0.0464
4	6.5×10^{-6}	0.2304	0.2561	0.4573	0.9438	0.0562
5	5.8×10^{-5}	0.2377	0.2861	0.3159	0.8398	0.1602
7	0.0012	0.5789	0.0071	0.1815	0.7687	0.2313
9	0.0014	0.1436	0.0790	0.1325	0.3565	0.6435
12	0.0013	0.0399	0.5167	0.0644	0.6223	0.3777
15	0.0037	0.1188	0.6337	0.0327	0.7889	0.2111
20	0.0203	0.0872	0.2575	0.0161	0.3811	0.6189
30	0.1127	0.1521	0.0469	0.0067	0.3184	0.6816
40	0.2160	0.2031	0.2182	0.0031	0.6404	0.3596
50	0.2662	0.1874	0.3099	0.0018	0.7653	0.2347
60	0.2545	0.1680	0.3413	0.0009	0.7647	0.2353
70	0.2051	0.1591	0.3388	0.0006	0.7036	0.2964
80	0.1442	0.1575	0.3139	0.0004	0.6160	0.3840
90	0.0893	0.1588	0.2750	0.0002	0.5233	0.4767
100	0.0475	0.1607	0.2305	0.0001	0.4388	0.5612

[a] Sum of equal probabilities in 2p_{+1} and 2p_{-1} states.

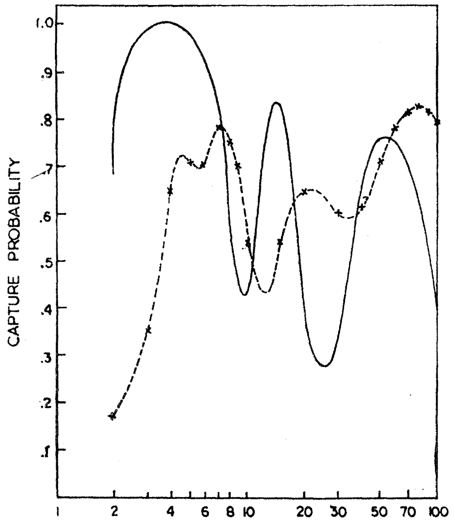

FIG. 1. Electron-capture probability is plotted versus incident ion energy at a fixed laboratory scattering angle θ of 1.2°. Unbroken line indicates present theory; dashed line indicates the experiment of Keever and Everhart (see Ref. 1).

We solve the above set of equations numerically by Runge-Kutta method. With the help of (3), it is seen that the unitarity of

$$\int_{-\infty}^{\infty} \bar{\Psi}_T \Psi_T dV$$

is preserved at all times, and we employ this fact as a check on the solutions of the differential equations, at any instant. To compute the capture cross sections

$$Q_i = 2\pi \int_0^{\infty} |Bi_{\infty}|^2 P dP,$$

we evaluate the necessary integrals numerically using the Gaussian quadrature method.

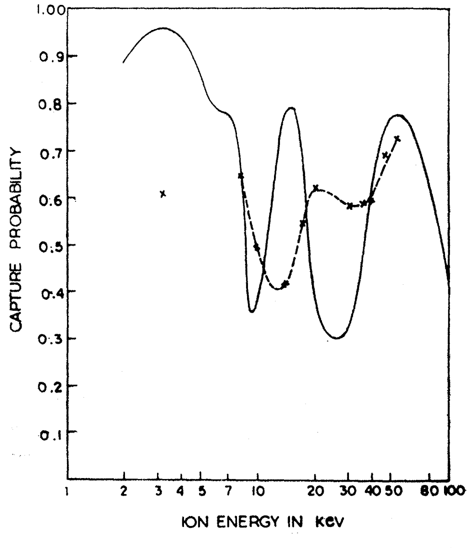

FIG. 2. The same as for Fig. 1, except that θ is 1.7°.

TABLE III. The cross sections of capture in the states $1s$, $2s$, $2p_0$, and $2p_{\pm 1}$ of the He^+ ion are given in units of πa_0^2, varying the incident ion energy E from 1.6 to 32.4 keV.

E (keV)	Capture cross section $1s$	$2s$	$2p_0$	$2p_{\pm 1}$[a]	Total
1.6	2.6×10^{-7}	0.3630	0.4154	0.5944	1.3727
3.6	6.4×10^{-6}	1.4372	1.6945	1.6521	4.7837
6.4	1.8×10^{-4}	2.5556	3.7773	3.2997	9.6327
10	4.8×10^{-4}	3.4261	5.7438	4.8035	13.9740
12	9.0×10^{-4}	4.0502	6.6594	5.5900	16.3010
14.4	1.43×10^{-3}	4.4853	7.2389	6.5345	18.2600
16	1.93×10^{-3}	4.5839	7.4141	7.1089	19.1090
19.6	4.26×10^{-3}	4.5041	7.6752	8.1401	20.3240
25.6	1.43×10^{-2}	4.1103	8.2404	9.1086	21.4740
32.4	3.22×10^{-2}	3.7318	8.6615	9.5071	21.9330

[a] Sum of equal probabilities in $2p_{+1}$ and $2p_{-1}$ states.

III. RESULTS AND DISCUSSION

At fixed scattering angles 1.2° and 1.7°, we calculate the probabilities of scattering of He^{++} and capture into different states of the He^+ ion, covering an energy range 2–100 keV. The results given in Tables I and II reveal that the capture probabilities in the excited states $2s$, $2p_{0,\pm 1}$ are much higher then those in the ground state. Further, there is little oscillation in the ground-state capture probability, whereas the excited-state capture probability is oscillatory. This observation runs counter to the tentative suggestions of Keever and Everhart,[1] that the accidental resonance process is not responsible for the oscillations in capture probability. Our results represented by the solid line in Figs. 1 and 2, (for fixed scattering angles 1.2° and 1.7°, respectively) have been compared with the experimental findings of Keever and Everhart.[1] The numbers of peaks and valleys in our curve are the same as in the experimental curve, except for a very small oscillation in the experiment in the range 4.5–7 keV in Fig. 1; but the positions of peaks and valleys do not show a quantitative agreement with

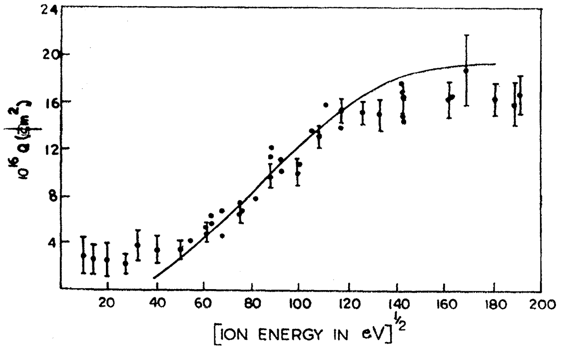

FIG. 3. Total capture cross section Q is plotted versus the square root of the incident ion energy in eV. Unbroken line indicates present theory. Closed circles represent the experiment of Fite, Smith, and Stebbings (see Ref. 2).

the experimental ones. One of the reasons for this difference may be the fact that the relation connecting impact parameter, scattering angle, and incident energy is unsatisfactory, inasmuch as it fails to take account of the influence of the particular electronic state on the trajectory.

In Table III we present our results for the cross sections of capture in the ground state and the excited states of the He^+ ion, in the energy range 1.6–32.4 keV. In Fig. 3 we compare our results of total cross section with the experimental findings of Fite, Smith, and Stebbings.[2] Here we have found a very good agreement. The general tendency of our theoretical results approaching zero in the zero-velocity limit of the α particle is a characteristic feature of accidentally resonant reactions, as has been remarked by Bates *et al.*[3] It seems clear that the predominantly large cross section for the capture into the $2s$ or $2p$ states compared with that in the ground state is due to the accidental resonance of the two states with the ground state of the hydrogen atom.

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Effective Operator Formalism in Optical Pumping*

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Real and virtual absorption of weak monochromatic light is analyzed with semiclassical radiation theory. The influence of the light on the atoms is described by an effective ground-state Hamiltonian operator, and the effect of the atoms on the light is described by a dielectric susceptibility operator. These operators are expressed explicitly in terms of familiar ground-state observables, angular factors, oscillator strengths, and plasma dispersion functions. The theory gives a comprehensive description of optical pumping, light shifts, and light modulation due to real and virtual absorption of light, and several new effects are predicted. Repopulation of the atomic ground state from a polarized excited state is not considered in this paper.

I. INTRODUCTION

A FORMAL theory of optical pumping was first developed by Barrat and Cohen-Tannoudji.[1] They show that for normal light intensities the pumping of the atomic ground state is due to two distinct processes: absorption by the ground-state atoms of light which is not completely isotropic or whose spectral intensity varies strongly in the region of the atomic absorption lines, and repopulation of the ground state by spontaneous emission from a polarized excited state. In their work the atoms are treated with the density matrix formalism while the light is represented by a many-photon state of the radiation field. Although this approach yields a detailed description of the evolution of the atoms, the corresponding influence of the polarized atoms on the light is treated only superficially.

In this paper we consider the effects due to the real and virtual absorption of light by atoms. We shall not be concerned with the repopulation of the atomic ground state by spontaneous emission from a polarized excited state. The interaction of the atoms with the light is treated semiclassically. The electric field of the incident light is represented by a quasimonochromatic wave[2]

$$\mathbf{E}(\mathbf{r},t)=(\mathbf{E}_0/2)e^{i(\mathbf{k}\cdot\mathbf{r}-\omega t)}+\text{c.c.}\,, \tag{I.1}$$

where the amplitude $\mathbf{E}_0$ is a slowly varying function of space and time and c.c. denotes complex conjugate. We shall assume that the incident light intensity is weak enough so that spontaneous emission from the excited state is much more probable than stimulated emission. We shall also assume that any external magnetic field which may be present is small enough that the Zeeman splittings of the atom are much less than the Doppler widths of the optical absorption lines or than the hfs splittings of the atomic states. Under these loose restrictions we show that the effect of real and virtual absorption of light by the atoms can be represented by an effective ground-state Hamiltonian operator $\delta\mathcal{H}$; i.e., as if the evolution of the atomic ground state were determined by a Schrödinger equation of the form

$$i\hbar(\partial\psi/dt)=(\mathcal{H}_0+\delta\mathcal{H})\psi\,. \tag{I.2}$$

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† Alfred P. Sloan Research Fellow.

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[2] This formalism has been extended to the case where several monochromatic light waves are present simultaneously.