Possible Resonance in Positron-Hydrogen Scattering

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The positron-hydrogen system is considered, with the view to determining whether a scattering resonance below the positronium threshold is likely to occur, as has been suggested by Bransden and Jundi. The likeliest mechanism for producing such a resonance would be the existence of a virtual bound state in the positronium-proton channel, brought about by the large dipole polarizability and mass of the positronium atom. A modification of Holøien's technique enables one to reject spurious solutions without the use of the projection-operator technique. A nonvariational adiabatic calculation seems to indicate that a resonance does exist, lying at 0.1 eV below the threshold. When, however, a variational treatment is employed, certain essential nonadiabatic terms appear. The resultant reduction in attraction serves to eliminate the apparent resonance. It is concluded that the previously reported resonance is probably an artifact.

I. INTRODUCTION

THE positron-hydrogen system above the threshold for positronium formation (6.8 eV) has recently been examined by Bransden and Jundi.[1] With the aid of the M-matrix method[2] they have extrapolated their results below the threshold, and have presented evidence that a resonance occurs in the e^+-H elastic channel. Their estimate of the position of this resonance corresponds to a state of the positronium-proton system, bound by about 0.02 eV (1.6×10^{-3} Ry). The present work is intended to examine the evidence for the existence of such a resonance.

The simplest method of locating such a resonance would be the projection-operator technique,[3] which has been very satisfactory in finding e^--H resonances below degenerate thresholds.[4] This technique effectively decouples the open and closed channel parts of the scattering wave function, and reduces the problem of resonances to that of bound states. The most likely physical mechanism which could produce binding is the electric polarization of the positronium atom in its ground state by the proton. Thus a wave function including this polarizability will be the basis of the present work.

If we construct an appropriate scattering trial function ψ including polarizability, the projection-operator prescription for computing the resonant energies is as follows:

(1) Construct a projection operator Q which removes the hydrogen ground-state component from ψ, and

(2) Carry out a Rayleigh-Ritz variational energy calculation using $Q\psi$ as the trial function.

Using the simple form $Q=1-|H\rangle\langle H|$, where $|H\rangle$ represents the hydrogen ground state $\phi_H(r)$, x is the positron coordinate, and the trial function has the form

$$\psi(\mathbf{r},\mathbf{x})=f(\mathbf{x})\phi_H(r)+\Phi(\mathbf{x},\mathbf{r}),\tag{1a}$$

one can write the closed-channel part of ψ as

$$Q\psi=\psi(\mathbf{r},\mathbf{x})-\phi_H(r)\int d^3r'\phi_H(r')\psi(\mathbf{r}',\mathbf{x}),\tag{1b}$$

$$Q\psi=\Phi(\mathbf{x},\mathbf{r})-\phi_H(r)\int d^3r'\phi_H(r')\Phi(\mathbf{x},\mathbf{r}').\tag{1c}$$

If, for example, Φ were a close-coupling expansion in excited states of the target, then $Q\psi=\Phi$. We wish, however, to write Φ in terms of the positronium atom in the field of a proton, so the second term in Eq. (1c) does not necessarily vanish.

Holøien[5] has used a simplification of the projection-operator method in searching for electron-atom resonances, and we will here apply a form of his approach to the positron problem. To do this we first neglect the second term in Eq. (1c), and use Φ itself for the energy calculation. Some of the resulting energies will correspond to functions Φ for which the integral in Eq. (1c) is very small; i.e., for which the projection onto the hydrogen ground state is very small. We follow Holøien in considering such states to be genuine resonances, although the energies thus obtained have no necessary upper bound character.

II. SCATTERING WAVE FUNCTION

Let us consider the motion of a positronium atom (Ps) in the field of a fixed proton (p). We will use a trial function of the following form

$$\Phi=[X(\mathbf{R})+F(\mathbf{R})G(R,\zeta,\cos\theta)]\phi(\zeta),\tag{2}$$

where $\phi(\zeta)=(8\pi)^{-\frac{1}{2}}e^{-\frac{1}{2}\zeta}$ is the positronium ground-state wave function, while $\mathbf{R}=\frac{1}{2}[\mathbf{x}+\mathbf{r}]$, $\zeta=\mathbf{x}-\mathbf{r}$, and $\cos\theta=(\mathbf{R}\cdot\zeta)/R\zeta$. The functions X and F will be deter-

[1] B. H. Bransden and Z. Jundi, Proc. Phys. Soc. (London) **92**, 880 (1967).

[2] See, for instance, K. Smith, in *Autoionization*, edited by A. Temkin (Mono Book Corp., Baltimore, Md., 1966).

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[4] T. F. O'Malley and S. Geltman, Phys. Rev. **137**, A1344 (1965); A. Temkin and J. F. Walker, Phys. Rev. **140**, A1520 (1965).

[5] E. Holøien, Proc. Phys. Soc. (London) **71**, 357 (1958); and A. Temkin, in *Autoionization*, edited by A. Temkin (Mono Book Corp., Baltimore, Md., 1966).

mined later, while G is to represent the adiabatic distortion of the positronium atom.

The Hamiltonian can be written in atomic units, with energies in rydbergs as

$$H = H_\zeta + V - \tfrac{1}{2}\nabla_R^2, \tag{3}$$

where

$$H_\zeta = -2[\nabla_\zeta^2 + (1/\zeta)], \quad [H_\zeta + \tfrac{1}{2}]\phi(\zeta) = 0,$$

$$V = 2\left[\frac{1}{|\mathbf{R}+\tfrac{1}{2}\zeta|} - \frac{1}{|\mathbf{R}-\tfrac{1}{2}\zeta|}\right] = \sum_{l(\text{odd})} v(R,\zeta)P_l(\cos\theta).$$

The first-order (in V) adiabatic form for G is obtained by solving the equation[6]

$$[G,H_\zeta]\phi = V\phi, \tag{4}$$

and since by symmetry only odd multipoles are retained in the expansion for the potential, it is a good approximation to keep only the dipole $[l=1]$ term. Then, $G = g(R,\zeta)P_1(\cos\theta)$ and Eq. (4) becomes

$$\frac{d^2g}{d\zeta^2} + \left(\frac{2}{\zeta} - 1\right)\frac{dg}{d\zeta} - \frac{2}{\zeta^2}g = f, \tag{5}$$

where $f = -\zeta/R^2$ for $\zeta \le 2R$ and $f = -8R/\zeta^2$ for $\zeta \ge 2R$. The properly continuous, regular solution of Eq. (5) with continuous first derivative is found to be

$$g(\zeta \le 2R) = \frac{1}{8R^2}[\zeta + \tfrac{1}{4}\zeta^2]$$

$$- \tfrac{3}{8}e^{-2R}\left(1 + \frac{1}{R}\right)^2\left[\frac{2}{\zeta^2}e^\zeta - \left(1 + \frac{2}{\zeta} + \frac{2}{\zeta^2}\right)\right]$$

$$g(\zeta \ge 2R) = -\frac{R}{2}\left[\frac{1}{\zeta} + \frac{1}{\zeta^2}\right] \tag{6}$$

$$+ \tfrac{3}{8}\left[1 - \frac{1}{R^2} + e^{-2R}\left(1 + \frac{1}{R}\right)^2\right]\left[1 + \frac{2}{\zeta} + \frac{2}{\zeta^2}\right].$$

III. ADIABATIC NONVARIATIONAL METHOD

Our first evaluation of χ and F will be nonvariational and resembles the polarized-orbital method[7] used previously for positron-hydrogen scattering.[8] We assume that $F = \chi$ in Eq. (2) and require χ to satisfy the equation

$$\langle[H-E][1+G]\rangle\chi = 0, \tag{7}$$

where $E = -\tfrac{1}{2} + \epsilon$, and the bracket is defined as

$$\langle q(\mathbf{R},\zeta)\rangle \equiv \int d^3\zeta\, \phi(\zeta)q(\mathbf{R},\zeta)\phi(\zeta). \tag{8}$$

A bound state in the Ps-p channel would occur if a normalizable solution of Eq. (7) can be found with $\epsilon < 0$, and it would represent a resonance in the elastic e^+-H channel near a positron energy $\tfrac{1}{2} + \epsilon$. Since $\langle G \rangle = 0$, Eq. (7) can be written explicitly as

$$[-\tfrac{1}{2}\nabla_R^2 + V_2]\chi = \epsilon\chi, \tag{9a}$$

where $V_2 \equiv \langle GV \rangle$ is the adiabatic dipole potential, listed in Table I. Before solving the eigenvalue problem of Eq. (9), one can check whether any bound states exist by solving the S-wave, zero-energy $[\epsilon=0]$ scattering problem. The number of nodes in the radial wave function will give the number of bound states. This radial function $U = R\chi$ is obtained by numerically integrating the equation

$$-\tfrac{1}{2}U'' + [V_2 - \epsilon]U = 0 \tag{9b}$$

outward from the origin in the usual way. The result for $\epsilon = 0$ is plotted in Fig. 1, and one sees that two bound states occur. The more compact of these is spurious, and results from the omission of the second term in Eq. (1c), but the state giving the second node may represent the resonance found in Ref. (1). The eigenvalues are then obtained numerically from Eq. (9b), by integrating outward from the origin and inward from the asymptotic region. Continuity of the logarithmic derivative determines ϵ. The lower eigenvalue is $\epsilon \approx -0.6$ Ry; this energy is close to that of the $1S$ state of hydrogen, and the corresponding eigenfunction peaks at $R \approx 1.5$, so this clearly is one of the spurious states which
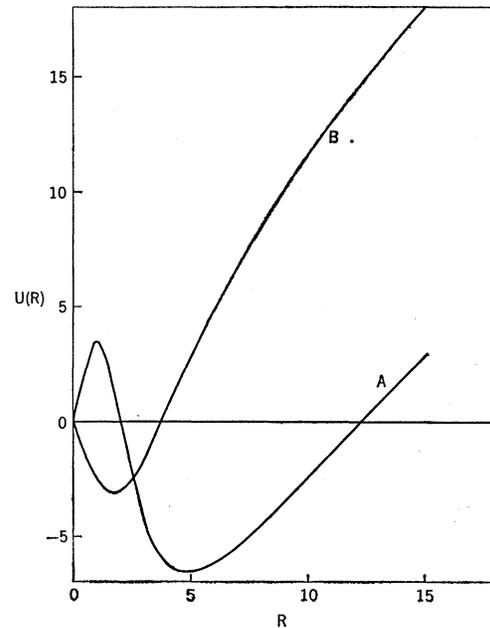

FIG. 1. Radial wave functions $U = R\chi$, for $\epsilon = 0$. Curve A is nonvariational and shows two nodes, while curve B is variational and has only one. The functions are normalized to unit slope asymptotically, with R measured in atomic units.

[6] A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. (London) A233, 70 (1955).

[7] A. Temkin and J. C. Lamkin, Phys. Rev. 121, 788 (1961).

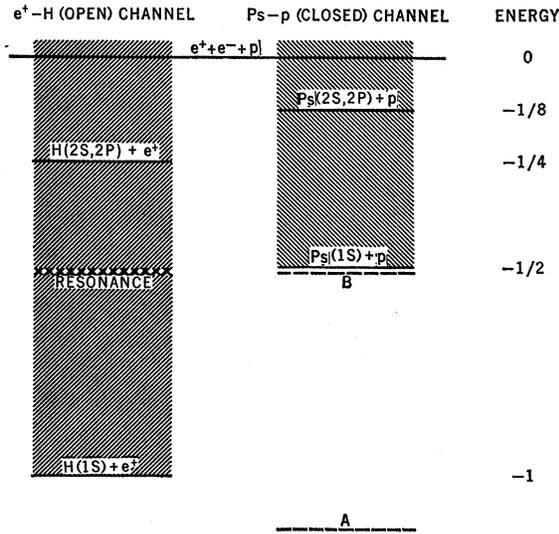[8] R. J. Drachman, Phys. Rev. 138, A1582 (1965).

FIG. 2. Energy-level diagram for the e^+-e^--p system. The two bound states found in the nonvariational method are shown: A is the spurious level, and B represents the resonance found below the Ps threshold. The diagonal hatching indicates the scattering continua. The terminology "open" or "closed" channel is meaningful only below $E=-\frac{1}{2}$.

would have been eliminated by the Q-operator technique. The second eigenvalue is $\epsilon=-7.5\times10^{-3}$ Ry, and represents a resonance lying 0.1 eV below the positronium threshold.[9] In Fig. 2 the low-lying e^+-e^--p states are shown on a level diagram in order to clarify the situation. The two bound states just discussed are in the closed channel below the ground state of positronium [$Ps(1S)+p$]. The spurious state is seen to be in the vicinity of the ground state of hydrogen [$H(1S)+e^+$], while the second state corresponds to a resonance in the open channel. In Sec. V we will discuss the relation between this resonance and that found in Ref. 1.

IV. VARIATIONAL METHOD

The assumptions made in Sec. III [that $F=\chi$ and that Eq. (7) holds] depend on the ability of the positronium atom to adjust adiabatically to the polarization induced by the electric field of the proton.[10] This in turn depends roughly on the smallness of the velocity of the positronium center-of-mass. The very tightly bound (spurious) lower state probably has too much kinetic energy to satisfy the adiabatic conditions, but the resonance state may satisfy them.

The variational method relaxes the above condition on F and determines both functions by free variation.

[9] An approximate form of V_2, derived by A. Temkin [Phys. Rev. **116**, 358 (1959) and used in Ref. 7] was also tried here and gave $\epsilon=-0.48$ Ry and $\epsilon=-2.5\times10^{-3}$ Ry. The second eigenvalue gives an apparent resonance at 0.03 eV below threshold, in good agreement with Ref. 1. This form of V_2 involves a step function in $g(R,\zeta)$, which is unsatisfactory for our later variational work.
[10] M. H. Mittleman and K. M. Watson, Phys. Rev. **113**, 198 (1959).

Eq. (7) is replaced by the following two equations:

$$\langle [H-E][\chi+FG]\rangle=0$$
$$\langle G[H-E][\chi+FG]\rangle=0, \quad (10)$$

whose solution corresponds to solving the Schrödinger equation in the restricted subspace spanned by the orthogonal vectors ϕ and $G\phi$. Explicitly, these result in the following system of differential equations[11]:

$$[\tfrac{1}{2}\nabla_R^2+\epsilon]\chi-V_2F=0$$

$$\left[N(\tfrac{1}{2}\nabla_R^2+\epsilon)+V_2-W-V_N\frac{d}{dR}\right]F-V_2\chi=0, \quad (11)$$

where

$$N\equiv\langle G^2\rangle, \quad W\equiv-\tfrac{1}{2}\langle G\nabla_R^2 G\rangle, \quad V_N\equiv-\tfrac{1}{2}\frac{dN}{dR}, \quad V_2\equiv\langle GV\rangle.$$

[These functions were evaluated numerically and are given in Table I.] Except for $R\to\infty$, the relation $F=\chi$ does not satisfy Eq. (11). Interesting features of Eq. (11) are the short-range potential W and the velocity-dependent term involving V_N.

Letting $\chi=R^{-1}U$ and $F=R^{-1}g$ one can write the S-wave, $\epsilon=0$ form of Eq. (11) as follows:

$$\tfrac{1}{2}U''=V_2 g$$
$$\tfrac{1}{2}Ng''-V_Ng'+[V_2-W+V_N/R]g=V_2U. \quad (12)$$

These equations resemble those of a two-state close-coupling calculation, and to treat them similar techniques are used.[12] Two linearly independent regular solutions of Eq. (12) exist for small R; their leading terms are

$$U_1=R, \quad g_1=0$$
and
$$U_2=0, \quad g_2=R. \quad (13)$$

Each of these solutions is integrated numerically from the origin out to a convenient intermediate point $\bar{R}$, at which point a linear combination

$$U_<(\bar{R})=AU_1(\bar{R})+BU_2(\bar{R}) \quad (14)$$

with undetermined coefficients represents the numerical value of U. A similar combination is formed for g. Three linearly independent regular solutions of Eq. (12) exist for large R. To find them, we use the asymptotic forms of the potentials given in Table I. Equation (12) becomes

$$\tfrac{1}{2}U''=-36R^{-4}g$$
$$\tfrac{1}{2}g''-2R^{-1}g'-(18/43)g=-(18/43)U, \quad (15)$$

where terms of order R^{-2} were neglected in the second

[11] These equations resemble those introduced by R. Damburg and E. Karule [Proc. Phys. Soc. (London) **90**, 637 (1967)].
[12] P. J. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962). (See especially pp. 477-479.)

TABLE I. Potentials needed for the numerical solution of the scattering problem (in Rydbergs).

R (a.u.)	$-V_2$	N	V_N	W
0	0	0	0	0
0.2	0.282	0.198	−0.920	0.801
0.4	0.745	0.661	−1.300	1.944
0.6	1.108	1.173	−1.197	2.613
0.8	1.306	1.586	−0.845	2.752
1.0	1.358	1.842	−0.436	2.536
1.5	1.135	1.873	+0.276	1.521
2.0	0.785	1.469	0.464	0.729
2.5	0.504	1.026	0.403	0.314
3.0	0.316	0.680	0.288	0.128
4.0	0.127	0.291	0.121	1.97(−2)
5.0	5.60(−2)	0.132	4.92(−2)	2.90(−3)
7.5	1.14(−2)	2.71(−2)	7.21(−3)	2.32(−5)
10.0	3.60(−3)	8.60(−3)	1.72(−3)	1.76(−7)
$R \to \infty$	$\sim 36R^{-4}$	$\sim 86R^{-4}$	$\sim 172R^{-5}$	exponential

line. The three solutions required for large R are

$$U_3 = 1 - 6/R^2, \quad g_3 = U_3,$$
$$U_4 = R - 18/R, \quad g_4 = U_4 - 43/9R, \quad (16)$$
$$U_5 = 0, \quad g_5 = e^{-\beta R}[1 + \beta R + \tfrac{1}{3}(\beta R)^2], \quad (\beta^2 = 36/43).$$

(Solutions 3 and 4 contain the first two terms of a series in inverse powers of R.) Each of these solutions is integrated numerically inward from an asymptotic point R_0 ($= 20$ in the present work) to the intermediate point $\bar{R}$ where the linear combination

$$U_>(\bar{R}) = CU_3(\bar{R}) + U_4(\bar{R}) + DU_5(\bar{R}) \quad (17)$$

represents the numerical value of U, and similarly for g. (The coefficient of U_4 is taken equal to unity, and U has the conventional normalization to unit slope at $R \to \infty$.) Four equations represent the matching conditions at $R = \bar{R}$:

$$U_< = U_>, \quad g_< = g_>, \quad U_<' = U_>', \quad g_<' = g_>'. \quad (18)$$

These determine the four constants A, B, C, D through a set of four linear algebraic equations. The function $U(R)$ thus obtained is plotted on Fig. 1. This is the principal result of the present work: The node representing the spurious state occurs at larger R than for the nonvariational case, and this decrease in effective attraction is sufficient to destroy the second node.[13] The variational treatment thus does not give any indication of a resonance below the Ps threshold. The radically different behavior produced by the inclusion of the nonadiabatic terms leads us to conclude that the resonance found in Ref. 1 is probably spurious.

V. DISCUSSION AND CONCLUSIONS

To explain the relation between the present work and that of Ref. 1, let us recall that the latter considered the

scattering of positrons on hydrogen above the threshold for positronium formation, using a polarized orbital type of wave function in both e^+-H and Ps-p channels. In our notation

$$\psi = \chi_1(\mathbf{x})[1 + G_H(\mathbf{x},\mathbf{r})]\phi_H(r)$$
$$+ \chi_2(\mathbf{R})[1 + G_{Ps}(\mathbf{R},\zeta)]\phi_{Ps}(\zeta). \quad (19)$$

If the Schrödinger equation $[H - E]\psi = 0$ is projected onto $\phi_H(r)$ and $\phi_{Ps}(\zeta)$ in turn, the coupled equations used in Ref. 1 are obtained [their Eq. (16)]. These are as follows:

$$[\nabla_x^2 + k_1^2 - V_1(x) - V_{2H}(x)]\chi_1(\mathbf{x})$$
$$= \int d^3 r \phi_H(r)[-\nabla_x^2 - k_1^2 + V(\mathbf{r},\mathbf{x})]$$
$$\times [1 + G_{Ps}(\mathbf{R},\zeta)]\phi_{Ps}(\zeta)\chi_2(\mathbf{R}) = 0$$

$$[\nabla_R^2 + k_2^2 - 2V_{2Ps}(R)]\chi_2(\mathbf{R})$$
$$= \int d^3 \zeta \phi_{Ps}(\zeta)[-\nabla_R^2 - k_2^2 + 2V(\mathbf{R},\zeta)]$$
$$\times [1 + G_H(\mathbf{x},\mathbf{r})]\phi_H(r)\chi_1(\mathbf{x}) = 0, \quad (20)$$

where the second-order potentials are the adiabatic polarization potentials of hydrogen [including several multipoles] and positronium [dipole distortion only], and where

$$V(\mathbf{r},\mathbf{x}) = 2[(1/x) - (1/|\mathbf{x} - \mathbf{r}|)], \quad (21)$$

and $V(\mathbf{R},\zeta)$ is given in Eq. (3). [A further neglect of all terms in G_H, G_{Ps} on the right-hand side of Eq. (20) does not concern us here.] If Eq. (20) is now solved, the eigenphases or reaction matrix satisfy a minimum principle, but only if certain nonadiabatic terms are added. These are complicated and involve cross-channel couplings, but for the diagonal Ps term the form is

$$\int d^3 R \chi_2(\mathbf{R}) \left[-\tfrac{1}{2}N(\nabla_R^2 + k_2^2) + W + V_N \frac{d}{dR} \right] \chi_2(\mathbf{R}), \quad (22)$$

where N, W, V_N were defined in Eq. (11), and a similar correction term appears in the diagonal H term. The authors of Ref. 1 emphasize that, since they have omitted the nonadiabatic correction terms their results cannot be considered quantitative. We have here attempted, by including terms of this type in an optimal variational calculation, to indicate that the most likely result of the quantitative extension of the work of Ref. 1 would be the disappearance of the resonance.

Recently, another above-threshold calculation has been reported,[14] which does not obtain the resonance discussed in Ref. 1. The method is very similar to that of Ref. 1, including both ground-state hydrogen and Ps as well as adiabatic polarization potentials. A unique coordinate system, introduced into the Ps-p channel to

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[13] Nonadiabatic effects are more important here than they are for e^+-H scattering (Ref. 8) just because of the very large polarizability of the Ps atom.

[14] M. F. Fels and M. H. Mittleman, Phys. Rev. **163**, 129 (1967).

simplify the form of the coupled equations, also provides a spurious centrifugal potential. It seems that this extra potential serves inadvertently to simulate the effect of the nonadiabatic terms we have discussed above, and hence to eliminate the resonance.

An interesting question may be raised now concerning the Ps-He$^+$ channel in e^+-He scattering. This system is the same as Ps-p at large distances, but its additional Van der Waals attraction might be just enough to produce the resonance. The cross section near threshold for e^+-He scattering has been measured,[15] although the

analysis of the experiment is not straightforward. It is possible that a resonance near threshold is needed to bring about agreement between experiment[15] and theory.[16]

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Measurement of High-Energy Charge-Transfer Cross Sections for Incident Protons and Atomic Hydrogen in Various Gases*

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(Received 8 February 1968)

Measurements of electron-capture cross sections σ_{10} and electron-loss cross sections σ_{01} for protons and atomic hydrogen in H_2, He, Ar, Kr, N_2, O_2, CO, CO_2, H_2O, CH_4, C_2H_4, C_2H_6, and C_4H_{10} are reported and compared with published theoretical estimates and experimental results. The energy range was 100 to 2500 keV. The results are presented in graphical form. By applying the additive rule, the cross sections σ_{10} and σ_{01} are estimated for hydrogen particles in carbon.

I. INTRODUCTION

A SUMMARY of experimental results of charge-transfer processes prior to 1958, for incident-particle energies less than 1.0 MeV, has been published by Allison.[1] A paper by Welsh et al.[2] reviews some of the charge-transfer results subsequent to 1958. Measurements by Welsh et al.,[2] Williams,[3] and Schryber[4] have extended the energy range for the various cross sections up to 13.8 MeV for the target gases H_2, He, Ar, and N_2.

Reviews of various theoretical formulations used in calculating charge-transfer cross sections have been presented by Bates and McCarroll,[5] Bates,[6] Dalgarno,[7]

and Bates and Williams.[8] Of particular interest to the present experiment are recent papers in which electron-capture cross sections have been calculated for protons on N, O, Ar, and Kr targets. Mapleton[9,10] has calculated cross sections for the capture of $2p$ electrons from atomic nitrogen and oxygen by means of the first Born approximation. He has also extended the first Born calculation to include capture from inner electron shells.[11] A first Born approximation has been applied by Nikolaev[12] to calculate the cross section for electron capture by protons in hydrogen, helium, lithium, nitrogen, neon, argon, and krypton. This calculation includes contributions to the cross section from inner electron shells of the target atom. Bates and Mapleton[13] have used a classical approach to calculate the electron-capture cross sections as a function of the atomic parameters of the target. This classical approach does not include the possibility of electron capture from inner

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