$$T_{2,2}=\tfrac{8}{3}z_v^{\,2}[s_4+t_2-\tfrac{3}{5}(s_5+t_3)]\ , \tag{A12}$$

$$T_{3,2}=\tfrac{64}{15}z_v^{\,3}y_0^{\,-1}[s_6+t_5-\tfrac{6}{5}(s_7+t_6)+\tfrac{9}{25}(s_8+t_7)]. \tag{A13}$$

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Auger Rates for Circular Orbits of $\alpha\pi^-e^-$, αK^-e^-, and $\alpha\bar{p}e^-$ Atoms

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Auger rates are estimated for some circular orbits of the $\alpha\pi^-e^-$, αK^-e^-, and $\alpha\bar{p}e^-$ atoms. It is found, as conjectured by Condo several years ago, that the Auger rate for a circular orbit depends sensitively on the multipolarity of the transition. In some instances, the multipolarity may be required by energy conservation to be large enough to permit a π^- or a K^- meson to decay rather than to eject an electron. In particular, the estimated Auger rates for those circular orbits of the $\alpha\pi^-e^-$, αK^-e^-, and $\alpha\bar{p}e^-$ atoms with binding energies most nearly equal to that of a He atom are, respectively, 2×10^{12}, 4×10^{5}, and $\lesssim10^{3}$ sec^{-1}. Radiative rates are also computed.

I. INTRODUCTION

Estimates of Auger rates for some states of the $\alpha\pi^-e^-$, αK^-e^-, and $\alpha\bar{p}e^-$ atoms are obtained in the present paper. These atoms are formed when π^- and K^- mesons and antiprotons are stopped in helium. In the particular states which are being considered here, the electron is in a $1s$ orbit, and the meson or the antiproton is in a circular orbit with large principal quantum number n. In a circular orbit, the orbital angular momentum l is given by $l=(n-1)$. For the sake of brevity, the particular atomic states which are being considered here are frequently referred to simply as circular orbits, and an antiproton is frequently referred to loosely as a meson.

The purpose of this investigation is to determine the extent to which the Auger rate for a circular orbit depends on the multipolarity of the transition. The circular orbits are distinguished by the fact that the magnitude $|\Delta n|$ of the change in the meson principal quantum number is equal to both the multipolarity of the Auger transition and the orbital angular momentum of the ejected electron. It was argued several years ago by Condo[1] that the Auger rate for a circular orbit would be extremely sensitive to the value of $|\Delta n|$, which in some instances might be required by energy conservation to be large enough to allow a π^- or a K^- meson to decay rather than to eject the electron, thereby accounting for the large values of the measured mean cascade times[2–4] for these particles in atomic orbits in liquid helium. Since the antiproton does not decay, radiative rates are also computed in the present paper.

The computation of the Auger rates, which is quite straightforward, is carried out in Sec. II by making use of some approximate wave functions and binding energies which are determined elsewhere.[5] The allowed values of $|\Delta n|$ are also determined in Ref. 5. The results obtained in Sec. II are found to be indeed sensitive to the values of $|\Delta n|$. In Sec. III, a detailed investigation is made of the extent to which inaccuracies in the wave func-

tions and binding energies, as determined in Ref. 5, could affect the values of the computed Auger rates. Energy is expressed in rydbergs throughout this paper; the unit of distance is the hydrogen Bohr radius; and the unit of mass is the electron mass.

II. CALCULATION OF AUGER AND RADIATIVE RATES

The wave function for the initial state of the mesonic atom is approximated with the product of two hydrogenic functions. One of these hydrogenic functions is characterized by the effective nuclear charge z_i and describes an electron in a $1s$ orbit around the α particle. The other function is characterized by the effective nuclear charge Z_i and describes a negative particle of mass M in a circular orbit around the α particle. The mass M is the reduced mass of the meson and α particle.

The wave function for the final state is also approximated with the product of two hydrogenic functions. One of these functions is a Coulomb distorted plane wave which describes an electron with wave vector $\vec{k}$ and energy k^2 moving in the attractive field of a point charge z_f. The other hydrogenic function describes a meson of reduced mass M bound in a circular orbit with principal quantum number $n - |\Delta n|$. The final meson wave function is characterized by the nuclear charge $Z_f = 2.0$.

The interaction which is responsible for Auger transitions may be expressed in the form

$$\frac{2}{|\vec{r}_e - \vec{r}_\mu|} = \sum_{L=0}^{\infty} H_L', \tag{2.1a}$$

$$H_L' = \frac{8\pi}{2L+1} \sum_{M=-L}^{L} Y_{LM}^*(\hat{r}_\mu) Y_{LM}(\hat{r}_e) \times \begin{pmatrix} r_\mu^L / r_e^{L+1}, & r_\mu < r_e \\ r_e^L / r_\mu^{L+1}, & r_\mu > r_e \end{pmatrix}, \tag{2.1b}$$

where $\vec{r}_e$ and $\vec{r}_\mu$ denote, respectively, the positions of the electron and the meson with respect to the α particle. The multipolarity of a given transition is the lowest value of L for which H_L' has a nonvanishing transition matrix element. For circular orbits, this multipolarity is equal to both the magnitude of the change Δn in the meson principal quantum number and the magnitude of the change Δl in its orbital angular momentum. Since the electron is initially in an s state, the ejected electron has orbital angular momentum $|\Delta n|$. The lowest allowed values of $|\Delta n|$ are determined by energy conservation and are calculated in Ref. 5.

It is easily verified that the Auger rate P_A for a circular orbit is given by

$$P_A = 2.62 \times 10^{14} k \sum \int d\Omega(\hat{k}) \times \left| \int \Psi_f^* H'_{|\Delta n|} \Psi_i \, d\tau_e \, d\tau_\mu \right|^2 \text{sec}^{-1}, \tag{2.2}$$

where the summation sign denotes an average and a sum, respectively, over the possible initial and final sublevels. In Eq. (2.2), the initial and final wave functions are denoted, respectively, by Ψ_i and Ψ_f. Although the interactions $H'_{|\Delta n|+2}$, $H'_{|\Delta n|+4}$, etc., also have nonvanishing transition matrix elements if n is fairly large, it is not necessary to take them into account because, as indicated by the numerical results given below, the centrifugal barrier experienced by the ejected electron causes the effects of these higher multipole interactions to be negligibly small. A straightforward calculation shows that the preceding expression for P_A is given more explicitly by

$$P_A = 1.65 \times 10^{17} (2|\Delta n| + 1)^{-1} \times [(n-1, |\Delta n|, 0, 0 \,|\, n-1, |\Delta n|, n - |\Delta n| - 1, 0)]^2 \times I^2 k \text{ sec}^{-1}, \tag{2.3}$$

where I is defined by

$$I = a \int_0^\infty L_{|\Delta n|}(kr_e) u_{1s}(r_e) G(r_e) r_e^2 \, dr_e, \tag{2.4}$$

and where a and $G(r_e)$ are defined by

$$a = \left(\frac{2ZM}{n}\right)^{|\Delta n| + 1/2} \left(\frac{M(2n - 2|\Delta n|)!}{(n - |\Delta n|)^3 (2n)!}\right)^{1/2} \left(\frac{8Zn(n - |\Delta n|)}{[Z(n - |\Delta n|) + 2n]^2}\right)^{n - |\Delta n|}, \tag{2.5}$$

$$G(r_e) = b^{-|\Delta n|} \left[(br_e)^{|\Delta n|} e^{-br_e} \sum_{\nu=0}^{(2n - 2|\Delta n| - 1)} \frac{1}{\nu!} (br_e)^\nu \right.$$

$$+\frac{(2n)!\,(br_e)^{-|\Delta n|-1}}{(2n-2|\Delta n|-1)!}\left(1-e^{-br_e}\sum_{\nu=0}^{2n}\frac{1}{\nu!}(br_e)^{\nu}\right)\Bigg], \tag{2.6}$$

the quantity b in Eq. (2.6) being defined by

$$b=\frac{M[Z(n-|\Delta n|)+2n]}{n(n-|\Delta n|)}\ . \tag{2.7}$$

In Eq. (2.4), the quantity $u_{1s}(r_e)$ is the radial wave function for the initial state of the electron, and, in the notation of Mott and Massey,[6] $L_{|\Delta n|}(kr_e)$ is the radial wave function for an electron with wave number k and orbital angular momentum $|\Delta n|$ moving in the attractive Coulomb field of a point charge z_f. The integral I was evaluated numerically with an electronic computer. The vector addition coefficient in Eq. (2.3) is expressed in the notation of Condon and Shortley.[7] This coefficient is easily evaluated.[8]

Figure 1 shows the values of P_A which are obtained if $z_f = 1.0$ and if z_i and Z_i are set equal to the effective charges which are determined by a variational calculation given in Ref. 5. These effective nuclear charges, which are denoted by z and Z, are determined by employing hydrogenic functions and minimizing the expectation value of the Hamiltonian

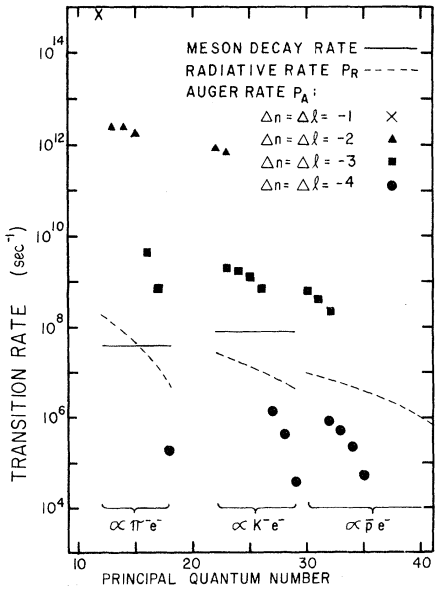

FIG. 1. Auger, radiative, and meson decay rates for circular orbits of the $\alpha\pi^-e^-$, αK^-e^-, and $\alpha\bar{p}e^-$ atoms.

$$H_b=-\nabla_e^{\,2}-\frac{4}{r_e}-\frac{1}{M}\nabla_\mu^{\,2}-\frac{4}{r_\mu}+\frac{2}{|\vec{r}_e-\vec{r}_\mu|}\ . \tag{2.8}$$

This expectation value is denoted by $E_c{}^v$. In obtaining the values of P_A which are shown in Fig. 1, it is assumed that $k=k_c{}^v$, where

$$(k_c{}^v)^2=E_c{}^v+\frac{4M}{(n-|\Delta n|)^2}\ . \tag{2.9}$$

As surmised by Condo,[1] the Auger rates for circular orbits are very sensitive to $|\Delta n|$: An increase of 1 in the value of $|\Delta n|$ generally causes P_A to decrease by 3 orders of magnitude. Detailed explanations of this dependence on $|\Delta n|$ may be found elsewhere.[1,9,10]

With only two exceptions, Fig. 1 shows Auger rates for $|\Delta n| = |\Delta n|_{\min}$, where $|\Delta n|_{\min}$ is the lowest energetically allowed value of $|\Delta n|$, as determined by the variational calculation given in Ref. 5. In order to emphasize the dependence of P_A on $|\Delta n|$, even if $|\Delta n|_{\min}$ is associated with a relatively low value of $(k_c{}^v)^2$, Fig. 1 shows values of P_A for both $|\Delta n|_{\min}=2$ and $|\Delta n|=3$ in the case of the αK^-e^- atom with $n=23$, and also for both $|\Delta n|_{\min}=3$ and $|\Delta n|=4$ in the case of the $\alpha\bar{p}e^-$ atom with $n=32$. The respective values of $(k_c{}^v)^2$ for this level of the αK^-e^- atom are 0.16 and 0.96 Ry; and for the $\alpha\bar{p}e^-$ atom they are 0.09 and 0.60 Ry. In both instances, the transition with the lower value of $|\Delta n|$ is much more favored.

As noted in Ref. 5, the variational calculation given there only leads to a lower limit to $|\Delta n|_{\min}$. However, some more elaborate calculations in Ref. 5 indicate that the only instance considered in the present paper for which this variational calculation appears to lead to an underestimate is the $n=29$ level of the αK^-e^- atom. In this case, $|\Delta n|_{\min}$ is probably 5 instead of 4.

Figure 1 also shows the meson decay rates and the radiative rates. The radiative rate P_R is calculated assuming that the initial and final states of the mesonic atom are adequately represented by products of hydrogenic functions whose effective nuclear charges are determined by the variational calculation given in Ref. 5. This rate is given by

$$P_R=1.34\times10^9E_\gamma{}^3\left(\frac{4z_iz_f}{(z_i+z_f)^2}\right)^3$$

$$\times\frac{n(n-1)^3}{M^2Z_f^2}\left(\frac{4n(n-1)Z_iZ_f}{[nZ_f+(n-1)Z_i]^2}\right)^{2n+1}\ \text{sec}^{-1}. \quad (2.10)$$

The initial state is a circular orbit with principal quantum number n, and the final state is a circular orbit with principal quantum number $n-1$. In Eq. (2.10) the effective nuclear charges for the electron and the meson are denoted by z_i and Z_i for the initial state, and by z_f and Z_f for the final state. The energy of the photon is denoted by E_γ. The radiative rates shown in Fig. 1 were computed assuming that E_γ is given with sufficient accuracy by the difference between the values of $E_c{}^v$ for the two states in question.

III. POSSIBLE INACCURACIES IN COMPUTED TRANSITION RATES

Because the values of P_A shown in Fig. 1 depend so sensitively on the values of Δn, it seems necessary to determine the extent to which the use of approximate wave functions and binding energies may affect the accuracy of these computed transition rates. Some rough estimates of possible inaccuracies can be obtained by repeating the calculations with different values of the effective charges and energy differences and trying to guess which values of these parameters might lead to more accurate results. For the atoms which are being considered here, all values of the effective nuclear charges which are in any way realistic must lie between 1.0 and 2.0. And since the variational energy $E_c{}^v$ is an overestimate of the binding energy, the value of k must lie between zero and $k_c{}^v$ for an energetically allowed transition.

Only two cases are given detailed consideration in estimating the accuracy of the computed Auger rates; but because in some respects these two cases represent contrasting physical situations, it is assumed that the scope of the investigation is sufficiently general. One case is the $\alpha\pi^-e^-$ atom with $n=18$, and the other is the αK^-e^- atom with $n=27$. Although in both instances $\Delta n=-4$, the relative values of the mean electron and meson orbital radii $\bar{r}_e$ and $\bar{r}_\mu$ are quite different. Table I gives the values of z, Z, $\bar{r}_e$, $\bar{r}_\mu$, and $(k_c{}^v)^2$ for these two cases, as determined by the variational calculation described in Ref. 5.

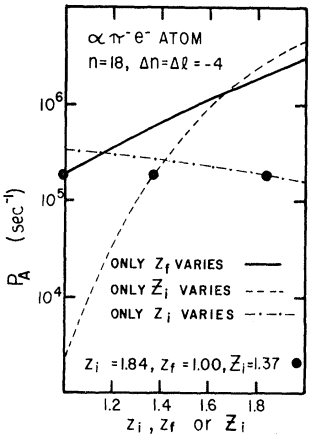

FIG. 2. Behavior of the calculated Auger rate P_A for the circular orbits of the $\alpha\pi^-e^-$ atom with $n=18$ if the values of z_i, z_f, and Z_i are varied separately. All calculations were performed with $k^2=(k_c{}^v)^2=0.46$ Ry.

Figures 2 and 3 show the behavior of P_A if the values of z_i, Z_i, and z_f are varied separately, with $k=k_c{}^v$ in each instance. Since the computed Auger rate is very sensitive to the values of these three parameters, particularly Z_i, it is apparent that in some instances the use of approximate wave functions may result in a substantial error.

More restricted limits on possible inaccuracies in the computed values of P_A can be determined if it can be established roughly what values of z_i, Z_i, and z_f give the most accurate wave functions for the particular purpose of computing Auger rates. The electron wave function depends more or less adiabatically on the position of the much more slowly moving meson. In particular, as r_μ becomes smaller the electron becomes more effectively shielded from the field of the α particle, and its wave function attains a greater spatial extent.[11] Since the ejected electron has a low energy and a relatively high orbital angular momentum, the amount of overlap between the initial and final electron wave functions becomes larger as r_μ becomes smaller, although the effect of this on the transition matrix element is surely offset to some extent by a decrease in the effectiveness of the perturbing multipole interaction. The behavior of

TABLE I. Effective nuclear charges, mean orbital radii, and Auger transition energies for some circular orbits of the $\alpha\pi^-e^-$ and αK^-e^- atoms. The unit of distance is the hydrogen Bohr radius, which is denoted by a_0.

Atom	n	z	Z	$\bar{r}_e$ (a_0)	$\bar{r}_\mu$ (a_0)	$(k_c{}^v)^2$ (Ry)
$\alpha\pi^-e^-$	18	1.84	1.37	0.82	0.92	0.46
αK^-e^-	27	1.36	1.87	1.10	0.47	0.52

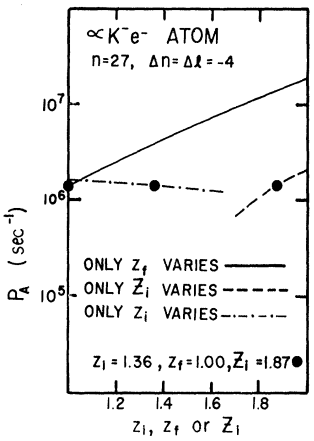

FIG. 3. Behavior of the calculated Auger rate P_A for the circular orbits of the $\alpha K^- e^-$ atom with $n=27$ if the values of z_i, z_f, and Z_i are varied separately. All calculations were performed with $k^2=(k_c^{\,v})^2=0.52$ Ry.

the initial wave function for relatively small values of r_μ is important because, as shown in Ref. 5, the initial and final meson radial wave functions are sharply peaked and rather well separated. The radial wave functions are particularly well separated if $|\Delta n|$ is relatively large, as it is in the two cases which are considered here. These meson wave functions overlap to the greatest extent at values of r_μ which are rather smaller than the mean orbital radius $\bar{r}_\mu$ for the initial state. In this region of greatest overlap between the meson wave functions, the meson in the initial state is less effectively shielded from the field of the α particle than it is if $r_\mu=\bar{r}_\mu$, because the spatial extent of the electron wave function increases as r_μ becomes smaller. Therefore, it seems reasonable to expect that those values of z_i and Z_i which give the most accurate wave functions, at least for the purpose of computing Auger rates, should satisfy the conditions $z_i<z$ and $Z_i>Z$. Also, it seems reasonable to assume that final-state interactions can be taken into account approximately by employing some value of z_f which satisfies the condition $1.0<z_f\leq z_i$.

An examination of Figs. 2 and 3 shows that any change in the values of z_i, Z_i, and z_f that is compatible with the preceding considerations would result in an increase in the computed Auger rate. However, the largest possible change in P_A is much different for the two cases being considered. Since the meson orbit is well inside that of the electron in the case of the $\alpha K^- e^-$ atom, there is less uncertainty about the adequacy of the approximate wave function for this system. In order to obtain rough limits on the amounts by which the computed values of P_A can vary if the effective charges are permitted to have any values which are at all compatible with the preceding considerations, the Auger rates for these two cases are shown in Fig. 4 as functions of z_i, it now being assumed that $Z_i=2.0$, $z_f=z_i$, and $k=k_c^{\,v}$. Since Figs. 2 and 3 indicate that P_A varies more rapidly with z_f than it does with z_i, not only the condition $Z_i=2.0$, but also the condition $z_f=z_i$, causes an increase in the computed value of P_A for all values of z_i in the interval $1.0\leq z_i\leq 2.0$. If it is further assumed that $z_i=z$, the values of P_A for the $\alpha\pi^- e^-$ and $\alpha K^- e^-$ atoms in Fig. 4 are found, respectively, to be 272 and 4 times larger than the values shown in Fig. 1. These numbers are probably substantial overestimates of the factors by which inaccuracies in the radial wave functions, or at least those inaccuracies which occur not too far from the α particle, cause the estimated Auger rates in these two instances to be in error. Another source of error, which is due to the behavior of the initial electron wave function at relatively large distances from the origin, is discussed below.

The inaccuracies which are introduced by assuming that $z_i=z$, $Z_i=Z$, and $z_f=1.0$ obviously depend on the relative values of $\bar{r}_e$ and $\bar{r}_\mu$. It is shown in Ref. 5 that those circular orbits of a mesonic atom with binding energies approximately equal to that of a He atom, which are generally supposed to be the circular orbits most likely to be formed when a meson is stopped in helium, have values of $\bar{r}_e$ substantially larger than $\bar{r}_\mu$. The $\alpha K^- e^-$ atom with $n=27$ being given detailed consideration in the present paper is an example of such circular orbits. Therefore, in these instances, the use of the variational wave functions obtained in Ref. 5

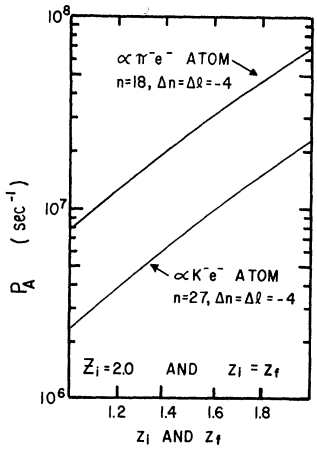

FIG. 4. Behavior of the calculated Auger rate P_A for some circular orbits of the $\alpha\pi^- e^-$ and $\alpha K^- e^-$ atoms if $Z_i=2.0$, and if z_f is set equal to z_i and then varied. The calculations were performed assuming that $k^2=(k_c^{\,v})^2=0.46$ Ry for the $\alpha\pi^- e^-$ atom with $n=18$ and $k^2=(k_c^{\,v})^2=0.52$ Ry for the $\alpha K^- e^-$ atom with $n=27$.

seems likely to lead to estimates of the Auger rates with errors which are negligible compared with the calculated rates for transitions with smaller values of $|\Delta n|$.

The preceding estimates attempt to take into account those correlations in the wave functions which depend on the radial coordinates r_e and r_μ. However, there are also correlations which depend on the angular coordinates $\hat{r}_e$ and $\hat{r}_\mu$. In particular, the electron wave function depends to some extent on the position of the much more slowly moving meson. The distortion of the electron wave function depends on r_e, r_μ, and $\hat{r}_e \cdot \hat{r}_\mu$. The magnitude of this distortion is largest if $r_e \simeq r_\mu$ and $\hat{r}_e \cdot \hat{r}_\mu \simeq 1$. For mesonic atoms with binding energies approximately equal to that of a He atom, the relative change in the electron wave function due to the dipole interaction of the electron with the meson is found in Ref. 5 to be less than ~20% if $r_e \simeq \bar{r}_\mu$. Therefore, it seems reasonable to assume that the effect of this distortion of the electron wave function on the Auger rate is not large compared with the other effects which are considered above.

Figure 5 shows the behavior of P_A if k^2 is varied, it being assumed that $z_i = z$, $Z_i = Z$, and $z_f = 1.0$. Since P_A increases as k^2 becomes larger, any inaccuracy in the value of $E_c{}^v$, unlike those inaccuracies in the radial wave functions which are discussed above, causes the Auger rate to be overestimated. The extent of this overestimate depends largely on the relative amount by which $(k_c{}^v)^2$ differs from the exact energy E_A of the Auger electron. Some fairly detailed estimates in Ref. 5 indicate

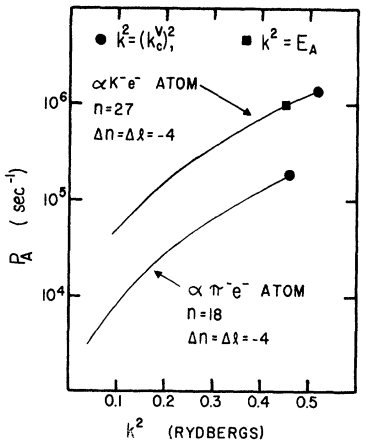

FIG. 5. Behavior of the calculated Auger rate P_A for some circular orbits of the $\alpha\pi^-e^-$ and αK^-e^- atoms if the value of the kinetic energy k^2 of the ejected electron is varied. The calculations were performed assuming that $z_i = 1.84$, $Z_i = 1.37$, and $z_f = 1.00$ for the $\alpha\pi^-e^-$ atom with $n = 18$ and $z_i = 1.36$, $Z_i = 1.87$, and $z_f = 1.00$ for the αK^-e^- atom with $n = 27$.

TABLE II. Some estimates of the kinetic energy of the ejected electron for Auger transitions of an αK^-e^- atom in a circular orbit with principal quantum number n.

n	$\Delta n = \Delta l$	$(k_c{}^v)^2$ (Ry)	E_A (Ry)
29	−5	0.51	0.43
	−4	0.04	
28	−4	0.27	0.20
27	−4	0.52	0.45
26	−3	0.19	
25	−3	0.41	
24	−3	0.67	
23	−3	0.96	
	−2	0.16	
22	−2	0.38	

that the magnitude of this difference probably does not exceed 0.1 Ry in each of the instances for which an Auger rate is given in Fig. 1. In the particular case of the αK^-e^- atom with $n = 27$, for which an estimate of E_A has been made in Ref. 5, this results in an inaccuracy of about 40%, as indicated in Fig. 5. Although for smaller values of E_A the relative inaccuracy can be larger, in most instances it would not be very much larger, because the values of $(k_c{}^v)^2$ for the two instances considered in Fig. 5 are fairly typical. Table II gives values of $(k_c{}^v)^2$ and, in two instances, estimates of E_A, as determined in Ref. 5, for some circular orbits of the αK^-e^- atom. With the exception of the level with $n = 29$, for which a transition with $\Delta n = -4$ is apparently not energetically allowed, the value of $(k_c{}^v)^2$ in most of these instances is probably large enough to allow it to be used as an approximate value of E_A without causing the Auger rate to be overestimated by more than about a factor of 2.

Since the final electron wave function is a rapidly increasing function of r_e, even at relatively large distances from the origin, it would seem necessary to investigate more carefully the behavior of the initial electron wave function at a distance of several hydrogen Bohr radii from the α particle in order to be sure that the results given in Fig. 1 do not seriously underestimate the Auger rates. This can be done by regarding the exact wave function Φ for a circular orbit as being expanded in eigenfunctions of the operator

$$H_c = -\nabla_e{}^2 - \frac{4}{r_e} - \frac{1}{M}\nabla_\mu{}^2 - \frac{4}{r_\mu} + H_0', \qquad (3.1)$$

where H_0' is the monopole interaction between the electron and the meson, as defined by Eq. (2.1b). The orbital angular momentum operators for both the electron and the meson commute with H_c. The exact wave function Φ for a circular orbit with principal quantum number n is composed predom-

inantly of eigenstates of H_c in which the meson has orbital angular momentum $n-1$ and the electron has orbital angular momentum zero. However, since to some extent the meson and the electron share the total orbital angular momentum of the atom, there are components of Φ in which the meson has orbital angular momentum n or $n-2$ and the electron has orbital angular momentum 1. In the contribution to Φ which is most likely to overlap appreciably with the final electron wave function at a distance of several Bohr radii from the origin, the electron is in an almost hydrogenic $2p$ state for which the effective nuclear charge is very nearly equal to 1. It is now assumed that, if the z component of the orbital angular momentum of the mesonic atom is m, this contribution to Φ, which is denoted by Φ_{2p}, can be adequately represented by

$$\Phi_{2p} \simeq b_{2p} u_{2p}(r_e) R_{n-1}(r_\mu) \times \sum_{\nu=-1}^{1} (1, n-2, \nu, m-\nu \mid 1, n-2, n-1, m) \times Y_{1,\nu}(\hat{r}_e) Y_{n-2,m-\nu}(\hat{r}_\mu) , \qquad (3.2)$$

where b_{2p} is an amplitude, $u_{2p}(r_e)$ is the normalized radial wave function for an electron in a $2p$ state with effective nuclear charge 1, and $R_{n-1}(r_\mu)$ is the normalized radial wave function for a meson in a circular hydrogenic orbit with principal quantum number $n-1$ and effective nuclear charge of 2. If the meson mean orbital radius $\bar{r}_\mu$ is substantially less than that of the electron in the initial state, or in other words if Z is not too much smaller than 2, this approximate representation of Φ_{2p} should be fairly satisfactory, at least for the purpose of determining whether or not the electron $2p$ state can possibly have an appreciable effect on the Auger rate. The effect on the Auger rate is likely to be overestimated, because in this representation of Φ_{2p} the meson is assumed to have orbital angular momentum $n-2$, and the lowest nonvanishing transition multipole matrix element is therefore surely larger than it would be if the meson were assumed to have orbital angular momentum n. Of course, assuming that the effective nuclear charge for the meson is 2 in this representation of Φ_{2p} is also likely to cause the Auger rate to be overestimated.

The amplitude b_{2p} is now assumed to be given accurately enough by an estimate which is made in Ref. 5. This estimate is obtained by first assuming that the meson is a stationary classical point charge situated on the z axis a distance $\bar{r}_\mu$ from the origin and then using perturbation theory to calculate, for the ground state of this system, the amplitude for the electron being in the $2p$ state with $m=0$ of the unperturbed Hamiltonian

$$H_{de} = -\nabla_e^2 - \frac{4}{r_e} + \begin{pmatrix} 2/\bar{r}_\mu, & r_e < \bar{r}_\mu \\ 2/r_e, & r_e > \bar{r}_\mu \end{pmatrix} . \qquad (3.3)$$

This semiclassical estimate is not likely to give the correct phase of b_{2p}.

In view of the approximations which have already been made, it would seem permissible to ignore the requirement that contributions to a transition amplitude be added coherently. Therefore, it is assumed that a rough indication of the importance of electron $2p$ states can be obtained by replacing Ψ_i and $H'_{|\Delta n|}$ in Eq. (2.2) by Φ_{2p} and $H'_{|\Delta n|-1}$, respectively. The rate which is then obtained is denoted by $P_A^{(2p)}$. Since $\bar{r}_\mu$ is much smaller than the mean orbital radius of the $2p$ electron, it is assumed that the multipole interaction $H'_{|\Delta n|-1}$ in the expression for $P_A^{(2p)}$ is given accurately enough for all values of r_e and r_μ by its exact form for $r_\mu < r_e$, as specified by Eq. (2.1b). It can then be shown that $P_A^{(2p)}$ is given by

$$P_A^{(2p)} = 1.65\times10^{17}[(n-2, |\Delta n|-1, 0, 0 \mid n-2, |\Delta n|-1, n-|\Delta n|-1, 0)]^2 B J^2 k \ \text{sec}^{-1} , \qquad (3.4)$$

where

$$B = \frac{|\Delta n|}{8(2|\Delta n|+1)(2|\Delta n|-1)} \left(\frac{n-|\Delta n|}{4M}\right)^{2|\Delta n|-2} \times \left(\frac{(2n-2|\Delta n|)(2n-2)}{(2n-|\Delta n|-1)^2}\right)^{2n-1} \frac{(2n-2)!}{(2n-2|\Delta n|)!} , \qquad (3.5)$$

$$J = \int_0^\infty L_{|\Delta n|}(kr_e) r_e^{-|\Delta n|+2} e^{-r_e/2} dr_e . \qquad (3.6)$$

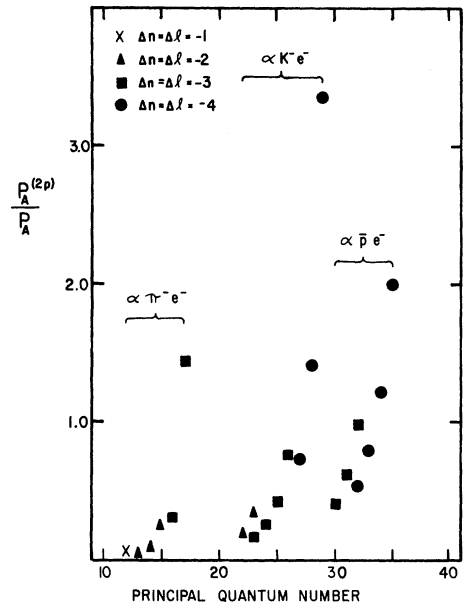

FIG. 6. Ratio $P_A^{(2p)}/P_A$ for some circular orbits of the $\alpha\pi^-e^-$, αK^-e^-, and $\alpha\bar{p}e^-$ atoms.

Figure 6 shows values of the ratio $P_A^{(2p)}/P_A$, where P_A is the computed Auger rate given in Fig. 1. These results indicate that in some instances the corrections due to the electron $2p$ states may be as important as some of the other corrections which have been considered. However, they are not large enough to affect the conclusions of the present paper.

A similar calculation of the effect of the electron $3d$ states was performed. It was found that these states have an entirely negligible effect on the Auger rate, probably because the wave function for the ejected electron is no longer a steeply rising function of r_e at distances from the origin where the $3d$ wave function is large.

The accuracy of the radiative rates shown in Fig. 1 also can be investigated by varying the values of the effective charges and transition energies. Since $\Delta n = -1$ for a radiative transition from a circular orbit, there is usually not too large a difference between the effective nuclear charges for the initial and final meson wave functions, and consequently for a given initial state the estimate of the matrix element for this process is more accurate than that for an Auger transition. For example, if both Z_i and Z_f in Eq. (2.10) are equated to the value of Z for the final state, the calculated radiative rate is increased by 47% in the case of the $\alpha\pi^-e^-$ atom with $n=18$ and by 2% in the case of the αK^-e^- atom with $n=27$. Also, in every instance it is found that replacing both z_i and z_f in Eq. (2.10) by the value of z for the final state causes P_R to change by less than 1%. If, as is indicated by some estimates that are made in Ref. 5, the errors in the values of E_γ are less than 0.01 Ry, the resulting inaccuracy in the calculated radiative rate is less than about 15% in every instance for which a value of P_R is given in Fig. 1.

IV. SUMMARY

The calculations presented in Secs. II and III establish that the Auger rates for circular orbits do indeed decrease very rapidly as $|\Delta n|_{\min}$ becomes larger; but due to inaccuracies in the wave functions that were used, the Auger rates shown in Fig. 1 are in some instances probably only accurate to within 1, or perhaps even 2, orders of magnitude. However, for those circular orbits with binding energies roughly equal to that of a He atom, the Auger rates shown in Fig. 1 are probably accurate to within a factor of 2 or 3. Furthermore, the circular orbits of the αK^-e^- atom with $n \geq 27$ have Auger rates which are less than the K^- decay rate, and the circular orbits of the $\alpha\bar{p}e^-$ atom with $n \geq 33$ have Auger rates which are less than the radiative rate.

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Multistate Impact-Parameter Calculation of Atom-Atom Excitation Cross Sections: Excitation of Atomic Hydrogen by Neon, Argon, and Krypton†

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Excitation cross sections for the collisions H(1*s*) + Ne, Ar, Kr → H(2*s*, 2p_0, 2$p_\pm$) + Ne, Ar, Kr are calculated over the velocity range of 0.3–5.0 a.u. in the distorted Born, two-state (for argon only), and four-state impact-parameter approximations that do not allow for electron exchanges between the colliding atoms. The results are compared with earlier first Born and scaled first Born calculations and with experimental data. The four-state cross sections, while greatly reduced from the first Born results, are still between three and ten times greater than experiment. Polarization fractions are also calculated from the four-state cross sections and compared with experimental data and with previous calculations.

I. INTRODUCTION

In a recent paper, to be referred to as I, Levy[1] presented a general method for evaluating the time-dependent matrix elements occurring in multistate impact-parameter calculations of atom-atom inelastic collisions. The method does not allow for electron exchanges between projectile and target atoms, but it does permit the inclusion of all the direct couplings.

First Born wave calculations[2] of excitation and ionization cross sections for H(1*s*) in collision with rare gases in their ground states gave values for the heavier target atoms that are many times larger than the experimental values, even at high incident velocities. However, the substitution of a velocity-dependent scaling factor $\eta_B(v_1)$ [determined by fitting theoretical ionization cross-section calculations to experimental results] for Z_B, the nuclear charge of the target atom B in the cross-section equations resulted in good agreement between theoretical and experimental excitation cross sections for neon, argon, and krypton targets.

While the use of velocity-dependent scaling factors was successful in this instance, it was not possible to isolate the physical effects most responsible for the large deviation of the first Born wave calculations from experiment.

In this paper, the effects of distortion, coupling to the initial state, and couplings among the final excited states (2p_0, 2p_+, 2p_-, and 2*s*) are considered in order to determine their importance as corrections to the first Born wave treatment.

II. THEORY

The general formulation of multistate impact-parameter calculations and, in particular, the means of evaluating the required time-dependent matrix elements have been presented in I and will not be discussed here in great detail.

We wish to solve the truncated set of coupled differential equations:

$$i\dot{a}_n(t) = \sum_{m=1}^{N} a_m(t) V_{nm}[\vec{R}(t)](e^{itE_{nm}}), \quad n = 1 \to N, \tag{1}$$

where $E_{nm} = E_n - E_m$ is the transition energy, (2)

and

$$V_{nm}[\vec{R}(t)] = \int d\vec{r}_A \int d\vec{r}_B \, \phi_i^{A*} \phi_u^{B*} \times V[\vec{r}_A, \vec{r}_B, \vec{R}(t)] \phi_j^A \phi_v^B \tag{3}$$