Probability of internal ionization during β^+ decay: Importance of the direct-collision mechanism

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A theory of the ionization of inner-shell electrons during β^+ decay is obtained by modifying a theory of inner-shell ionization during β^- decay presented previously. The theory includes the contributions of both the shakeoff and direct-collision mechanisms and yields results whose relative accuracy is of order $Z\alpha$. Numerical results for the K-shell ionization probability are presented for several nuclides, including ^{58}Co, ^{64}Cu, and ^{65}Zn; they demonstrate that, contrary to the β^- case, the direct-collision mechanism plays an essential role in inner-shell ionization during β^+ decay, confirming a conjecture by Law. When compared with the results of recent experiments, they are found to give significantly better agreement than do the results of previous theoretical work.

Inner-shell ionization during β decay is a subject whose beginnings may be traced to two pioneering theoretical papers by Feinberg[1] and Migdal.[2] In these seminal works the two basic mechanisms by which an internal ionization event can occur were identified as (i) the shakeoff (SO) mechanism which attributes the transition to the sudden change in nuclear charge, and (ii) the direct-collision (DC) mechanism according to which the transition results from a Coulomb interaction between the emerging β particle and an inner-shell electron. Feinberg, in particular, stressed the predominance of the SO mechanism, estimating that the relative contribution of the DC mechanism to P_K, the total probability per β decay for internal ionization of the K shell, is of order $|B_K/\bar{E}_\beta|$, where B_K is the binding energy of a K-shell electron and $\bar{E}_\beta$ is the average kinetic energy of the β particle.

Subsequent theoretical studies[3] were strongly influenced by Feinberg's assessment and resulted in the development of a more refined theory for the SO process—based on relativistic hydrogenic wave functions—culminating in the SO theory of Law and Campbell,[4,5] as corrected by Isozumi, Shimizu, and Mukoyama.[6] And in all of these studies the contribution of the DC mechanism was either completely ignored or corrected for by means of Born-approximation results of simple *ad hoc* prescriptions based on Feinberg's estimate.

These theoretical advances were paralleled by a steady increase in the number and precision of experiments devoted to the measurement of P_K; indeed, since 1970 a large number of reports on high-precision experiments have appeared in the literature.[7] By 1977 it was quite clear that a systematic discrepancy between the predictions of the corrected SO theory and experiment existed with respect to P_K. Indeed, for over 20 different β^- emitters the calculated values of P_K were found to be roughly $\frac{1}{2}$ the experimentally determined values.[8]

This striking disagreement led many authors to suggest that, Feinberg's estimate not withstanding, the contribution from the DC mechanism may be much larger than had been assumed previously and that a more refined theoretical treatment was needed. In response, theoretical studies of the internal ionization process in which both the SO and DC contributions were included *ab initio* were undertaken by Batkin *et al.*[9] and by the present author.[10–12] Since the principal purpose of these calculations was to provide a definitive assessment of the relative importance of the two basic mechanisms (rather than to generate accurate numerical values for P_K), nonrelativistic hydrogenic wave functions were employed in both to simplify the analysis. However, the two calculations did differ with regard to the choice of Green's function, that used by the present author yielding the more accurate results.

To facilitate these calculations an angular momentum expansion was used to represent the wave function of each of the outgoing electrons. This resulted in a partial-wave expansion for the DC amplitude and for P_K, a result of the form

$$P_K = P_K(\mathrm{SO}) + P_K(I) + \sum_{l=0}^{\infty} P_K^{(l)}(\mathrm{DC}) , \tag{1}$$

where $P_K(\mathrm{SO})$ is the K-shell ionization probability due to SO alone and $P_K(I)$ is the contribution associated with interference between the SO and DC amplitudes. The last set of terms represents the partial-wave expansion for $P_K(\mathrm{DC})$, the K-shell ionization probability due to DC alone.

Focusing on β^- emitters having low β end-point energies E_0 and relatively large values for the ratio B_K/E_0, the present author (Ref. 11) obtained essentially exact numerical results for P_K for three nuclides of interest. The criteria by which they were selected insured rapid convergence of the partial-wave expansion while identifying, via Feinberg's estimate, situations for which the DC contribution should be relatively large. However, for all three cases it was found that the inclusion of the DC contribution in the calculation of P_K resulted in an increase in the result due to SO alone of not more than 15%, demonstrating that the DC mechanism cannot account for the factor of 2 discrepancy between experiment and the predictions of SO theory.

At about the same time a very different approach towards a more refined treatment of the internal ionization process was developed by Law and Suzuki.[13] These authors maintained the traditional view that the DC mechanism is not very important, and suggested that the discrepancy between SO theory and experiment could be resolved by considering the many-body aspects of the problem, and by evaluating the wave functions involved in the initial and final states more exactly. To this end, Law and Suzuki performed a calculation of $P_K(\mathrm{SO})$ using a relativistic self-consistent-field approach and assuming that the final state of the atom corresponds to a fully relaxed system with a K vacancy. Indeed, in this way they found that, for β^- emitters, generally good agreement between theory and experiment could be obtained, the remaining discrepancy being at most of the order of 10%. Law and Suzuki suggested that this remaining difference was due to a small DC contribution, a supposition consistent with the results of Intemann.[11]

However, when Law and Suzuki applied their theory to the β^+ emitter ^{64}Cu, they obtained for $P_K(\mathrm{SO})$ a value which is about a factor of 2 smaller than the results of two recent experiments.[14,15] Since then, additional measurements have been reported on two other β^+ emitters, ^{58}Co and ^{65}Zn.[16–18] Again, the measured values were found to be larger than the predictions of the Law-Suzuki theory by factors of 2 to 3.

To explain this striking failure of SO theory, Law[19] has recently advanced the proposition, based on an admittedly crude mathematical argument, that while the DC contribution will be (necessarily) quite small for β^- decay, it can be quite large for β^+ decay, and indeed may very well be sufficient to bring about agreement between theory and experiment for the β^+ case.

To confirm Law's conjecture, we have investigated the relative importance of the DC contribution to P_K for β^+ emitters using a suitably modified form of the theory previously developed by us for the study of internal ionization during β^- decay.[20] This theory is based on nonrelativistic hydrogenic wave functions and a Coulomb Green's function originally developed by Glauber and Martin,[21] and it yields results whose relative accuracy is of order $Z\alpha$. Thus for the relatively low-Z β^+ emitters that are in fact of interest, quite good results should be obtained.

The lowest-order Feynman diagrams corresponding to the process of internal ionization during β^+ decay are shown in Fig. 1. The amplitudes M_{SO} and M_{DC} describe

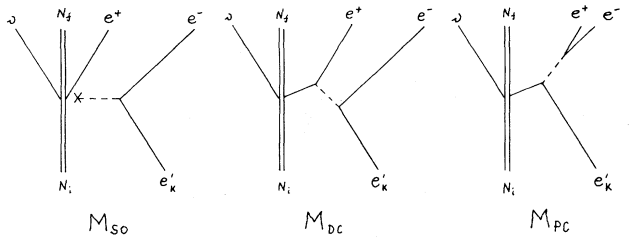

FIG. 1. Feynman diagrams for internal ionization during β^+ decay.

the SO and DC mechanisms, respectively, and are analogous to the two amplitudes which arise in the study of the β^- case. The amplitude M_{PC}, on the other hand, involves the (virtual) annihilation and creation of electron-positron pairs; it arises only in the β^+ case and, in principle, provides another channel for the process. However, because the available energy is generally much less than $2mc^2$, the amplitude M_{PC} is expected to be very small; indeed, in the approximation employed in this paper (as in I)—neglect of retardation effects and the use of nonrelativistic wave functions—the amplitude M_{PC} is identically equal to zero.

Thus, to apply the results of I to the β^+ case one need only change the sign of the charge of the outgoing β particle in the expressions for M_{SO} and M_{DC} obtained in I, and omit the exchange terms since the two final charged leptons are no longer indistinguishable. The effects of these modifications on the final result for P_K are readily traceable and may be summed up as follows.

For the β^+ case, Eqs. (37)—(41) of I are replaced by

$$P_K=\int_1^{W_K-1}dE_1\int_1^{W_K-E_1}dE_2\lambda_K(E_1,E_2)\ , \tag{2}$$

with

$$\lambda_K(E_1,E_2)=\frac{2^6\alpha^2(a')^3}{\pi\lambda_\beta}P_1P_2F_-(a,P_1)F_+(a,P_2)\times(W_K-E_1-E_2)^2(C_{\mathrm{SO}}+C_I+C_{\mathrm{DC}})\ , \tag{3}$$

$$F_\pm(a,P)=\pm(2\pi a/P)[\exp(\pm 2\pi a/P-1]\ , \tag{4}$$

$$\lambda_\beta=\int_1^{W_0-1}dE\,PF_+(a,P)(W_0-1-E)^2\ , \tag{5}$$

and

$$C_{\mathrm{SO}}=[f(P_1)]^2\ , \tag{6a}$$

$$C_I=-2f(P_1)\mathrm{Re}[U_0(P_1,P_2)]\ , \tag{6b}$$

$$C_{\mathrm{DC}}=\sum_{l=0}^{\infty}[(2l+1)\,|\,U_l(P_1,P_2)\,|^2+l\,|\,V_l(P_1,P_2)\,|^2+(l+1)\,|\,W_l(P_1,P_2)\,|^2]\ . \tag{6c}$$

Except as noted below, all quantities appearing in the above equations are defined as in I,[22] but with the understanding that now (P_1,E_1) refer to the ionized electron while (P_2,E_2) refer to the outgoing positron.

The energy-dependent functions U_l, V_l, and W_l which appear in (6) were originally defined in I by means of (A13)—(A15), along with (A7) and (23c). For the β^+ case, these definitions must be modified as follows: In (A13), $2a\rightarrow -2a$; in (A13)—(A15), $\eta\rightarrow-\eta$ and $a\rightarrow -a$ in $f_l(P_2,t_2)$, $f_{l-1}(P_2,t_2)$, and $f_{l+1}(P_2,t_2)$, respectively; in (A7), $a/P_2\rightarrow -a/P_2$ everywhere including the phase shift $\delta_{l'}(P_2)$.

As described in I, a considerable amount of numerical integration is required for the evaluation of the functions U_l, V_l, and W_l, the amount of computer time needed in-

TABLE I. Contributions to theoretical P_K probabilities for $^{151}_{62}$Sm in units of 10^{-7} assuming allowed β^- or β^+ decay. End-point energy is the same for both modes.

Mode	P_K(SO)	$P_K(I)$	$P_K^{(0)}$(DC)	$P_K^{(1)}$(DC)	$P_K^{(2)}$(DC)	P_K/P_K(SO)
β^- (actual)	7.09	−1.53	1.84	0.957	0.027 8	1.18
β^+ (hypothetical)	0.0903	0.0808	0.0351	0.158	0.003 66	4.07

creasing rapidly with l. This severely limits the number of terms in the partial-wave expansion for P_K(DC) which it is practical to evaluate; in our computations we have truncated the expansion for P_K(DC) which appears in (1) after the $l=2$ term.

For β emitters with very low end-point energies the partial-wave expansion for P_K(DC) is rapidly convergent and, as we have demonstrated elsewhere,[11] no appreciable error is incurred in truncating the expansion for P_K(DC) as described above. However, for the three β^+ emitters for which experimental data is currently available, the end-point energies are relatively large and truncation cannot be expected to yield accurate results. For this reason we prefer to examine first a somewhat hypothetical situation for which the truncated results are essentially exact, and where we have a controlled setting in which to compare the contributions of the SO and DC mechanisms for both β^- and β^+ decays.

The nuclide we have chosen is ^{151}Sm, a β^- emitter with an end-point energy of 76 keV, for which we have already reported theoretical results for P_K. Using the modified theory described above, we have computed the various contributions to P_K for ^{151}Sm under the assumption that this nuclide is a β^+ emitter with the same end-point energy as for the actual β^- case. The results of these computations, along with those of our earlier work,[11] are displayed in Table I.

It is evident from the values shown in the table that, relative to P_K(SO), both $P_K(I)$ and P_K(DC) are much larger for the β^+ case. Indeed, for this case $P_K(I)$ is comparable to P_K(SO) while P_K(DC) is twice as large. Furthermore, the interference term $P_K(I)$ is now positive and reinforces the contributions due to SO and DC alone whereas for the β^- case $P_K(I)$ is negative and, to a large extent, cancels the contribution due to DC alone. As a result, with the inclusion of the DC amplitude one obtains a total P_K which is four times larger than P_K(SO) for the β^+ case. By contrast, for the β^- case the resulting increase is only about 18%. Thus, at least for low end-point energy transitions, we have striking confirmation of the conjecture of Law.

At this point it is appropriate to consider why the DC amplitude is so much larger for the β^+ case.[23] Now, changing the sign of the charge of the β particle alters the Green's function which appears in $M_{\rm DC}$ as well as the wave function describing the final state of the β particle, this wave function appearing in both $M_{\rm SO}$ and $M_{\rm DC}$. Also, the antisymmetrization requirement (exchange terms) is omitted for β^+ decay. Of these three modifications, the latter two affect both amplitudes whereas the modification of the Green's function affects only $M_{\rm DC}$. Indeed, the principal effect of changing the sign of the charge in the final-state wave function appears to be the replacement of the Fermi function appropriate to an electron by one appropriate to a positron, this Fermi function being common to all the contributions to P_K. Thus, it appears that it is the modification of the Green's function that is responsible for the prominence of the DC mechanism in β^+ decay. To confirm this, we have run our computer program for ^{151}Sm with and without the final-state wave function and antisymmetrization modifications only, and have verified that the ratio P_K(DC)/P_K(SO) is indeed completely unaffected by these particular changes.

The nature of the modification of the Green's function $G_E(\vec{r},\vec{r}')$ is readily understood by recalling its familiar expansion in terms of the stationary states $\psi_\alpha(\vec{r})$,

$$G_E(\vec{r},\vec{r}')=\sum_\alpha \frac{\psi_\alpha(\vec{r})\psi_\alpha^\dagger(\vec{r}')}{(E_\alpha-E)}+\int d\alpha \frac{\psi_\alpha(\vec{r})\psi_\alpha^\dagger(\vec{r}')}{(E_\alpha-E)}\ , \tag{7}$$

in which the sum extends over all the bound states for a β^- particle in a nuclear Coulomb field while the integral is over the continuum of unbound states. For application to the β^+ case this expansion must be modified by deleting the entire bound-state sum and changing the sign of the charge of the β particle everywhere that it appears in each continuum wave function. Unfortunately, with the particular representation that was employed in I, we cannot exercise separate control over the sign of the β-particle charge and the presence or absence of the bound-state con-

TABLE II. Contributions to theoretical P_K probabilities in β^+ decay in units of 10^{-4}.

Z	E_0 (keV)	B_K/E_0	P_K(SO)	$P_K(I)$	$P_K^{(0)}$(DC)	$P_K^{(1)}$(DC)	$P_K^{(2)}$(DC)	P_K/P_K(SO)	$l_{\max}$
$^{58}_{27}$Co	474	0.0150	8.45	−0.657	0.593	1.02	3.75	1.56	8.6
$^{64}_{29}$Cu	656	0.0127	7.44	−0.852	0.434	0.661	2.92	1.43	10.0
$^{65}_{30}$Zn	330	0.0272	6.05	0.001	0.657	1.37	4.28	2.04	6.1

tribution. Thus, we cannot directly assess the relative importance of these two alterations experienced by the Green's function. However, we have run our computer programs with the Coulomb field "turned off" in the intermediate state for both the β^+ and β^- cases. This has the effect of eliminating the bound-states contribution for the β^- case and replacing the continuum Coulomb states by their free particle counterparts for both cases. The numerical results obtained strongly suggest that the loss of the bound states and the change in the sign of the charge for the continuum states are both important modifications, their roles being such that their effects tend to compensate one another. Hence, the effect of switching off the Coulomb field is found to be much more pronounced for the β^+ case where no compensation can occur.

Having established the importance of the DC process for the hypothetical β^+ emitter ^{151}Sm, we then considered ^{58}Co, ^{64}Cu, and ^{65}Zn, three allowed β^+ emitters for which experimental values for P_K are currently available. For all three of these nuclides the end-point energy is much larger than for ^{151}Sm; hence the partial-wave expansion for P_K(DC) will converge much more slowly and truncation after $l=2$ will yield no more than a lower limit for P_K(DC). Nevertheless, as is evident from the results displayed in Table II, even with truncation the prominence of the DC contribution is already unmistakable.

As expected, the first three partial-wave contributions to P_K(DC) now show no tendency towards convergence, and the listed values for $l_{\max}$ are indicative of the number of terms which must be included before we can expect to approach convergence. Nevertheless, the truncated results for P_K(DC) are already quite substantial, the most definitive of these being that for ^{65}Zn. For this particular nuclide it may be said that with the inclusion of the DC mechanism the resulting value for P_K is at least a factor of 2 larger than the value resulting from SO alone.

It should also be noted that for ^{58}Co and ^{64}Cu $P_K(I)$ is negative and relatively small—of the order of 10% of P_K(SO)—while for ^{65}Zn the interference term is practically zero. In contrast, for our hypothetical low end-point β^+ emitter ^{151}Sm $P_K(I)$ is positive and comparable in magnitude to P_K(SO). That interference effects are much more important for low-energy phenomena is, of course, to be expected from general quantum-mechanical considerations.

Although our truncated results fail to include fully the DC contribution to P_K, the results of Table II suggest that they do represent a substantial part of P_K(DC). Thus, it is of interest to place these results in perspective by comparing them with the recent theoretical results of Law and Suzuki[13] and with the available experimental data. This we have done in Table III, quoting experimental values from the references listed and attributing to Law and Suzuki those predictions by them which come closest to the experimental values.

TABLE III. K-shell internal ionization probabilities in β^+ decay.

Nuclide	$P_K(\times 10^{-4})$			
	Theory		Experiment	
	LS	Present work		Reference
^{58}Co	9.22	13.2	13.8±2.4	16
			16.6±2.1	17
^{64}Cu	8.25	10.6	13.2±0.8	14
			13.3±1.1	15
^{65}Zn	6.60	12.4	16.1±3.0	18

Now the predictions of Law and Suzuki were obtained from a SO calculation—using wave functions obtained from a relativistic self-consistent-field approach—and it is interesting to compare them with the nonrelativistic hydrogenic SO results which are listed in Table II under the column heading P_K(SO). It is immediately evident that the inclusion of relativistic and many-body effects causes the results of nonrelativistic hydrogenic SO theory to increase by only about 10%, an insignificant change considering the magnitude of the disagreement between theory and experiment. Rather, as the results of the present work show, it is the inclusion of the final-state interaction (i.e., the DC mechanism) which so greatly increases the predictions of SO theory and, the limitations inherent in the present work notwithstanding, leads to results which approach much more closely to the experimental values for P_K.

Whether a complete calculation of P_K(DC) will close the gap between theory and experiment for the case of β^+ decay remains to be seen. Presumably, agreement to better than about 10% will also require the inclusion of relativistic and many-body effects. To this end, further theoretical work is to be encouraged.

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[22]However, it should be noted that for the β^+ case $a'=(Z+1)\alpha$ where, as in I, Z is the charge number of the daughter nucleus.
[23]For a more intuitive explanation than is given in this paper, see the discussion contained in Ref. 19.