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Probability of internal ionization during nuclear β decay: Effect of final-state interaction

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A full calculation of the probability of ionization of a K-shell electron during nuclear β decay, including the effect of final-state interaction (direct-collision mechanism), has been carried out using nonrelativistic hydrogenic wave functions. Numerical results are presented for $^{63}_{28}$Ni, $^{107}_{46}$Pd, and $^{151}_{62}$Sm; they are found to be larger than the predictions of shake-off theory by 12–15%. A comparison with other recent theoretical results is made; significant differences are found.

It has long been recognized that there are two basic mechanisms by which an inner-shell electron can be ionized when a radioactive nuclide undergoes β decay: (i) The shake-off (SO) mechanism which attributes the ionization process to the sudden change in the nuclear charge and (ii) the direct-collision (DC) mechanism according to which an orbital electron is Coulomb scattered by the emerging β particle. In his pioneering paper[1] on internal ionization, Feinberg identified the predominant mechanism to be the SO process, with the DC process estimated to contribute, in most cases, only a small correction.

As a consequence of Feinbergs's assessment, essentially all subsequent theoretical studies on internal ionization dealt only with SO, leading to a highly refined model for this process.[2] Detailed calculations were carried out for the K shell, resulting in extensive numerical results for $P_K(\mathrm{SO})$, the total K-shell internal ionization probability per β decay due to the SO process. In these studies the contribution of the DC process was either totally ignored or corrected for by employing results based on the Born approximation or simple *ad hoc* prescriptions, procedures which are admittedly crude at best.

Theoretical developments were complemented by experimental work, undertaken by many groups,[3] devoted primarily to the determination of $\bar{P}_K$, the probability per β decay for the production of a hole in the K shell. Particularly during the last ten years, the application of high-resolution devices and new techniques has resulted in experimental data of sufficient precision to make possible a definitive test of the theoretical model. Indeed, until a few years ago there appeared to be good agreement between the theoretical results of Law and Campbell[4,5] and recent experimental data, agreement which was predicated on the assumptions that the contributions to $\bar{P}_K$ from shake-up transitions is very small and that the DC process can be neglected. However, due to the efforts of Isozumi, Shimizu, and Mukoyama,[6] it is now recognized that the Law-Campbell results for $P_K(\mathrm{SO})$ are too large by a factor of 2 due to a counting error. With this adjustment the most refined theoretical calculations of $P_K(\mathrm{SO})$ now yield results[7] which are consistently about one-half of the measured values of $\bar{P}_K$ for over 20 isotopes.

In an attempt to explain this discrepancy it has often been suggested that the contribution of the DC process, $P_K(\mathrm{DC})$ may be much larger than has been assumed on the basis of Feinberg's estimate.[6,8–13] Indeed, Feinberg[14] himself pointed out some years ago that his frequently quoted estimate, $P_K(\mathrm{DC})/P_K(\mathrm{SO}) \simeq B_K/E_\beta$, where B_K is the K-shell binding energy and E_β is the average β-particle kinetic energy, implies that the DC contribution will not be unimportant at very low energies. This is especially significant for nuclides with high Z values and small decay energies; for such nuclides the DC contribution to P_K may, in fact, be quite appreciable.

Stimulated by such conjecture, we have undertaken a complete calculation of the K-shell internal ionization probability, one in which both the SO and DC mechanism are included *ab initio*. Because of the complexity of the calculation we have limited our initial effort to allowed transitions and employed nonrelativistic hydrogenic forms to describe the various electronic states. Preliminary results of this work have been reported at a recent conference.[15] In this

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paper we report the first essentially exact results obtained from such a model for the K-shell internal ionization probability.

Ignoring the presence of those atomic electrons not participating in the internal ionization process, we regard the initial state of the system as consisting of a radioactive parent nucleus, of charge number Z', and a single K electron. Then the final state of interest consists of a daughter nucleus of charge number Z, a neutrino, and two unbound electrons. The amplitude for such a transition, mediated by the β interaction, is given by

$$M=(1-P_{12})\int d\vec{r}\,\phi_{1,2}^{(Z)\dagger}(0,\vec{r})\phi_K^{(Z')}(\vec{r})B\phi_\nu(0)\,, \quad (1)$$

for an allowed β transition when the nuclear matrix elements are reduced to nonrelativistic form. $\phi_{1,2}^{(Z)}$, $\phi_K^{(Z')}$, and ϕ_ν are the wave functions for the two final electrons, the initial K electron, and the final neutrino, respectively. The operator P_{12} interchanges the two final electrons and B is a 4×4 matrix containing the operative nuclear matrix elements.

The principal difficulty associated with the evaluation of Eq. (1) originates in the need to develop a reasonably accurate form for the wave function representing the final two-electron state, one in which two unbound electrons are moving under the combined influence of the nuclear Coulomb field and their own mutual repulsion. Provided that $Z \gg 1$, this is most readily accomplished by treating the electron-electron interaction as a perturbation on the nuclear Coulomb interaction and applying conventional time-independent perturbation theory. Working to first order, we obtain for the transition amplitude,

$$M=M_{\rm SO}+M_{\rm DC}\,, \quad (2)$$

with

$$M_{\rm SO}=(1-P_{12})\phi_1^{(Z)\dagger}(0)B\phi_\nu(0) \times\int d\vec{r}\,'\,\phi_2^{(Z)\dagger}(\vec{r}\,')\phi_K^{(Z')}(\vec{r}\,') \quad (3)$$

and

$$M_{\rm DC}=\alpha(1-P_{12})\int d\vec{r}\int d\vec{r}\,'\,\phi_1^{(Z)\dagger}(\vec{r})G_E(\vec{r},0) \times B\phi_\nu(0)\frac{1}{|\vec{r}-\vec{r}\,'|}\phi_2^{(Z)\dagger}(\vec{r}\,') \times\phi_K^{(Z')}(\vec{r}\,')\,. \quad (4)$$

Appearing in Eqs. (3) and (4) are continuum hydrogenic wave functions $\phi_1^{(Z)}$ and $\phi_2^{(Z)}$, corresponding to an unperturbed final state, and the Dirac-Coulomb Green's function $G_E(\vec{r},\vec{r}\,')$, characterized by an energy $E=E_1+E_2-E_K$ with E_1, E_2, and E_K denoting the total energy of each of the two final electrons and of the initial K electron, respectively.

The two contributions to M are readily identified with the SO and DC mechanisms, the latter accounting for the final-state interaction in first approximation. Due to the near orthogonality of $\phi_2^{(Z)}$ and $\phi_K^{(Z')}$ (since $Z'=Z-1$), the two contributions to M are of the same order in the fine-structure constant α. Thus both must be considered in a lowest-order calculation. Indeed, because the DC amplitude describes Coulomb scattering of the β particle from a virtual intermediate state, the DC process, like the SO process with which it is coherent, is a one-step process, i.e., one in which the two final electrons and the neutrino share statistically in the total available energy.

When calculating the DC amplitude, it is important to recognize that the summation over intermediate states, implied by the presence of the Green's function, is not restricted by the possible occupation of these states by other electrons. Although certain transitions are indeed forbidden when the intermediate state is occupied, the absence of these terms in the intermediate-states summation is exactly compensated for by the occurrence of processes in which the ionization of the obstructing electron precedes the transition of the β particle.

The calculation of $M_{\rm SO}$ in hydrogenic approximation is a relatively simple task, even when fully relativistic wave functions are employed. The evaluation of $M_{\rm DC}$, on the other hand, is far more difficult. Indeed, heretofore $M_{\rm DC}$ has not been fully evaluated nonrelativistically even in the Born approximation.

Born-approximation results are, of course, of little interest since $M_{\rm DC}$ exerts its greatest influence at very low energies where Coulomb effects are important. However, in this region relativistic effects are of secondary significance, although they cannot be completely ignored, even for low Z atoms, due to the presence of the intrinsically relativistic neutrino. Thus, we have sought to evaluate the DC amplitude exactly, obtaining results limited only by the use of nonrelativistic hydrogenic wave functions for the electronic states.

The Green's function needed for such a calculation is that simplified form of the Dirac-Coulomb Green's function introduced by Glauber and Martin[16] in their study of radiative electron capture and first applied to the study of β-decay processes by Spruch and Gold.[17] For ϕ_K we use the standard hydrogenic form; for the continuum hydrogenic wave function needed to describe the state of each final electron, we employ the expansion in angular momentum eigenstates appropriate to a scattering state.

The evaluation of $M_{\rm DC}$ can, for the most part, be carried out by means of standard analytical methods; however, some numerical integration is required. While the calculations are straightforward, their details are quite complicated. They will be described elsewhere as part of a broader study of the internal ionization process in which energy spectra and various correlation functions are examined for effects of

the DC amplitude. For now, we wish only to describe the form of the final expression for P_K and display the results of numerical computation for several nuclides of interest.

For P_K we have obtained a final result of the form

$$P_K = P_K(\mathrm{SO}) + P_K(\mathrm{I}) + \sum_{l=0}^{\infty} P_K^{(l)}(\mathrm{DC}) \ , \qquad (5)$$

where $P_K(\mathrm{SO})$ is the K-shell ionization probability due to (SO) alone and $P_K(\mathrm{I})$ is the contribution resulting from interference between the SO and DC amplitudes. The remaining terms represent the partial-wave expansion for $P_K(\mathrm{DC})$, the contribution due to DC alone.

It is evident from Eq. (5) that the SO and DC contributions are not purely additive, as has often been assumed, since an interference term survives the final integrations. But because of the spherical symmetry of the SO amplitude with respect to the relative direction of the two final electrons, only the s-wave part of M_{DC} contributes to $P_K(\mathrm{I})$.

Because the DC mechanism is important only at very low energies, its overall effect on P_K will be most pronounced for nuclides for which the K-shell binding energy B_K is large and the β end-point energy E_0 is small. The energy imparted to a K electron during its (virtual) collision with the β particle is then necessarily quite small, resulting in a limitation on the electron's final angular momentum estimated as $l_{\max} = r_0 P_{\max}$, where r_0 is the nuclide's first Bohr radius and $P_{\max}$ is the maximum momentum permitted the ejected electron by energy conservation. Beyond $l = l_{\max}$, the partial-wave expansion for $P_K(\mathrm{DC})$ should converge quite rapidly, an expectation which is borne out very well by the numerical results displayed in Table I.

While the ratio B_K/E_0 is not very large for $^{63}_{28}$Ni, it is the best candidate available from among known allowed β emitters. The other nuclides shown better satisfy our criteria of low decay energy and large B_K/E_0 ratio, but they decay by first forbidden transitions. The results shown for them are valid only in the ξ approximation.

Examination of the column headed $P_K(\mathrm{I})$ reveals that the SO and DC amplitudes interfere destructively, the interference being sufficiently strong to largely cancel $P_K^{(0)}(\mathrm{DC})$. This considerably reduces the overall effect of the DC mechanism on P_K.

For $^{107}_{46}$Pd and $^{151}_{62}$Sm, $P_K^{(1)}(\mathrm{DC})$ is considerably smaller than $P_K^{(0)}(\mathrm{DC})$, while for $^{63}_{28}$Ni these first two contributions are comparable. Considering the respective values of $l_{\max}$, this is not unexpected. In all three cases $P_K^{(2)}(\mathrm{DC})$ is at least an order of magnitude smaller than $P_K^{(1)}(\mathrm{DC})$, an indication of the rapidity with which the angular momentum expansion converges for low end-point energy transitions. For $^{107}_{46}$Pd and $^{151}_{62}$Sm, $P_K^{(2)}(\mathrm{DC})$ contributes only about 1% to $P_K(\mathrm{DC})$; for $^{63}_{28}$Ni its contribution is about 5%. Since the error associated with truncation of the expansion is comparable to the $l=2$ contribution, our numerical results for $P_K(\mathrm{DC})$ should be accurate to a few percent. The truncation error in the tabulated results for P_K is then never more than about 1%.

Thus, it appears that even under the most favorable circumstances the DC mechanism contributes only about 12–15% to the total P_K. While not an insignificant contribution, alone it is not nearly enough to account for the existing wide-spread discrepancy between theory and experiment.

To further refine the theoretical model relativistic and screening effects must be included; it is known that such corrections substantially increase $P_K(\mathrm{SO})$ and their influence on the total P_K is expected to be similar. For low-energy transitions this can be done by extending the calculations outlined in this paper to the relativistic domain and using wave functions which incorporate the effects of screening. But to determine if agreement between theory and experiment can thereby be achieved will require further theoretical work. [Indeed, Law and Suzuki[18] have recently used a relativistic self-consistent-field approach to include many-body effects in the determination of $P_K(\mathrm{SO})$, thereby achieving much better agreement with recent experimental results.]

After completion of this Communication there came to our attention a recent paper by Batkin *et al.*[19] reporting theoretical P_K probabilities for several nuclides, including two of those listed in Table I. From

TABLE I. Contributions to theoretical P_K probabilities in β decay in units of 10^{-4}. The first entry is an allowed (A) transition, followed by two first forbidden (1f) transitions. All theoretical results shown assume the transition to be allowed.

Z	Type	E_0 (keV)	B_K/E_0	$P_K(\mathrm{SO})$	$P_K(\mathrm{I})$	$P_K^{(0)}(\mathrm{DC})$	$P_K^{(1)}(\mathrm{DC})$	$P_K^{(2)}(\mathrm{DC})$	P_K	$P_K(\mathrm{SO})/P_K$	$l_{\max}$
$^{63}_{28}$Ni	A	67	0.134	2.06	−0.195	0.265	0.249	0.0241	2.41	0.86	2.4
$^{107}_{46}$Pd	1f	35	0.729	0.0037	−0.00062	0.00069	0.00045	0.000012	0.0042	0.88	0.6
$^{151}_{62}$Sm	1f	76	0.638	0.0071	−0.0015	0.0018	0.00095	0.000028	0.0084	0.85	0.7

their numerical results these authors conclude that the DC contribution is significant in all cases considered by them, the most dramatic being that of $^{151}_{62}$Sm for which they find that the DC contribution is *larger* than that of SO, comprising 55% of the total P_K.

The calculations of Batkin *et al.* are quite similar to those upon which our results are based, differing from ours only through the use of a more relatistic representation for the Fermi function and a completely nonrelativistic form for the Coulomb Green's function. Now it is easily shown that, for a low endpoint energy transition, refining the Fermi function serves only to alter the various contributions to P_K by a common multiplicative factor, leaving unaffected their relative importance. However, by using a fully nonrelativistic Green's function in their calculation, Batkin *et al.* have neglected terms greater than order $Z\alpha$; whereas by using the Glauber and Martin Green's function, we have neglected only terms of order $Z\alpha$. Evidently, the employment of this more accurate Coulomb Green's function in the calculation of M_{DC} results in a substantial reduction in the relative size of the contribution to P_K made by the DC mechanism. This is not entirely unexpected since a similar effect is known to occur in the theory of K-shell internal ionization during K electron capture.[20]

I wish to acknowledge a valuable conversation with Dr. J. Law regarding the work of Batkin *et al.*

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