PHYSICAL REVIEW A VOLUME 27, NUMBER 2 FEBRUARY 1983

Inner-shell ionization during nuclear β decay

Robert L. Intemann
Department of Physics, Temple University, Philadelphia, Pennsylvania 19122
(Received 9 August 1982)

A theory is developed of the ionization of inner-shell electrons during β decay. For allowed transitions it is shown that in the lowest order of the coupling constants the transition amplitude for the process is a sum of two terms, one of which attributes the ionization process to the sudden change in nuclear charge, and the other to a virtual scattering of an inner-shell electron by the emerging β particle. For the K-shell specific calculations are carried out using nonrelativistic hydrogenic wave functions and a Coulomb Green's function due to Glauber and Martin. Results whose relative accuracy is of order $Z\alpha$ are obtained for energy spectra, angular correlation functions, and the total internal ionization probability; numerical results are presented for the nuclides ^{63}Ni, ^{107}Pd, and ^{151}Sm. The role of the virtual-scattering mechanism is assessed and a comparison with other recent theoretical work is made.

I. INTRODUCTION

It is well known that nuclear β decay is sometimes accompanied by ionization (or excitation) of the electron cortege of the daughter atom, a higher-order process commonly referred to as internal ionization. A satisfactory description of the process requires that the decay be treated as a transformation of the whole atom, a formidable theoretical task which was first undertaken by Feinberg[1] and Migdal[2] in two pioneering papers. As these authors were first to recognize, there are two basic mechanisms by which an internal ionization transition can proceed, viz., (i) the shake-off (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 (virtual) Coulomb scattering of an orbital electron by the emerging β particle.

On the basis of estimates made by Feinberg[1] it became generally accepted that the dominant contribution to the internal-ionization probability comes from the SO mechanism, with the DC mechanism contributing, at most, a small correction. As a result, the SO process became the focus for subsequent theoretical work,[3–11] with detailed calculations usually restricted to the determination of P_K(SO), the total K-shell internal-ionization probability per β decay due to SO alone. In these studies the DC contribution was either completely ignored or corrected for by means of Born-approximation results[8] or simple *ad hoc* prescriptions based on Feinberg's estimate.[12] Of these SO calculations the most refined is that of Law and Campbell.[11]

The development of the theory of the SO process was paralleled by extensive experimental work, especially during the last ten years, primarily devoted to the measurement of $\bar{P}_K$, the probability per β decay for the production of a hole in the K shell. On the seemingly reasonable assumptions that the contribution to $\bar{P}_K$ from shake-up transitions is unimportant and the DC mechanism can be ignored [so that $\bar{P}_K \approx P_K$(SO)], excellent agreement with the Law-Campbell theory was obtained for a large number of nuclides.[13]

However, in 1977 it was pointed out by Isozumi, Shimizu, and Mukoyama[14] that, because of a counting error, the Law-Campbell results for P_K(SO) are too large by a factor of 2. And while initially this assertion generated a good deal of controversy, it was soon confirmed by Cooper and Åberg[15] and now there is general agreement that such an adjustment of the Law-Campbell results is indeed necessary. Thus, the previously established good agreement between theory and experiment was fortuitous, the revised theoretical values for P_K(SO) being roughly one-half the experimentally determined values for $\bar{P}_K$.

To explain this discrepancy, Isozumi, Shimizu, and Mukoyama[14] suggested that the DC contribution to $\bar{P}_K$ may be much larger than had been assumed from Feinberg's estimate so that a satisfactory theory of the internal-ionization process must take both mechanisms fully into account. Indeed, this suggestion has been offered with increasing frequency by various experimental groups[16–22] as a way of reconciling their data with the predictions of SO theory. Also, Feinberg himself has pointed out that his frequently quoted estimate

$$P_K(\mathrm{DC})/P_K(\mathrm{SO}) \approx B_K/E_\beta \ ,$$

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 has particular significance for nuclides with large charge number and a very small decay energy. For such nuclides the DC contribution to P_K, the total K-shell internal-ionization probability per β decay, may be quite pronounced.

Stimulated by such speculation regarding the role of the DC mechanism, we have undertaken a theoretical study of the internal-ionization process in which both the SO and DC mechanisms are included *ab initio*. In this paper we limit our considerations to allowed transitions and the use of nonrelativistic hydrogenic wave functions to describe the initial and final electronic states. Admittedly, such a treatment will not yield accurate quantitative results for heavy nuclides, but to obtain such is not our purpose. Rather we wish to examine the relative importance of the DC mechanism for the K-shell internal-ionization process, particularly under those circumstances which ought to be most favorable to the DC mechanism. To do this we shall carry out exact calculations within an approximation scheme whose relative accuracy is of order $Z\alpha$.

Some results of our work, including values for P_K and the various contributions to it for several nuclides of interest, have already been reported.[23,24] In the sections that follow we shall describe the calculations upon which these results are based. We shall also examine the DC mechanism for its influence on energy spectra and certain angular-correlation functions.

After completion of this study there came to our attention a recent paper by Batkin *et al.*[25] in which a similar investigation of the role of the DC mechanism is described. However, in their treatment Batkin *et al.* employ a completely nonrelativistic Coulomb Green's function rather than the more accurate Glauber-Martin Green's function which is utilized in our work. Consequently, as we have already pointed out,[24] Batkin *et al.* have omitted from their calculations terms larger than order $Z\alpha$; whereas in the calculations presented in this paper only terms of order $Z\alpha$ have been neglected.

II. TRANSITION AMPLITUDE FOR INTERNAL IONIZATION

The Hamiltonian for the radioactive system is

$$H = H_0 + H_\beta \ , \tag{1}$$

where H_β is the weak-interaction Hamiltonian responsible for β decay,

$$H_\beta = C_V \int d\vec{r}\, \bar{\psi}_p(\vec{r})\gamma_\mu(1+\lambda\gamma_5)\psi_n(\vec{r})\bar{\psi}_e(\vec{r}) \times \gamma_\mu(1+\gamma_5)\psi_\nu(\vec{r}) \ , \tag{2}$$

and the $\psi(\vec{r})$'s are the field operators for the quantized fields associated with the various particles. The Dirac γ matrices are defined by $\vec{\gamma} = -i\beta\vec{\alpha}$, $\gamma_4 = \beta$; they therefore obey the anticommutation relations $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$ ($\mu = 1,2,3,4$) and are Hermitian. We have $\gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4$, $\bar{\psi} = \psi^\dagger\gamma_4$, and $\lambda = |C_A/C_V|$, where C_V and C_A are the vector and axial-vector coupling constants of the β interaction.

The unperturbed Hamiltonian H_0 is the sum of nuclear, atomic, and neutrino contributions:

$$H_0 = H_N + H_A + H_\nu \ , \tag{3}$$

in which H_ν is the Hamiltonian for the free neutrino field and H_N is the Hamiltonian of the nucleus (in the absence of the weak interaction). The atomic Hamiltonian is usually written as

$$H_A = \int d\vec{r}\, \psi_e^\dagger(\vec{r}) h_C(\vec{r}) \psi_e(\vec{r}) + \tfrac{1}{2} \int d\vec{r} \int d\vec{r}\,' \psi_e^\dagger(\vec{r}\,')\psi_e^\dagger(\vec{r}) \frac{\alpha}{|\vec{r}-\vec{r}\,'|} \times \psi_e(\vec{r})\psi_e(\vec{r}\,') \ , \tag{4}$$

a form in which the vector part of the electromagnetic interaction and associated retardation effects are neglected. The single-particle Dirac-Coulomb Hamiltonian $h_C(\vec{r})$ is given by

$$h_C(\vec{r}) = \alpha\cdot\vec{\mathrm{P}} + \beta - \alpha Z/r \ , \tag{5}$$

where Z is the nuclear charge-number operator. The units employed are those in which $m = c = \hbar = 1$ and $e^2 = \alpha \approx \frac{1}{137}$.

From the Feynman-Dyson expansion for the S matrix the lowest-order matrix element for a β-decay transition from an initial state i to a final state f (assumed to be eigenstates of H_0) is easily obtained, and from it the familiar Fermi's golden rule for the partial transition rate w_{if},

$$w_{if} = 2\pi |M|^2 \delta(E_i - E_f) \ , \tag{6a}$$

$$M = \langle f | H_\beta | i \rangle \ . \tag{6b}$$

To find the total transition rate, (6a) must be summed over all final states and averaged over all initial states, operations which will be considered shortly.

For simplicity we restrict our considerations to allowed transitions[26] where, with the nuclear part reduced to nonrelativistic form, the transition matrix element simplifies to

$$M = \langle a';k' | H_\beta | a;k \rangle = C_V \langle a' | \bar{\psi}_e(0)\mathcal{B}\psi_\nu(0) | a \rangle \ , \tag{7}$$

where a (a') labels the initial (final) leptonic state and k (k') labels the initial (final) nuclear state. The nuclear matrix elements operative in allowed transitions are contained in $\mathscr{B}$, viz.,

$$\mathscr{B}=B_\mu\gamma_\mu(1+\gamma_5)\ ,$$
$$B_\mu=(i\lambda\langle k'\mid\vec{\sigma}\mid k\rangle,\langle k'\mid 1\mid k\rangle)\ . \tag{8}$$

The basic model adopted in all theoretical studies is one in which only those leptons which participate in the rearrangement process are included in the specification of the leptonic states. All other electrons are regarded as inert and it is assumed that their influence on the process, largely one of shielding, can be corrected for later. In this case,

$$\mid a\rangle=\mid e_\alpha\rangle$$
and
$$\mid a'\rangle=\mid e_1,e_2,\nu\rangle\ , \tag{9}$$

where e_α denotes the initial bound electron and e_1 and e_2 denote the two final electrons, taken to be in continuum states. With this simplification and the introduction of a configuration-space representation, the transition matrix element takes on the form

$$M=C_V\langle e_1,e_2,\nu\mid\bar{\psi}_e(\vec{0})\mathscr{B}\psi_\nu(\vec{0})\mid e_\alpha\rangle$$
$$=C_V(1-P_{12})\int d\vec{r}\,\phi_{1,2}^{(z)\dagger}(\vec{0},\vec{r})\phi_\alpha^{(z')}(\vec{r})\times\gamma_4\mathscr{B}\phi_\nu(\vec{0})\ , \tag{10}$$

in which $\phi_{1,2}^{(z)}$ and $\phi_\alpha^{(z')}$, labeled by the appropriate eigenvalues of the nuclear charge-number operator, and ϕ_ν are the normalized wave functions representing the two-electron final state, the initial state of the orbital electron, and the final state of the neutrino, respectively. P_{12} is the exchange operator which interchanges the two final electrons.

The evaluation of (10) requires the construction of a reasonably accurate form for the two-electron wave function $\phi_{1,2}$ which satisfies the equation

$$[h_C(\vec{r}_1)+h_C(\vec{r}_2)+\alpha/r_{12}]\phi_{1,2}^{(z)}(\vec{r}_1,\vec{r}_2)=E_{1,2}\phi_{1,2}^{(z)}(\vec{r}_1,\vec{r}_2)\ , \tag{11}$$

in which the nuclear charge-number operator appearing in h_C has taken on the eigenvalue Z. Were there available a solution of this equation based on the self-consistent-field method, its use would permit the evaluation of (10) directly, yielding results which include the effects of the final-state interaction. Unfortunately, no such continuum solution of (11) is known and one's only recourse is to perturbation theory.

Provided that $Z\gg 1$, it is appropriate to treat the electron-electron interaction as a perturbation on the nuclear Coulomb interaction of the electrons. The unperturbed wave function is simply the product of two continuum hydrogenic wave functions and the perturbed wave function, calculated to first order by conventional perturbation theory, is

$$\phi_{1,2}^{(z)}(\vec{r}_1,\vec{r}_2)=\phi_1^{(z)}(\vec{r}_1)\phi_2^{(z)}(\vec{r}_2)+\alpha\sum_{l,n}{}'\phi_l^{(z)}(\vec{r}_1)\phi_n^{(z)}(\vec{r}_2)\int d\vec{r}\,'_1\int d\vec{r}\,'_2\phi_l^{(z)\dagger}(\vec{r}\,'_1)\phi_1^{(z)}(\vec{r}\,'_1)\frac{1}{r'_{12}}\phi_n^{(z)\dagger}(\vec{r}\,'_2)\phi_2^{(z)}(\vec{r}\,'_2)+\mathscr{O}(\alpha^2) \tag{12}$$

(the prime on the summation implying that terms for which the energy denominator vanishes are to be omitted from the sum). With the introduction of (12), the transition matrix element (10) may be written as

$$M=M_{\rm SO}+M_{\rm DC}\ , \tag{13a}$$

with

$$M_{\rm SO}=C_V(1-P_{12})\bar{\phi}_1^{(z)}(\vec{0})\mathscr{B}\phi_\nu(\vec{0})\int d\vec{r}\,\phi_2^{(z')\dagger}(\vec{r})\phi_\alpha^{(z)}(\vec{r})\ , \tag{13b}$$

$$M_{\rm DC}=C_V\alpha(1-P_{12})\int d\vec{r}\int d\vec{r}\,'\phi_2^{(z)\dagger}(\vec{r}\,')\phi_\alpha^{(z')}(\vec{r}\,')\frac{1}{\mid\vec{r}-\vec{r}\,'\mid}\phi_1^{(z)\dagger}(\vec{r})G_E(\vec{r},\vec{0})\mathscr{B}\phi_\nu(\vec{0})\ . \tag{13c}$$

Appearing in (13c) is the Dirac-Coulomb Green's function

$$G_E(\vec{r},\vec{r}\,')=\sum_\sigma\frac{\phi_\sigma^{(z)}(\vec{r})\bar{\phi}_\sigma(\vec{r}\,')}{(E-E_\sigma)} \tag{14}$$

with $E=E_1+E_2-E_\alpha$, the total energies of the two final electrons and the initial electron being given by E_1, E_2, and E_α, respectively.

The overlap integral appearing in (13b) is readily shown to be of order α as a consequence of the near orthogonality of ϕ_2 and ϕ_α (since $Z=Z'+1$). Thus, $M_{\rm SO}$ and $M_{\rm DC}$ are of the same order in the coupling constants and the contributions of both terms must be considered in determining M to lowest order.

In Fig. 1 are shown Feynman diagrams associated with the internal-ionization amplitude (10) and the leading terms in its perturbation expansion. (In addition to the diagrammatic expansion shown, there

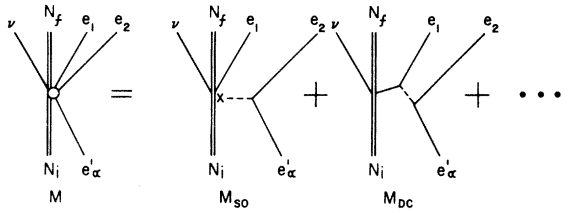

FIG. 1. Feynman diagrams for internal ionization during β decay.

is also a similar expansion for the exhange term, differing only by an interchange of the two final electrons e_1 and e_2.) In the amplitude M_{SO} correlation effects are neglected and the transition is attributed to the sudden change in nuclear charge and the resulting imperfect wave-function overlap. The final-state interaction is accounted for (to lowest order in α) by the amplitude M_{DC} according to which the transition results from a (virtual) direct collision between the orbital electron and the emerging β particle.

For purposes of calculating M_{DC}, it is convenient to introduce the integral representation

$$\frac{1}{|\vec{r}-\vec{r}'|}=\lim_{\epsilon\to 0}\frac{1}{2\pi^2}\int_{-\infty}^{\infty}d\vec{k}\,\frac{\exp[i\vec{k}\cdot(\vec{r}-\vec{r}')]}{(k^2+\epsilon^2)} \tag{15}$$

and express the Dirac-Coulomb Green's function $G_E(\vec{r},\vec{r}')$ in terms of the analogous Green's function for the second-order form of the Dirac equation,

$$G_E(\vec{r},\vec{r}')=[-\vec{\gamma}\cdot\vec{\nabla}+1+\gamma_4(E+a/r)]g_E(\vec{r},\vec{r}')\ . \tag{16}$$

Then the DC amplitude may be written as

$$M_{DC}=\frac{C_V\alpha}{2\pi^2}(1-P_{12})\lim_{\epsilon\to 0}\int_{-\infty}^{\infty}\frac{d\vec{k}}{(k^2+\epsilon^2)}J_1J_2\ , \tag{17a}$$

with

$$J_1=\int d\vec{r}\,\phi^{\dagger}_{P_1}(\vec{r})\phi_\alpha(\vec{r})e^{-i\vec{k}\cdot\vec{r}} \tag{17b}$$

and

$$\begin{aligned}J_2&=\int d\vec{r}\,\phi^{\dagger}_{P_2}(\vec{r})G_E(\vec{r},\vec{0})\mathcal{B}\phi_\nu(\vec{0})e^{i\vec{k}\cdot\vec{r}}\\&=\int d\vec{r}\,\phi^{\dagger}_{P_2}(\vec{r})\{[-\vec{\gamma}\cdot\vec{\nabla}+1+\gamma_4(E+a/r)]g_E(\vec{r},\vec{0})\}\mathcal{B}\phi_\nu(\vec{0})e^{i\vec{k}\cdot\vec{r}}\\&=\int d\vec{r}\,\bar{\phi}_{P_2}(\vec{r})e^{i\vec{k}\cdot\vec{r}}(E+E_2+2a/r+\vec{\alpha}\cdot\vec{k})g_E(\vec{r},\vec{0})\mathcal{B}\phi_\nu(\vec{0})\ ,\end{aligned} \tag{17c}$$

where we have integrated by parts and used the fact that ϕ_{P_2} satisfies the Dirac equation in obtaining (17c).

The evaluation of the transition amplitude will be described in Sec. III. For now we simply note the connection between the transition amplitude and the total transition rate for the internal ionization of an electron initially in the state α. The partial transition rate is given by (6a); hence, the rate for transitions to a group of final states in the differential momentum ranges $d\vec{P}_1$, $d\vec{P}_2$ is

$$dw_\alpha=2\pi\int d\vec{P}_\nu\sum_{\substack{\text{final}\\\text{spins}}}|M|^2\delta(E_1+E_2+E_\nu-E_\alpha-\Delta E)d\vec{P}_1d\vec{P}_2\ , \tag{18}$$

where ΔE is the energy released in the nuclear transformation. The spin summation in (18) is over the spin states of the three final leptons. Also, a summation over all final nuclear spin states and an average over all initial nuclear spin states are implicitly assumed. If averaging with respect to the directions of $\vec{P}_\nu$ is denoted by angular brackets with a subscript ν, the result of integrating (18) over all final states of the unobserved neutrino may be written as

$$dw_\alpha=8\pi^2\sum_{\substack{\text{final}\\\text{spins}}}\langle|M|^2\rangle_\nu(W_\alpha-E_1-E_2)^2d\vec{P}_1dP_2\ , \tag{19}$$

with $W_\alpha=E_0+2-B_\alpha$, where B_α is the binding energy of an electron in the state α and E_0 is the β end-point energy. Transforming to the energy scale and integrating over all directions for $\vec{P}_1$ and $\vec{P}_2$, we obtain for the double-differential energy spectrum

$$\frac{dw_\alpha}{dE_1dE_2}=8\pi^2P_1P_2(W_\alpha-E_1-E_2)^2\int d\Omega_1\int d\Omega_2\sum_{\substack{\text{final}\\\text{spins}}}\langle|M|^2\rangle_\nu\ . \tag{20}$$

Then, for P_α, the total internal-ionization probability per β decay, we have

$$P_\alpha=\frac{1}{2w_\beta}\int_1^{W_\alpha-1}dE_1\int_1^{W_\alpha-E_1}dE_2\frac{dw}{dE_1dE_2}\ , \tag{21}$$

where w_β is the rate for ordinary β decay and, because of the indistinguishability of the two final electrons, we have divided by 2 to avoid double counting the internal-ionization events.

Of particular interest are results for the internal ionization of K-shell electrons. These are obtained from (20) and (21) by setting $\alpha=K$ and summing (20) over the spin states of the initial electron. Hence,

$$P_K=\frac{4\pi^2}{w_\beta}\int_1^{W_k-1}dE_1\int_1^{W_K-E_1}dE_2P_1P_2(W_K-E_1-E_2)^2\int d\Omega_1\int d\Omega_2\sum_{\substack{\text{all}\\ \text{spins}}}\langle\,|M|^2\rangle_\nu\ . \tag{22}$$

III. CALCULATION OF TRANSITION RATE

For the purpose of detailed calculation we limit our considerations to the internal ionization of K-shell electrons. It is this case which has been investigated most extensively; it is also the one for which the DC contribution is expected to be most important. Our task is to evaluate M as given by (13) and (17) and then obtain the transition rate from (20).

The evaluation of M_{SO} is straightforward and relatively simple; it has been calculated by many workers and there are available for it expressions of greater accuracy than we shall need. By comparison, the evaluation of M_{DC} is much more difficult. Indeed, while M_{SO} has been evaluated analytically using relativistic hydrogenic wave functions, a closed analytical form for M_{DC} has not been obtained even in the nonrelativistic Born-approximation limit.

Born-approximation results are, of course, of little interest since M_{DC} is expected to exert its greatest influence at very low energies where Coulomb effects cannot be neglected. At the same time, however, relativistic effects will be of secondary importance, although they cannot be completely ignored, owing to the presence of the intrinsically relativistic neutrino. Therefore, it is appropriate to undertake an analysis of the DC amplitude in which nonrelativistic hydrogenic wave functions are utilized, thereby preserving a relative accuracy of order $Z\alpha$.

Concomitant with the use of nonrelativistic hydrogenic forms for the initial and final electron states, we may employ the simplified form for the second-order Green's function $g_E(\vec{r},\vec{0})$ which was first studied by Glauber and Martin.[27] For the β-decay case this approximate second-order Green's function is given by[28]

$$g_E'(r,0)=\frac{i\mu}{2\pi}e^{i\mu r}\int_0^\infty dS\left[\frac{1+S}{S}\right]^{i\eta}e^{2i\mu rS} \tag{23a}$$

with

$$\mu=(E^2-1)^{1/2},\quad \eta=aE/\mu,\quad a=Z\alpha\ . \tag{23b}$$

For the initial K electron we employ the familiar form

$$\phi_K(r)=[(a')^3/\pi]^{1/2}e^{-a'r}\chi_K \tag{24}$$

with

$$a'=(z-1)\alpha\ ,$$

while for each of the final electrons we use a continuum hydrogenic wave function written as

$$\phi_{\vec{P}}(\vec{r})=\frac{\chi}{(2\pi)^{3/2}}\sum_{l=0}^{\infty}i^l(2l+1)R_l(Pr)P_l(\hat{P}\cdot\hat{r}) \tag{25a}$$

with

$$R_l(Pr)=e^{\pi a/2P}\frac{|\Gamma(l+1-ia/P)|}{(2l+1)!}(2Pr)^le^{-iPr}e^{-i\delta_l(P)}F(ia/P+l+1,2l+2,2iPr) \tag{25b}$$

and

$$e^{2i\delta_l(P)}=\Gamma(l+1-ia/P)/\Gamma(l+1+ia/P)\ . \tag{25c}$$

In the above expressions, χ is a two-component Pauli spinor, $\vec{P}$ is the momentum of a final electron, P_l is a Legendre polynomial, $\Gamma(z)$ is the gamma function, and $F(b,c,x)$ is the confluent hypergeometric function. As given by (25), $\phi_{\vec{P}}$, describes an in-state normalized on the momentum scale.

Although a closed-form expression for the nonrelativistic Coulomb scattering state $\phi_{\vec{P}}$ is well known, its employment would render the calculation of (13c) intractable at an early stage, necessitating a prohibitive amount of numerical work. Furthermore, results based on such an approach are not readily generalizable to the relativistic domain. Thus, we have chosen instead a partial-wave expansion for $\phi_{\vec{P}}$.

The use of such as expansion will, of course, lead to results for M_{DC} and the transition rate which are also in the form of partial-wave expansions and, at first glance, it might appear that any calculational advantage will be offset by the need to evaluate a large number of terms in order to achieve an accurate final result. The DC mechanism is however expected to be important only at very low energies, its effects being most pronounced for nuclides with large Z and a small decay energy. Here, the amount of energy that can be transferred to a K electron during its collision with the β particle is necessarily quite small, thereby limiting the electron's final angular momentum.

Recognizing that the first Bohr orbit $(1/a)$ is the only natural length associated with this process and denoting by P_{max} the maximum momentum acquirable by the ejected electron, we may estimate the maximum angular momentum the electron is likely to have as $l_{max}=P_{max}/a$; above l_{max} a partial-wave expansion for M_{DC} should be rapidly convergent. As can be seen from Table I, l_{max} is in the neighborhood of 1 or 2 for those nuclides of particular interest. For them, truncation of the partial-wave expansion after only a few terms should yield quite accurate results.

We begin our calculations by rederiving a well-known result for M_{SO}. Substituting (24) and (25) into (13b) and employing for the confluent hypergeometric function the contour-integral representation,

$$F(a,b,x)=\frac{i}{2\pi}\frac{\Gamma(1-a)\Gamma(b)}{\Gamma(b-a)} \times \oint_C dt\, e^{tx}(-t)^{a-1}(1-t)^{b-a-1} , \quad (26)$$

where C is a contour enclosing the interval $0\le t\le 1$ on the real axis in the positive sense, we obtain upon integration

$$M_{SO}=\alpha C_V(1-P_{12})\chi_2^\dagger \mathscr{B}\phi_\nu(\vec{0})\chi_1^\dagger\chi_K I_{SO}(P_1,P_2) , \quad (27a)$$

with

$$I_{SO}(P_1,P_2)=-\frac{1}{\pi^2}[(a')^3/\pi]^{1/2}D(P_1,P_2)f(P_1) , \quad (27b)$$

$$D(P_1,P_2)=e^{\pi a/2P_1}\Gamma(1-ia/P_1) \times e^{\pi a/2P_2}\Gamma(1-ia/P_2) , \quad (27c)$$

and

$$f(P_1)=\exp[-(2a/P_1)\tan^{-1}(P_1/a')]/[P_1^2+(a')^2]^2 . \quad (27d)$$

Now considering M_{DC}, we start by introducing into (17b) and (17c) the Rayleigh expansion,

$$e^{i\vec{k}\cdot\vec{r}}=\sum_{l=0}^{\infty} i^l(2l+1)j_l(kr)P_l(\hat{k}\cdot\hat{r}) , \quad (28)$$

where j_l is the spherical Bessel function and $\hat{k}\cdot\hat{r}=\cos\theta$, θ being the angle between the vectors $\vec{k}$ and $\vec{r}$. After integrating over $d\Omega_{\vec{r}}$ we have

$$J_1=\frac{[2(a')^3]^{1/2}}{\pi}\chi_1^\dagger\chi_K\sum_{l=0}^{\infty}(-1)^l(2l+1)P_l(\hat{k}\cdot\hat{P}_1)\mathscr{R}_l \quad (29)$$

and

$$J_2=(2/\pi)^{1/2}\chi_2^\dagger\sum_{l=0}^{\infty}(2l+1)P_l(\hat{k}\cdot\hat{P}_2)[(E+E_2+\vec{\alpha}\cdot\vec{k})\mathscr{S}_l^{(2)}+2a\mathscr{S}_l^{(1)}]\mathscr{B}\phi_\nu(\vec{0}) \quad (30)$$

with

$$\mathscr{R}_l(P_1,k)=\int_0^\infty dr\, r^2R_l^*(P_1r)j_l(kr)e^{-a'r} \quad (31)$$

TABLE I. Characteristics of some β^--emitting nuclides with very low end-point energies.

Nuclide	Type	E_0 (keV)	B_K/E_0	P_{max} (mc)	l_{max}
$^{63}_{28}$Ni	A	67	0.134	0.49	2.4
$^{107}_{46}$Pd	$1f$	35	0.729	0.19	0.6
$^{151}_{62}$Sm	$1f$	76	0.638	0.33	0.7

and

$$\mathscr{S}_l^{(n)}(P_2,k)=\int_0^\infty dr\, r^n R_l^*(P_2 r) j_l(kr) g_E'(r,0) e^{-\lambda r} . \tag{32}$$

To ensure convergence of the integral in (32), we have inserted the factor $e^{-\lambda r}$ with the understanding that the limit $\lambda \to 0$ will be taken at an appropriate point in our calculation.

It is now convenient to substitute (29) and (30) into (17a) and integrate over $d\Omega_{\vec{k}}$. This leads to the following expansion for M_{DC}:

$$M_{\mathrm{DC}}=\alpha C_V(1-P_{12})\chi_2^\dagger I_{DC}(\vec{\mathrm{P}}_1,\vec{\mathrm{P}}_2)\mathscr{B}\phi_\nu(\vec{0})\chi_1^\dagger\chi_K \tag{33a}$$

with

$$I_{\mathrm{DC}}(\vec{\mathrm{P}}_1,\vec{\mathrm{P}}_2)=-(4/\pi^2)[(a')^3/\pi]^{1/2}\sum_{l=0}^{\infty}(-1)^l\{(2l+1)A_l P_l(\hat{P}_1\cdot\hat{P}_2)-[l(2l-1)]^{1/2}B_l^{l-1}\Lambda_{l-1}^l(\hat{P}_1\cdot\hat{P}_2)$$
$$+[(l+1)(2l+3)]^{1/2}B_l^{l+1}\Lambda_{l+1}^l(\hat{P}_1\cdot\hat{P}_2)\} \tag{33b}$$

and

$$\Lambda_{l'}^l(\hat{P}_1\cdot\hat{P}_2)=[4\pi/(2l+1)]^{1/2}\sum_{\mu=1,0,-1}(-1)^\mu C(l',1,l;0,\mu,\mu)\alpha_{-\mu}Y_l^\mu(\hat{P}_1\cdot\hat{P}_2) , \tag{33c}$$

where $C(l',1,l;0,\mu,\mu)$ are Clebsch-Gordan coefficients, α_μ are the spherical components of the Dirac matrices $\vec{\alpha}$, and Y_l^μ are the spherical harmonics. The functions A_l, B_l^{l-1}, B_l^{l+1}, containing the energy dependence of I_{DC}, are defined by

$$A_l(P_1,P_2)=-[(E+E_2)S_l^{(2)}(P_1,P_2)+2aS_l^{(1)}(P_1,P_2)] \tag{34a}$$

with

$$S_l^{(n)}(P_1,P_2)=\lim_{\epsilon\to 0}\int_0^\infty \frac{k^2dk}{(k^2+\epsilon^2)}\mathscr{R}_l(P_1,k)\mathscr{S}_l^{(n)}(P_2,k) \tag{34b}$$

and

$$B_l^{l'}(P_1,P_2)=\lim_{\epsilon\to 0}\int_0^\infty \frac{k^3dk}{(k^2+\epsilon^2)}\mathscr{R}_l(P_1,k)\mathscr{S}_{l'}^{(2)}(P_2,k) . \tag{34c}$$

The determination of M_{DC} is now reduced to the evaluation of the functions A_l, $B_l^{l\pm1}$. This is described in the appendix where it is shown that these functions may be written in the convenient form

$$A_l(P_1,P_2)=(D/4)U_l(P_1,P_2),\quad B_l^{l-1}(P_1,P_2)=(D/4)V_l(P_1,P_2),\quad B_l^{l+1}(P_1P_2)=(D/4)W_l(P_1,P_2) , \tag{35}$$

where D is given by (27c) and the functions U_l, V_l, and W_l are defined by (A13), (A14), and (A15), respectively. With the use of (35), (27) and (33) may be combined into the following expression for the internal-ionization transition amplitude:

$$M=-(\alpha C_V/\pi^2)[(a')^3/\pi]^{1/2}D(P_1,P_2)(1-P_{12})\chi_2^\dagger K(\vec{\mathrm{P}}_1,\vec{\mathrm{P}}_2)\mathscr{B}\phi_\nu(\vec{0})\chi_1^\dagger\chi_k \tag{36a}$$

with

$$K(\vec{\mathrm{P}}_1,\vec{\mathrm{P}}_2)=f(P_1)+\sum_{l=0}^{\infty}(-1)^l\{(2l+1)U_l(P_1,P_2)P_l(\hat{P}_1\cdot\hat{P}_2)-[l(2l-1)]^{1/2}V_l(P_1,P_2)\Lambda_{l-1}^l(\hat{P}_1\cdot\hat{P}_2)$$
$$+[(l+1)(2l+3)]^{1/2}W_l(P_1,P_2)\Lambda_{l+1}^l(\hat{P}_1\cdot\hat{P}_2)\} . \tag{36b}$$

A final result for P_K may now be obtained by substituting (36) into (22) and performing the angular integration and spin summations. This leads to

$$P_K=\tfrac{1}{2}\int_1^{W_K-1}dE_1\int_1^{W_K-E_1}dE_2\lambda_K(E_1,E_2) \tag{37}$$

with the β-normalized double-differential energy spectrum given by

$$\lambda_K(E_1,E_2)=\frac{2^6\alpha^2(a')^3}{\pi\lambda_\beta}P_1P_2F(a,P_1)F(a,P_2)(W_K-E_1-E_2)^2(C_{\rm SO}+C_I+C_{\rm DC})\ , \tag{38}$$

where we have introduced the nonrelativistic Fermi function by

$$F(a,P)=(2\pi a/P)/[1-\exp(-2\pi a/P)]\ . \tag{39}$$

In obtaining (38) we have also written the rate for ordinary β decay as

$$w_\beta=(C_V^2/\pi^3)(\vec{\mathrm{B}}\cdot\vec{\mathrm{B}}^*+B_4B_4^*)\lambda_\beta$$

with

$$\lambda_\beta=\int_1^{W_0-1}dE\,PF(a,P)(W_0-1-E)^2 \tag{40}$$

and $W_0=E_0+2$. Lastly, the coefficients determining the relative importance of the two mechanisms and the extent of their interference are given by

$$C_{\rm SO}=f^2+\tilde{f}^2-f\tilde{f}\ , \tag{41a}$$

$$C_I=\mathrm{Re}[f(\tilde{U}_0-2U_0)+\tilde{f}(U_0-2\tilde{U}_0)]\ , \tag{41b}$$

$$C_{\rm DC}=\sum_{l=0}^{\infty}\{(2l+1)[\,|U_l|^2+|\tilde{U}_l|^2-\mathrm{Re}(U_l\tilde{U}_l^*)]+l[\,|V_l|^2+|\tilde{V}_l|^2-\mathrm{Re}(V_l\tilde{V}_l^*)]$$
$$+(l+1)[\,|W_l|^2+|\tilde{W}_l|^2-\mathrm{Re}(W_l\tilde{W}_l^*)]\}\ , \tag{41c}$$

where $f=f(P_1)$, $\tilde{f}=f(P_2)$, $U_l=U_l(P_1,P_2)$, $\tilde{U}_l=U_l(P_2,P_1)$, and similarly for V_l and W_l.

IV. ANGULAR-CORRELATION FUNCTIONS

As we have already reported,[24] the value of P_K is not greatly affected by the inclusion of the DC mechanism. This is owing, in part, to the fact that the contribution to P_K from the interference term is negative and largely cancels the contribution due to the DC process alone. As we shall see in Sec. V, the same is true for the energy spectra whose shapes show very little change when the DC amplitude is included.

It is therefore of interest to examine some of the simpler angular-correlation functions. Since $M_{\rm SO}$ is spherically symmetric, any correlation in the distribution of the final electrons is evidence for the presence of the DC mechanism. Furthermore, because such a correlation can manifest itself through the interference term where it is amplified by the much larger SO amplitude, its effect can be quite pronounced.

A. Electron-electron angular correlation

To study the angular correlation between the directions of emission of the two final electrons we once again substitute (36) into (22), but now we only perform the spin summation and not the angular integration. The result obtained is

$$\frac{1}{w_\beta}\frac{dw_K(\theta)}{dE_1dE_2}=\lambda_K(E_1,E_2)\frac{d\Omega_{12}}{4\pi}\mathcal{G}(E_1,E_2,\theta)\ , \tag{42}$$

where $\lambda_K(E_1,E_2)$ is given by (38), $d\Omega_{12}$ is the element of solid angle about the direction of $\vec{\mathrm{P}}_2$ relative to $\vec{\mathrm{P}}_1$, and the angular correlation function $\mathcal{G}$ is given by

$$\mathcal{G}(E_1,E_2,\theta)=(C_{\rm SO}+\mathcal{C}_I+\mathcal{C}_{\rm DC})/(C_{\rm SO}+C_I+C_{\rm DC}) \tag{43a}$$

with $C_{\rm SO},C_I,C_{\rm DC}$ given by (41) and

$$\mathcal{C}_I=\sum_{l=0}^{\infty}(-1)^l(2l+1)P_l$$
$$\times\mathrm{Re}[f(2U_l-\tilde{U}_l)+\tilde{f}(2\tilde{U}_l-U_l)]\ , \tag{43b}$$

$$\mathcal{C}_{\rm DC}=\sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(-1)^{l+l'}[Q_{ll'}+R_{ll'}+S_{ll'}$$
$$-(T_{ll'}+\tilde{T}_{l'l}^*)] \tag{43c}$$

with

$$Q_{ll'}=[(2l+1)(2l'+1)P_lP_{l'}]$$
$$\times[U_lU_{l'}^*+\tilde{U}_l\tilde{U}_{l'}^*-\tfrac{1}{2}(U_l\tilde{U}_{l'}^*+\tilde{U}_lU_{l'}^*)]\ , \tag{43d}$$

$$R_{ll'}=[P_l^{(1)}P_{l'}^{(1)}+ll'P_lP_{l'}] \times[V_lV_{l'}^*+V_l\tilde{V}_{l'}^*-\tfrac{1}{2}(V_l\tilde{V}_{l'}^*+\tilde{V}_lV_{l'}^*)]\ , \tag{43e}$$

$$S_{ll'}=[P_l^{(1)}P_{l'}^{(1)}+(l+1)(l'+1)P_lP_{l'}] \times[W_lW_{l'}^*+\tilde{W}_l\tilde{W}_{l'}^*-\tfrac{1}{2}(W_l\tilde{W}_{l'}^*+\tilde{W}_lW_{l'}^*)]\ , \tag{43f}$$

$$T_{ll'}=[P_l^{(1)}P_{l'}^{(1)}-l(l'+1)P_lP_{l'}] \times[V_lW_{l'}^*+\tilde{V}_l\tilde{W}_{l'}^*-\tfrac{1}{2}(V_l\tilde{W}_{l'}^*+\tilde{V}_lW_{l'}^*)]\ , \tag{43g}$$

where the argument of the Legendre polynomial P_l and associated Legendre functions P_l^m is $\cos\theta=\hat{P}_1\cdot\hat{P}_2$.

For SO alone we have $\mathcal{G}(E_1,E_2,\theta)=1$, a well-known result implying no correlation between the directions of emission of the two final electrons. On the contrary, the result (43) shows that such a correlation does arise through the DC mechanism, manifesting itself especially through the interference term $\mathcal{C}_I$.

Also, for later use we define the integrated angular correlation function by

$$G(\theta)=\frac{\int_1^{W_K-1}dE_1\int_1^{W_K-E_1}dE_2\lambda_K(E_1,E_2)\mathcal{G}(E_1,E_2,\theta)}{\int_1^{W_K-1}dE_1\int_1^{W_K-E_1}dE_2\lambda_K(E_1,E_2)}\ . \tag{44}$$

As with $\mathcal{G}(E_1,E_2,\theta)$, $G(\theta)=1$ for SO alone.

B. Distribution of electrons from polarized nuclei

Implicit in the expression $\sum_{\text{spins}}|M|^2$ is a sum over all final nuclear spin states and an average with respect to all initial nuclear spin states. Thus far in our calulations we have assumed that the initial nuclear population is unpolarized. If, on the contrary, the initial nuclei, whose states $|J,M\rangle$ are characterized by the angular-momentum quantum numbers J and M, are polarized, (36) leads not to (38) but rather to

$$\frac{1}{w_\beta}\frac{dw_K^{(M)}(\theta_1)}{dE_1dE_2}=\lambda_K(E_1,E_2)\frac{d\Omega_1}{4\pi}[1+\mathcal{F}(E_1,E_2)a_K\,|\,\vec{\mathcal{P}}_M\,|\cos\theta_1] \tag{45}$$

with

$$\mathcal{F}=(F_I+F_{\rm DC})/(C_{\rm SO}+C_I+C_{\rm DC})\ , \tag{46a}$$

$$F_I=\mathrm{Re}[f(2W_0-\tilde{W}_0)+\tilde{f}(2\tilde{W}_0-W_0)]\ , \tag{46b}$$

$$F_{\rm DC}=-2\sum_{l=0}^{\infty}\mathrm{Re}\{l[U_l^*V_l+\tilde{U}_l^*\tilde{V}_l-\tfrac{1}{2}(\tilde{U}_l^*V_l+U_l^*\tilde{V}_l)]+(l+1)[U_l^*W_l+\tilde{U}_l^*\tilde{W}_l-\tfrac{1}{2}(\tilde{U}_l^*W_l+U_l^*\tilde{W}_l)]\}\ , \tag{46c}$$

after the Ω_{12} integration has been performed. Here $\vec{\mathcal{P}}_M=\langle J,M\,|\,\vec{J}\,|\,J,M\rangle/J$ is the polarization vector of the initial nuclear state and θ_1 is the angle between the vectors $\vec{\mathcal{P}}_M$ and $\vec{P}_1$; a_K is an energy-independent coefficient whose value depends on the initial and final nuclear angular momenta J and J' and the type of transition as follows: For a pure Fermi transition,

$$a_K=0\ ;$$

for a pure Gamow-Teller transition,

$$a_K=\begin{cases}-J/(J+1), & J'=J+1\\ 1/(J+1), & J'=J\\ 1, & J'=J-1\ ;\end{cases}$$

for a mixed transition,

$$a_K=\left[\frac{\lambda^2|R|^2}{(J+1)}-\frac{\lambda J(R+R^*)}{[J(J+1)]^{1/2}}\right]\times(1+\lambda^2|R|^2)^{-1}\ ;$$

where

$$R=\langle f||\vec{\sigma}||i\rangle/\langle f||1||i\rangle$$

is the ratio of the reduced nuclear matrix elements for Gamow-Teller- and Fermi-type transitions. If we now integrate (45) with respect to E_2, we obtain

$$\frac{1}{w_\beta}\frac{dw_K^M(\theta_1)}{dE_1}=\lambda_K(E_1)\frac{d\Omega_1}{4\pi}W_M(\theta_1)\ , \tag{47}$$

a result in which the one-electron energy distribution is given by

$$\lambda_K(E_1)=\int_1^{W_K-E_1} dE_2\lambda_K(E_1,E_2)\ , \tag{48}$$

and the angular distribution function is defined by

$$W_M(\theta_1)=1+\mathscr{D}(E_1)a_K\mid\vec{\mathscr{P}}_M\mid\cos\theta_1 \tag{49}$$

with the energy-dependent coefficient

$$\mathscr{D}(E_1)=\frac{1}{\lambda_K(E_1)}\int_1^{W_K-E_1} dE_2\lambda_K(E_1,E_2)\times\mathscr{F}(E_1,E_2)\ . \tag{50}$$

For the SO process alone, $\mathscr{F}(E_1,E_2)=0$ and the one-electron distribution is spherically symmetric. As is evident from (49) and (50), this symmetry is perturbed by the action of the DC mechanism, the extent of the resulting asymmetry depending largely on the magnitude of $\mathscr{D}(E_1)$. We shall examine the behavior of this function in Sec. V.

V. RESULTS AND CONCLUSIONS

To illustrate the results of our calculations we have chosen the three nuclides listed in Table I. Although the ratio B_K/E_0 is not very large for ^{63}Ni, it is the best candidate available from among known allowed β emitters. The two other nuclides shown better satisfy our criteria of low decay energy and large B_K/E_0 ratio, but they decay by nonunique first-forbidden transitions. For them our results are valid only in the ξ approximaton which, however, is well satisfied because of the low end-point energy.

We consider first the composite energy spectrum $\lambda_K(E_1)$ obtained from (38) and (48). As is evident from these equations, $\lambda_K(E_1)$ is of the form

$$\lambda_K=\lambda_K(\mathrm{SO})+\lambda_K(I)+\sum_{l=0}^{\infty}\lambda_K^{(l)}(\mathrm{DC})\ , \tag{51}$$

where $\lambda_K(\mathrm{SO})$ is the spectrum due to SO alone, $\lambda_K(I)$ describes the interference between the SO and DC amplitudes, and $\lambda_K^{(l)}(\mathrm{DC})$ represent the partial-wave contributions to $\lambda_K(\mathrm{DC})$, the spectrum due to DC alone.

On the basis of our estimates for $l_{\max}$ we have truncated the series for $\lambda_K(\mathrm{DC})$ after the $l=2$ term. Computer codes have been developed for the evaluation of the functions U_l, V_l, and W_l, defined by (A13)–(A15), for $l=0,1,2$ and with them we have obtained the results displayed in Figs. 2–4.

It is evident from curves D_0, D_1, and D_2 of Fig. 2 that the partial-wave expansion for $\lambda_K(\mathrm{DC})$ converges rapidly at all energies for ^{63}Ni and, even though $l_{\max}=2.4$ in this case, the contributions from partial waves with $l\geq 3$ are clearly negligible. For ^{107}Pd and ^{151}Sm convergence of the series for

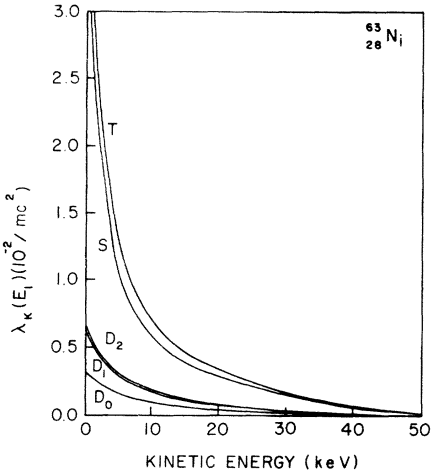

FIG. 2. Composite energy spectrum of ejected K electrons and β particles for internal ionization during β decay by ^{63}Ni. Curve S is the spectrum due to SO alone; curves D_0, D_1, and D_2 are the $l=0,1,2$ partial sums of the contribution from DC alone. Overall spectrum is described by curve T.

$\lambda_K(\mathrm{DC})$ is even more rapid as is to be expected from the corresponding values for $l_{\max}$. Indeed, in Figs. 3 and 4 the curves D_1 and D_2 are indistinguishable. Thus, for all three cases our results for $\lambda_K(E_1)$ may be regarded as essentially exact within the framework defined by our approximation scheme.

From the curves D_2 and S of all three figures it is

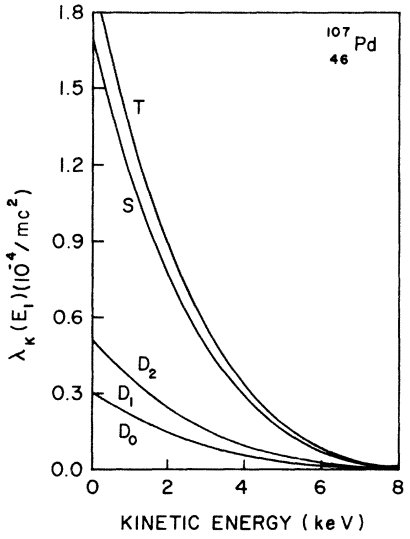

FIG. 3. Composite energy spectrum of ejected K electrons and β particles for internal ionization during β decay by ^{107}Pd. Curve S is due to SO alone and curves D_0, D_1, and D_2 are the first three partial sums of the DC contribution. Curve T represents the overall spectrum.

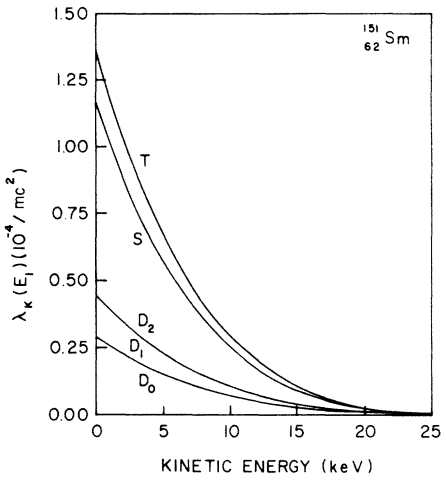

FIG. 4. Composite energy spectrum of ejected K electrons and β particles for internation ionization during β decay by ^{151}Sm. Curve S is due to SO alone and curves D_0, D_1, and D_2 are the first three partial sums of the DC contribution. Curve T represents the overall spectrum.

clear that λ_K(DC) is never more than about one third to one half of λ_K(SO). But while such a contribution is quite substantial, the overall effect of the DC mechanism on the composite energy spectrum is, in fact, considerably smaller because of an equally substantial, but negative, contribution from $\lambda_K(I)$. When both of these contributions are added to λ_K(SO), one obtains a total λ_K which, for the three nuclides considered, differs from λ_K(SO) by only about 12—15 % at all energies.

In view of the significant role played by the interference term it is worth remarking that this term is Coulombic in origin. As Feinberg[1] has shown, when a plane-wave approximation is employed for the intermediate and final states of the β particle, $\lambda_K(I)$ vanishes and the SO and DC contributions to λ_K are purely additive. However, when Coulomb effects are included, this is no longer the case although it is only the s-wave part of the expansion for $M_{\rm DC}$ which contributes to $\lambda_K(I)$.

Because the overall effect of the DC mechanism on λ_K (and P_K) is not very great, even under favorable conditions, it is of interest to consider correlation effects since these can arise only through the DC amplitude. Since such effects are more sensitive to the higher partial waves, we shall examine only ^{107}Pd and ^{151}Sm since our expansion for $M_{\rm DC}$ is more rapidly convergent for these nuclides than for ^{63}Ni. Although these two cases involve nonunique first-forbidden transitions, angular-correlation functions are expected to be relatively insensitive to shape-factor corrections.

Undoubtedly, the simplest correlation to observe is that between the directions of emission of the two final electrons. To illustrate this correlation, we have plotted in Fig. 5 the integrated angular-correlation function $G(\theta)$, given by (44), for ^{107}Pd. The effect is indeed substantial. For example, in an electron-electron coincidence experiment, the counting rate is predicted to vary by about a factor of 2 when the angle between the two detectors ranges from 90° to 180°. Such experiments, while admittedly very difficult, are to be encouraged since they are capable of furnishing direct evidence for the presence of the DC mechanism as well as a more stringent test of the theory developed in this paper.

Another correlation function of some interest is that associated with the angular distribution of electrons from a polarized source. As we have shown in Sec. IV, the composite one-electron momentum distribution is, in this case, characterized by the angular distribution function $W_M(\theta_1)$, defined by (49). The extent to which this function can depart from unity is limited by the magnitude of the energy-dependent coefficient $\mathscr{D}(E_1)$, defined by (50), especially at low energies where most of the internal-ionization events occur. In Fig. 6 we have plotted $\mathscr{D}(E_1)$ for ^{151}Sm; the results are disappointing. Over the entire energy range this function is only of order 10^{-2}, making polarization effects far too small to be of any experimental interest. The situation with respect to ^{107}Pd is much the same.

To further refine the theoretical model, relativistic and screening effects must be included. In view of the dominance of the SO process, a reasonable estimate of the resulting corrections may be obtained by considering their influence on the SO amplitude alone. For the model used in this paper, this can readily be done for P_K. By combining results of Isozumi, Shimizu, and Mukoyama[14] with those from Table I of Ref. 24, it is found that relativistic effects increase P_K(SO) by a factor of 1.05, 1.08, and 1.21 for the nuclides listed with $Z=28$, 46, and 62,

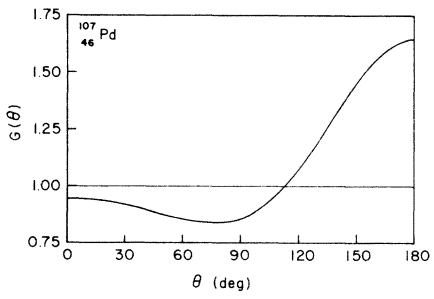

FIG. 5. Plot of integrated angular-correlation function $G(\theta)$ for ^{107}Pd obtained using first three terms of partial-wave expansion.

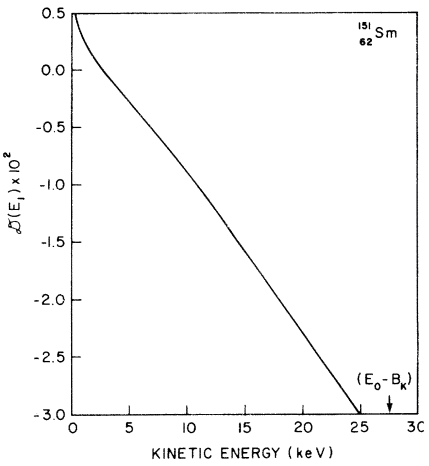

FIG. 6. Plot of asymmetry coefficient $\mathscr{D}(E_1)$ for ^{151}Sm obtained using first three terms of partial-wave expansion.

respectively. Similarly, combining results from Isozumi, Shimizu, and Mukoyama[14] with those from Mukoyama and Shimizu,[19] it is found that screening effects increase the relativistic hydrogenic results for P_K(SO) by a factor of 1.36 (1.21) for the nuclide with $Z=28$ ($Z=62$). When combined, these factors yield an overall correction factor of 1.43 for ^{53}Ni and 1.46 for ^{151}Sm.

For the DC process corrections of comparable magnitude are to be expected and a completely satisfactory theory will have to take them into account. For low-energy transitions this may be done by extending the calculations of this paper to the relativistic domain and using wave functions which incorporate the effects of screening.

An advantage of the perturbation approach used in this paper is that it permits a detailed and accurate treatment of the DC amplitude, particularly important for the study of correlation phenomena. However, because of the complex structure of $M_{\rm DC}$, the extent to which one can modify the wave functions to incorporate many-body effects is limited. On the other hand, the DC amplitude plays only a minor role as far as the calculation of λ_K and P_K are concerned. Here, because of the much simpler structure of $M_{\rm SO}$, it is possible to use more elaborate procedures to include many-body effects. Indeed, recently Law and Suzuki[29] have utilized a relativistic self-consistent-field approach to include many-body effects in a calculation of $M_{\rm SO}$, thereby achieving much better agreement with recent experimental results for $\bar{P}_K$.

The results of Law and Suzuki are very encouraging and point up the importance of many-body effects. However, DC effects are not included in their results and estimates of the DC contribution to $\bar{P}_K$ by Law and Suzuki yield results about an order of magnitude smaller than expected, an indication of the difficulty of properly accounting for the DC amplitude in their approach. It therefore seems likely that the two approaches will have to be combined in an appropriate way in order to adequately describe all aspects of the internal-ionization phenomenon; further theoretical work to this end is to be encouraged.

APPENDIX

Evaluation of the functions $A_l(P_1,P_2)$ and $B_l^{l\pm1}(P_1,P_2)$ begins with the calculation of $\mathscr{S}_l^{(n)}(P_2,k)$ and $\mathscr{R}_l(P_1,k)$ defined by (31) and (32), respectively. For this purpose we introduce into these equations the forms (23a), (25b), (26), and, for the spherical Bessel function,

$$j_l(kr)=\frac{1}{2i^l}\int_{-1}^{1} du\, e^{ikru}P_l(u)\ . \tag{A1}$$

The r integration is now elementary and leads to the following results:

$$\mathscr{S}_l^{(n)}(P_2,k)=-(\mu/8\pi^2)(-2iP_2)^l e^{\pi a/2P_2}\Gamma(-l+ia/P_2)e^{2i\delta_l(P_2)}(l+n)!$$
$$\times\int_{-1}^{1} du_2 P_l(u_2)\int_0^{\infty} dS\left[\frac{1+S}{S}\right]^{i\eta}\oint_C \frac{dt_2 f_l(P_2,t_2)}{[\lambda+iP_2(2t_2-1)-iku_2-i\mu(1+2S)]^{l+n+1}} \tag{A2}$$

with $\mathrm{Im}\,t_2<\lambda/2P_2$ as the condition for convergence, and

$$\mathscr{R}_l(P_1,k)=(i/4\pi)(-2iP_1)^l e^{\pi a/2P_1}\Gamma(-l+ia/P_1)e^{2i\delta_l(P_1)}(l+2)!$$
$$\times\int_{-1}^{1} du_1 P_l(u_1)\oint_C \frac{dt_1 f_l(P_1,t_1)}{[a'-iku_1+iP_1(2t_1-1)]^{l+3}} \tag{A3}$$

with $\mathrm{Im}\,t_1<a'/2P_1$ along C to ensure convergence. Also, for convenience, we have introduced the definition

$$f_l(P,t)=(-t)^{-ia/P+l}(1-t)^{ia/P+l}\,. \tag{A4}$$

Substitution of (A2) and (A3) into (34) and completion of the k integration by the method of residues then yields

$$S_l^{(n)}(P_1,P_2)=N_l^l(P_1,P_2)(D/4)\int_0^\infty dS\left[\frac{1+S}{S}\right]^{i\eta}\oint_C dt_1 f_l(P_1,t_1)\oint_C dt_2 f_l(P_2,t_2)I_l^{(n)} \tag{A5}$$

and

$$B_l^{l'}(P_1,P_2)=N_l^{l'}(P_1,P_2)(D/4)\int_0^\infty dS\left[\frac{1+S}{S}\right]^{i\eta}\oint_C dt_1 f_l(P_1,t_1)\oint_C dt_2 f_{l'}(P_2,t_2)I_l^{l'}\,, \tag{A6}$$

where

$$N_l^{l'}(P_1,P_2)=-(\mu/4\pi^2)(2P_1)^l(2P_2)^{l'}e^{2i\delta_l(P_1)}e^{2i\delta_{l'}(P_2)}\frac{\Gamma(-l+ia/P_1)\Gamma(-l+ia/P_2)}{\Gamma(1-ia/P_1)\Gamma(1-ia/P_2)}\,, \tag{A7}$$

$$I_l^{(n)}=(-i)^n(-1)^{l+1}(2l+n+2)!\int_0^1 du_1 P_l(u_1)u_1^{l+n}\int_0^1 du_2 P_l(u_2)u_2^{l+2}/(Au_1+Bu_2)^{2l+n+3}\,, \tag{A8}$$

$$\begin{aligned}I_l^{l'}=&(-1)^{l'+1}(l'+2)(l+l'+3)!\int_0^1 du_1 P_l(u_1)u_1^{l'+1}\int_0^1 du_2 P_{l'}(u_2)u_2^{l+1}/(Au_1+Bu_2)^{l+l'+4}\\&+(-1)^{l'}(l+l'+4)!A\int_0^1 du_1 P_l(u_1)u_1^{l'+2}\int_0^1 du_2 P_{l'}(u_2)u_2^{l+1}/(Au_1+Bu_2)^{l+l'+5}\end{aligned} \tag{A9}$$

with $A=P_2(2t_2-1)-\mu(1+2S)-i\lambda$ and $B=P_1(2t_1-1)-ia'$.

By repeated integration by parts and extensive use of well-known recursion relations for the Legendre polynomials, both integrations in (A8) and (A9) may be completed. The results are

$$I_l^{(n)}=(-i)^n(-1)^{l+1}(2l+n)!\left[\frac{1}{(2l+1)A^nB^2(A+B)^{2l+1}}+\frac{1}{AB(A+B)^{2l+n+1}}\right] \tag{A10}$$

and

$$\begin{aligned}I_l^{l'}=(-1)^{(l+l'-1)/2}(l+l'+2)!\Bigg[&\frac{1}{(l+l'+2)A^{l'-l+1}B^{l-l'+1}(A+B)^{l+l'+2}}\\&+\frac{1}{A^{(l'-l+1)/2}B^{(l-l'+1)/2}(A+B)^{l+l'+3}}\Bigg]\,.\end{aligned} \tag{A11}$$

With the aid of (34a) we may now write

$$\begin{bmatrix}A_l(P_1,P_2)\\B_l^{l-1}(P_1,P_2)\\B_l^{l+1}(P_1,P_2)\end{bmatrix}=D(P_1,P_2)/4\begin{bmatrix}U_l(P_1,P_2)\\V_l(P_1,P_2)\\W_l(P_1,P_2)\end{bmatrix}\,, \tag{A12}$$

where, from (A5) and (A6), we have

$$U_l(P_1,P_2)=-N_l^l(P_1,P_2)\int_0^1 dx\,x^{-i\eta}(1-x)^{-2}\oint_C dt_1 f_l(P_1,t_1)\oint_C dt_2 f_l(P_2,t_2)[(E+E_2)I_l^{(2)}+2aI_l^{(1)}]\,, \tag{A13}$$

$$V_l(P_1,P_2)=N_l^{l-1}(P_1,P_2)\int_0^1 dx\,x^{-i\eta}(1-x)^{-2}\oint_C dt_1 f_l(P_1,t_1)\oint_C dt_2 f_{l-1}(P_2,t_2)I_l^{l-1}\,, \tag{A14}$$

$$W_l(P_1,P_2)=N_l^{l+1}(P_1,P_2)\int_0^1 dx\,x^{-i\eta}(1-x)^{-2}\oint_C dt_1 f_l(P_1,t_1)\oint_C dt_2 f_{l+1}(P_2,t_2)I_l^{l+1}\,. \tag{A15}$$

The final evaluation of (A13)–(A15), for which we have transformed the integration variable S to $x=S/(1+S)$, is straightforward but laborious and we shall not present it in detail. Of the three remaining integrations only one of the contour integrals can be done analytically. For example, one can perform the t_1 integration by observing that $I_l^{(n)}$ and $I_l^{l\pm1}$ have poles in the t_1 plane at $t_1'=(P_1+ia')/2P_1$ and at $t_1''=t_1'-A/2P_1$ and applying the method of residues. The remaining two integrations must then be performed numerically. By means of standard techniques their execution is straightforward but with the amount of computing time required increasing rapidly with l.

[1]E. L. Feinberg, J. Phys. (Moscow) 4, 423 (1941).
[2]A. B. Migdal, J. Phys. (Moscow) 4, 449 (1941).
[3]J. S. Levinger, Phys. Rev. 90, 11 (1953).
[4]H. M. Schwartz, J. Chem. Phys. 21, 45 (1953).
[5]A. Winther, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 27, No. 1 (1952).
[6]A. E. S. Green, Phys. Rev. 107, 1646 (1957).
[7]R. M. Weiner, Phys. Rev. 144, 127 (1966).
[8]P. Stephas and B. Crasemann, Phys. Rev. 164, 1509 (1967).
[9]T. A. Carlson, C. W. Nestor, Jr., T. C. Tucker, and F. B. Malik, Phys. Rev. 169, 27 (1968).
[10]A. J. Mord, Nucl. Phys. A192, 305 (1972).
[11]J. Law and J. L. Campbell, Nucl. Phys. A185, 529 (1972).
[12]J. Law and J. L. Campbell, Phys. Rev. C 12, 984 (1975).
[13]Reviews of experimental data in comparison with various theoretical results are contained in the following references: M. S. Freedman, in Annu. Rev. Nucl. Sci. 24, 209 (1974); R. J. Walen and C. Briançon, in *Atomic Inner-Shell Processes,* edited by B. Crasemann (Academic, New York, 1975), Vol. 1. A more recent comparison of available data with the (uncorrected) Law-Campbell theory may be found in Ref. 12.
[14]Y. Isozumi, S. Shimizu, and T. Mukoyama, Nuovo Cimento A 41, 359 (1977).
[15]J. W. Cooper and T. Åberg, Nucl. Phys. A298, 239 (1978).
[16]J. L. Campbell, L. A. McNelles, and J. Law, Can. J. Phys. 49, 3142 (1971).
[17]Y. Isozumi, T. Muoyama, and S. Shimizu, Phys. Rev. Lett. 29, 298 (1972).
[18]H. H. Hansen, Phys. Rev. C 14, 281 (1976).
[19]T. Mukoyama and S. Shimizu, J. Phys. G 4, 1509 (1978).
[20]J. Dobrinic, A. Ljubicic, and Y. Isozumi, Can. J. Phys. 57, 1489 (1979).
[21]G. Schupp and M. S. Freedman, Phys. Rev. C 21, 348 (1980).
[22]C. E. Laird, P. C. Hummel, and H. C. Liu, Phys. Rev. C 21, 723 (1980).
[23]R. L. Intemann, in *Inner-Shell and X-Ray Physics of Atoms and Solids,* edited by D. J. Fabian, H. Kleinpoppen, and L. M. Watson (Plenum, New York, 1981).
[24]R. L. Intemann, Phys. Rev. A 26, 3012 (1982).
[25]I. S. Batkin, I. V. Kopytin, Yu. G. Smirnov, and T. A. Churakova, Yad. Fiz. 33, 48 (1981) [Sov. J. Nucl. Phys. 33, 25 (1981)].
[26]It is demonstrated in Ref. 25 that internal-ionization results obtained assuming an allowed transition hold also for nonunique first-forbidden transitions in the ξ approximation.
[27]R. J. Glauber and P. C. Martin, Phys. Rev. 104, 158 (1956).
[28]L. Spruch and W. Gold, Phys. Rev. 113, 1060 (1959).
[29]J. Law and A. Suzuki, Phys. Rev. C 25, 514 (1982).