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Mechanisms contributing to K electron ejection in nuclear β decay

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Theoretical calculations of shake-off and shake-up autoionization probabilities for K electrons are presented, using the formalism presented previously. Total K electron ejection probabilities P_K are obtained by summing shake-off and shake-up contributions. The role of direct collision is discussed. Agreement between these P_K values and 33 recent experimental results produced by different techniques is generally good. The comparison permits critical assessment of the remaining weaknesses of the theory.

[RADIOACTIVITY K vacancy creation in β-decay calculations.]

I. INTRODUCTION

There has been a great deal of progress in the field of atomic electron ejection during nuclear β decay in recent years, both on the theoretical and experimental fronts. The earliest work of Feinberg[1,2] and Migdal[3] laid the theoretical foundation for the understanding of the process. However, there was only agreement to a factor of 2 to 3 between the theoretical and experimental estimates for the probability of K electron ejection. There was also little incentive for detailed theoretical extensions of Feinberg's calculations due to large uncertainties attached to the experimental estimates.

This situation has changed recently, as the application of high resolution devices such as semiconductor detectors and magnetic spectrometers has provided experimental data[4-6] of much higher precision and accuracy than hitherto available. The confrontation of these measurements with previous calculations has revealed disagreements which stimulated the development of a new theoretical treatment[7-9]; this differs from its predecessors[1,3,10-12] by taking into account fully the effect of the Pauli principle for the β particle and the ejected atomic electron. The encouraging agreement between the predictions of this theory and the data has in turn stimulated a spate of experiments of high quality. These allow one to test the theory on a finer basis and to assess the role of mechanisms other than the predominant shake-off effect which contributes to the electron ejection probability. One secondary contribution, viz. shake-up to bound states was calculated[13] for five radionuclides studied in our laboratory, but calculations have not been available for many other cases of interest.

The present paper may serve several purposes. First, all numerical approximations are removed from our earlier calculations of shake-off probabilities and the calculations are extended to nuclides not previously treated. Shake-up probabilities are also calculated, so that comparison of the sum of shake-off plus shake-up with experiment will throw some light on the direct-collision[2] mechanism of electron ejection. This comparison necessitates a review of experimental data, which we confine to recent work with high-resolution spectroscopy. We have discussed earlier data elsewhere.[7] Although our objectives do not include an over-all review, we have compared results from other models[1,3,11,12,14,15] with our own. A full review of atomic shaking in all radioactive decay processes was presented recently by Freedman[16]; however, 19 of the 33 measurements utilized in this paper have appeared in the short time since the review.

II. THEORY OF INNER SHELL VACANCY CREATION

We shall present only a brief account of the main aspects of earlier theoretical work here. A detailed description of the early development of the topic referred to as internal ionization or autoionization in β decay has been presented previously[5,9] and need not be repeated here.

Previous workers[11,12] have used differing definitions of K-shell autoionization probabilities. Here P_K is defined simply as the probability per nuclear disintegration that an atomic K vacancy is created. This is generally subdivided into two parts

$$P_K = P_K(\mathrm{SO}) + P_K(\mathrm{SU}). \tag{1}$$

Most theoretical effort has been devoted to the dominant shake-off (SO) process, i.e., ejection

to the continuum of a previously bound electron. Shake-up (SU) to unoccupied bound states makes a much smaller contribution. It has also been generally felt that apart from decays of very low β energy, direct collisions (DC) will contribute a minor fraction of the total K vacancies formed. Furthermore, as is evident from Feinberg's original paper[1] [his Eq. (10)], the DC process is by no means a simply additive contribution, although most workers would amend Eq. (1) by adding on a $P_K(\mathrm{DC})$ contribution.

A. Shake-off

Several early estimates of $P_K(\mathrm{SO})$ were made with hydrogenic wave functions, but the first extensive set of predictions with better wave functions was that of Carlson *et al.*[11] These workers, like some of their predecessors[17] computed $P_K[=P_K(\mathrm{SO})+P_K(\mathrm{SU})]$ via the equation

$$P_K = 1 - P_{KK} - P_F, \tag{2}$$

where P_{KK} equals the probability for K electron to remain and P_F equals the sum of probabilities for excitation to occupied levels. By using nonrelativistic Hartree-Fock wave functions for $Z<30$ and relativistic Hartree-Fock-Slater functions for $Z>30$, Carlson *et al.* ensured the most accurate representation of the atomic states to be found in existing autoionization calculations. However, it now appears to be generally accepted that the above predictions only afford a fair estimate of autoionization probabilities. This is because the mechanism of nuclear decay and the phase space sharing between the emitted antineutrino and electrons are neglected. It is more realistic, although less convenient from a calculational viewpoint, to treat the entire process as one single radioactive decay mode, where two electrons (one of which originates from nuclear decay) share the available decay energy simultaneously with the antineutrino. Stephas and Crasemann[12] attempted such a treatment and encountered difficulties arising from approximations used in their treatment and from the requirement that their formalism include the antisymmetrizations of the two electrons. These were overcome (almost simultaneously with the publication of the present treatment) by their associate Mord[14,15] who calculated values of $P_K(\mathrm{SO})$ which is denoted as ${}_1P_K$ in his papers, and also by Shimizu.[18] {It should be noted that Mord[14] makes an error in evaluating the decay matrix element M [his Eqs. (3-3) to (3-6)], although his final expression for P_K is numerically correct. The correct evaluation of his Eq. (3-3) would give his Eq. (3-4) multiplied by 2. Shimizu misquotes our result in his Eq. (12) for the antisymmetrization factor Ξ, which should be multiplied by 2.}

The new departure taken in the theoretical work[7] of the present authors was to incorporate in an exact fashion the demand of the Pauli principle, namely, the antisymmetrization of the final state two electron wave function. This was done conveniently by using a second quantization formalism. This approach differs from others by dropping entirely any distinction between the two electrons emitted when β decay is accompanied by shake-off. Since no measurements can distinguish between the electrons as regards their origin, a formalism which treats the two electrons on an equal footing is most apposite to the situation.

We first treat the case of a one electron model in which the initial state contains only one K-shell electron. The final state antineutrino is also conveniently included in the initial state giving

$$|i\rangle = |e_K; k; \nu\rangle$$

with k labeling the nuclear state. The final state consists of two electrons in the field of the daughter nucleus (k') and can be expressed as

$$|f\rangle = |e'_s e'_p; k'\rangle,$$

where the two electron state is antisymmetrized. The operator causing the transition is taken to be the V–A form of the β-decay Hamiltonian with the nuclear part reduced to the nonrelativistic form

$$H_\beta = \frac{G}{\sqrt{2}} \left\{ \int d^3x [\psi_p^\dagger(x)\psi_n(x)] [\bar{\psi}_e(x)\gamma_0(1-\gamma_5)\psi_\nu(x)] + \frac{C_A}{C_V} \int d^3x [\psi_p^\dagger(x)\vec{\sigma}\psi_n(x)] \times [\bar{\psi}_e(x)\vec{\gamma}(1-\gamma_5)\psi_\nu(x)] \right\}. \tag{3}$$

The $\psi(x)$'s are second quantized fields which annihilate a particle at x, and $\bar{\psi}(x)=\psi^\dagger(x)\gamma_0$ creates a particle at x. Dirac γ matrices obey the usual anticommutation relations $\{\gamma^\mu, \gamma^\nu\}=2g^{\mu\nu}$ with metric $g^{\mu\nu}=(+1,-1,-1,-1)$ and have the following properties

$$(\gamma_0)^+ = \gamma_0, \quad (\vec{\gamma})^+ = -\vec{\gamma}, \quad \gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3.$$

(The convention and normalization we are using correspond to those of Gasiorowicz.[19])

The Fermi golden rule gives for the partial decay rate (i.e., the rate of generation of K vacancies in the case of shake-off),

$$\lambda = 2\pi |\langle f|H_\beta|i\rangle|^2 \rho(E_s, E_p, E_\nu).$$

The evaluation of $|\langle f|H_\beta|i\rangle|^2$ for allowed transitions and various assumed approximations is performed in the Appendix. The result for shake-off

is

$$\lambda^{SO}(p)dp = \frac{G_V^2\xi}{2\pi^3}p^2dp\int_0^{s_0(p)}\frac{s^2ds}{2\pi^2}(W_K - E_p - E_s)^2\{M^2(E_s)F(Z', E_p) + M^2(E_p)F(Z', E_s) - M(E_s)M(E_p)[F(Z', E_s)F(Z', E_p)]^{1/2}\eta\} \quad (4)$$

with the further approximation that $\eta = \{[(E_p+m)/2m][(E_s+m)/2m]\}^{1/2} \approx 1$. $W_K = W_0 - B_K$ equals the available transition energy; W_0 is the decay energy including two electron rest masses. The corresponding expression for β decay, in which the K-shell electron remains in the daughter K shell is

$$\lambda^0(p)dp = \frac{G_V^2\xi}{2\pi^3}p^2dpF(Z', E_p)(W_0 - m - E_p)^2, \quad (5)$$

where a very small exchange contribution has been neglected.

In calculating K-shell shake-off probabilities with this formalism, we used[7] unscreened relativistic hydrogenic wave functions. The relevant matrix element is given by Eq. (29) of Ref. 7.

It should be emphasized that Eq. (4) gives the differential rate of generation of K vacancies $N(2e, \nu, V)$ (where V indicates creation of one K vacancy) in a one electron atom, which is equivalent *separately* to the rate of emission of K electrons and to the rate of emission of associated β particles. It is *not* equal to the *sum* of these rates. Equation (5) corresponds to normal β decay (e, ν). In each case we refer to the detection of one electron with momentum between p and $p+dp$. The total normal β-decay rate is [cf. Eq. (5)]

$$\Lambda = \int_0^{\bar{P}_0}\lambda^0(p)dp, \quad (6)$$

where $\bar{P}_0$ is the maximum emitted electron momentum given by $\bar{P}_0^2 = (W_0 - m)^2 - m^2$. To reflect the real world, where the occupation number is 2 (except for ^{3}H decay) the value of $\lambda(p)$ must be doubled. Hence the total K shake-off probability per β decay is

$$P_K(\mathrm{SO}) = \frac{\int_0^{P_0}2\lambda^{SO}(p)dp}{\Lambda}, \quad (7)$$

where $P_0^2 = (W_K - m)^2 - m^2$. The factor of 2 arises naturally if one takes an initial state with two K-shell electrons and a final state of three electrons, both states being fully antisymmetrized, by a simple extension of the method indicated in the Appendix.

B. Shake-up

In the Carlson *et al.*[11] calculations, the shake-up contributions in which only one electron is ejected while the other is excited to an unfilled level are automatically included. This event can be labeled (e, ν, V) where one K vacancy V is created. Within the one electron model this is easily calculated using the techniques indicated in the Appendix and Ref. 13. It is given by

$$\lambda^{SU}(p)dp = \frac{G_V^2\xi}{2\pi^3}p^2dp\sum_s{}'\{|\langle e_s'|e_K\rangle|^2F(Z', E_p) + |\langle e_p'|e_K\rangle|^2|\phi_S(0)|^2 - |\langle e_s'|e_K\rangle\langle e_p'|e_K\rangle|[F(Z', E_p)|\phi_S(0)|^2]^{1/2}\}(W_K - E_p - E_s)^2, \quad (8)$$

where $|\phi_S(0)|^2$ is the electron density evaluated at the nuclear radius. The summation $\sum_s'$ is over unfilled levels only. The approximation used involves neglecting the exchange terms (second and third in $\{\}$) since they are weighted by $|\phi_S(0)|^2$, and also setting the relativistic total energy E_s equal to m since the binding energies of the unfilled levels are small compared to the K-shell binding energy B_K. The shake-up probability per β decay is thus

$$P_K(\mathrm{SU}) = \frac{\int_0^{P_0}2\lambda^{SU}(p)dp}{\Lambda}, \quad (9)$$

where again the factor of 2 makes the transition from the one electron model to the real system.

The shake-up matrix element is given by Eq. (A10) in Campbell and Law.[13]

C. Direct-collision mechanism

Because the final state electrons can interact, the two electron wave function should have some correlation built into it. Since no solutions as yet exist based on a self-consistent field formalism which allows for the final state interaction, one has to resort to perturbation methods. In practice we use hydrogenic wave functions for the two electrons and attempt to account for final state interactions. We take

$$H = h(1) + h(2) + Qv = H_0 + Qv, \quad (10)$$

where $h(i)$ are single particle Hamiltonians, v is the final state interaction, and Q is the Pauli operator which projects out occupied levels. The correlated two electron wave function can be represented by

$$|e_p' e_s'\rangle = |e_p' e_s'\rangle_0 + \frac{Q}{E_p + E_s - H_0 + i\eta} v |e_p' e_s'\rangle , \quad (11)$$

in the independent pair approximation in analogy with the Bethe-Goldstone[20] equation and $+i\eta$ allows for the outgoing wave boundary condition. We also have

$$H_0 |e_p' e_s'\rangle_0 = (E_p + E_s) |e_p' e_s'\rangle_0 . \quad (12)$$

In the evaluation of the transition matrix element we have to determine

$$\langle e_K | \psi_e(0) | e_p' e_s'\rangle = \langle e_K | \psi_e(0) | e_p' e_s'\rangle_0 + \frac{\langle e_K | \psi_e(0) Q v | e_p' e_s'\rangle}{E_p - E_s - H_0 + i\eta} . \quad (13)$$

The first term gives the uncorrelated contribution. In the evaluation of the right hand side (RHS) of Eq. (13) one will have two parts, a direct part $(\mathrm{RHS})_D$ and an exchange part $(\mathrm{RHS})_E$. Considering only the direct part, one has to first order

$$(\mathrm{RHS})_D = \langle e_K | e_s'\rangle \phi_{e_p'}(0) + \sum_{\alpha\beta}{}'' \frac{\langle e_K | e_\beta\rangle \phi_{e_\alpha}(0) \langle e_\alpha e_\beta | v | e_p' e_s'\rangle}{E_p + E_s - E_\alpha - E_\beta + i\eta} , \quad (14)$$

where $\phi(0)$ are the unperturbed wave functions evaluated at the nuclear radius, and E_α, E_β are the intermediate state energies. The summation is over allowed states only, and we have dropped the subscript 0 for convenience. The second term of Eq. (14) (direct-collision contribution) thus reduces to

$$\sum_\alpha{}' \phi_{e_\alpha}(0) \frac{\langle e_\alpha e_K | v | e_p' e_s'\rangle}{E_p + E_s - E_\alpha - E_K + i\eta} , \quad (15)$$

which can be broken up by using the symbolic representation

$$\frac{1}{x + i\eta} = \frac{P}{x} - i\pi\delta(x) , \quad (16)$$

where P stands for principal part, into

$$\sum_d{}' \phi_d(0) \frac{\langle e_d e_K | v | e_p' e_s'\rangle}{E_p + E_s - E_K - E_d} + P \int \frac{d^3P_\alpha}{(2\pi)^3} \phi_{e_\alpha}(0) \frac{\langle e_\alpha e_K | v | e_p' e_s'\rangle}{E_p + E_s - E_\alpha - E_K} - i\pi\phi_{e_\alpha}(0) \frac{P_\alpha E_\alpha}{(2\pi)^3} \langle e_\alpha e_K | v | e_p' e_s'\rangle , \quad (17)$$

where $E_\alpha = E_p + E_s - E_K$ in the third term of Eq. (17), and $\sum_d'$ sums over allowed discrete levels. The first term in Eq. (14) is usually referred to as the shake-off contribution M_{SO} and the second term the direct-collision part M_{DC}. The evaluation of Eq. (17) for M_{DC} is complicated and Feinberg[1,2] essentially estimated part of this contribution. He also made the approximation of neglecting the interference term, namely (in obvious notation)

$$|M_{SO} + M_{DC}|^2 \sim |M_{SO}|^2 + |M_{DC}|^2$$

which then produces an *additive* probability $P_K(\mathrm{DC})$. As has been noted by Feinberg and also by considering Eq. (17), only part of the correction is purely additive. Feinberg's estimates suggested that

$$\frac{P_K(\mathrm{DC})}{P_K(\mathrm{SO})} \sim \frac{B_K}{E_\beta} , \quad (18)$$

where E_β is the β-particle energy. However, since the neglected interference and other terms may enhance or cancel, we will tentatively use an *ad hoc* additive estimate for $P_K(\mathrm{DC})$,

$$P_K(\mathrm{DC}) = \frac{B_K}{E_0} [P_K(\mathrm{SO}) + P_K(\mathrm{SU})] , \quad (19)$$

where E_0 is the β end point energy.

Until recently, experimental data have not been precise enough to test this correction. There are now sufficient data of high quality to permit one to draw some tentative conclusions about its magnitude.

D. Shape factors and forbidden decays

As noted previously, the above model assumes an allowed decay approximation. Forbidden decays were tentatively accommodated by inserting a phenomenological shape factor[21],

$$S = 1 + aE + b/E + cE^2 , \quad (20)$$

where a, b, c are fitted to the shape of the normal β-decay spectrum by the *ad hoc* replacement $F \to FS$ in Eqs. (4) and (8) for first forbidden decays (1f, 1fu). The total shake-off probability seems to be insensitive to the shape factor as included above, e.g. in ^{89}Sr, $P_K(\mathrm{SO})$ is 8.215×10^{-4} with $S = 1$ and 8.212×10^{-4} with $S = 1 - 0.054E$. However, the electron-vacancy coincidence momentum spectrum will be affected mainly due to modification of the interference term in Eq. (4). For second forbidden decays, Daniel[21] gives a form for the shape

TABLE I. Theoretical P_K probabilities in β decay for various models: P_K(FM): Feinberg-Migdal (Refs. 1 and 3); P_K(C): Carlson *et al.* (Ref 11); P_K(SC): Stephas-Crasemann (Ref. 12); P_K(LC): current model; P_K(+DC): P_K(LC) plus DC correction; P_K(SO), P_K(SU): separate contributions of SO and SU to P_K(LC); P_K(MSO): Mord (Refs. 14 and 15) SO calculations. The first group is allowed (A) decay, followed by first forbidden unique (1fu), first forbidden (1f), and second forbidden (2f). The values in [ ] are calculated for assumed allowed. All P_K values are in units of 10^{-4}.

Z	Type	E_0 (keV)	B_K/E_0	P_K (fm)	P_K(C)	P_K(SC)	P_K(LC)	P_K(expt.)	P_K(+DC)	P_K(SO)	P_K(SU)	P_K(MSO)	Shape factor
$^{3}_{1}$H	A	18.6	0.003	2977		2934	3188		3198	512.1	2676		
$^{6}_{2}$He	A	3510	0.0002	2306	2690	2294	2761		2761	935.2	1826		
$^{32}_{15}$P	A	1710	0.0014	29.53	39.6	29.07	53.64		53.72	49.32	4.32	31.5	
$^{33}_{15}$P	A	248	0.010	29.53	39.6	27.44	47.64		48.12	43.43	4.20		
$^{35}_{16}$S	A	167.4	0.017	26.26	33.7	23.36	38.80		39.46	35.16	3.64	28.4	
$^{45}_{20}$Ca	A	252	0.018	17.46	21.5	15.42	25.70	24.3 ± 3.9	26.16	23.33	2.37		
$^{63}_{28}$Ni	A	67	0.134	9.45	11.5	4.31	5.20		5.90	4.34	0.86	4.0	
$^{95}_{41}$Nb	A	160	0.125	4.55	5.66	2.12	2.67		3.00	2.42	0.25		
$^{114}_{49}$In	A	1987	0.015	3.30	3.60	2.91	5.42	5.40 ± 0.14	5.50	5.24	0.18		
$^{89}_{38}$Sr	1fu	1463	0.012	5.18	6.54	4.71	8.64	8.6 ± 0.7	8.74	8.21	0.42		$a=-0.054$
$^{90}_{38}$Sr	1fu	546	0.031	5.18	6.54	4.16	6.86	6.0 ± 0.9	7.07	6.46	0.40	5.22	$a=-0.054$
$^{90}_{39}$Y	1fu	2270	0.008	4.95	6.23	4.62	8.65	7.2 ± 1.2	8.72	8.24	0.41	6.10	$a=-0.0066$
$^{204}_{81}$Tl	1fu	765	0.115	1.79	2.08	0.83	1.14	1.10 ± 0.08	1.27	1.08	0.06	0.84	$a=-0.02$
$^{79}_{34}$Se	1f	154	0.087	6.29	8.03	3.64	4.91		5.34	4.50	0.41		
$^{107}_{46}$Pd	1f	35	0.729	3.76	4.59	0.0142	0.0142		0.026	0.0081	0.0061	0.0065	
$^{143}_{59}$Pr	1f	930	0.047	2.50	3.03	1.79	2.91	2.91 ± 0.21	3.05	2.80	0.120	2.43	$b=0.06$
$^{147}_{61}$Pm	1f	225	0.209	2.40	2.88	0.660	0.771	0.90 ± 0.09	0.932	0.710	0.061		
$^{151}_{62}$Sm	1f	76	0.639	2.35	2.82	0.023	0.023	0.023 ± 0.003	0.038	0.0173	0.0058	0.0143	
$^{169}_{68}$Er	1f	335	0.177	2.10	2.47	0.687	0.836	1.0 ± 0.2	0.984	0.775	0.061	0.715	
$^{185}_{74}$W	1f	429	0.167	1.93	2.25	0.662	0.823	1.0 ± 0.25	0.960	0.766	0.057	0.705	
$^{203}_{80}$Hg	1f	214	0.400	1.81	2.10	0.138	0.146	0.13 ± 0.04	0.204	0.126	0.020		
$^{210}_{83}$Bi	1f	1160	0.080	1.74	2.04	1.05	1.48	1.23 ± 0.1	1.60	1.425	0.050	1.31	$a=0.578$ $b=28.466$ $c=-0.658$
$^{99}_{43}$Tc	2f	292	0.076	4.08	5.17	2.03 [2.49]	3.13 [3.56]	3.9 ± 0.2	3.37 [3.83]	2.97 [3.38]	0.16 [0.18]	 [3.08]	$d=2.0$
$^{135}_{55}$Cs	2f	210	0.178	2.77	3.39	0.559 [0.919]	0.682 [1.10]		0.803 [1.30]	0.623 [1.019]	0.059 [0.083]		$d=10.0$

TABLE II. Experimental P_K probabilities in β decay in units of 10^{-4}.

Nuclide	Decay type	E_0 (keV)	B_K/E_0	P_K	Ref.
Ca	A	252	0.018	24.3 ± 3.9	30
Sr	1fu	1463	0.012	8.6 ± 0.7	30
				7.3 ± 1.5	25
Sr	1fu	546	0.031	6.5 ± 0.8	30
				5.4 ± 1.0	33
				3.6 ± 0.4	32
Y	1fu	2270	0.008	7.4 ± 1.5	30
				7.0 ± 1.0	33
				5.0 ± 1.1	32
Nb	A	160	0.125	4.4 ± 1.6	32
Tc	2f	292	0.076	3.9 ± 0.3	30
				3.89 ± 0.16	34
In	A	1987	0.015	5.4 ± 0.4	29
Pr	1f	930	0.047	2.88 ± 0.20	28
				2.94 ± 0.22	31
				3.01 ± 0.32	25
Pm	1f	225	0.209	0.98 ± 0.08	5
				0.81 ± 0.09	30
				0.84 ± 0.08	25
Sm	1f	76	0.639	0.023 ± 0.003	5, 13, 25
				0.024 ± 0.003	25
Er	1f	335	0.177	1.0 ± 0.2	5
W	1f	429	0.167	1.0 ± 0.2	30
				1.0 ± 0.3	13
Hg	1f	214	0.400	0.11 ± 0.035	35
				0.15 ± 0.045	36
Tl	1fu	765	0.115	1.0 ± 0.1	6
				1.18 ± 0.06	26
				1.12 ± 0.09	31
				1.06 ± 0.03	27
Bi	1f	1160	0.080	1.23 ± 0.1	25
				1.2 ± 0.1	5
				1.21 ± 0.05	27

of the normal β-decay spectrum as

$$S(E, E_\nu) = (E^2 - 1) + dE_\nu{}^2 . \quad (21)$$

We have used this form for ^{99}Tc and ^{135}Cs, again by the *ad hoc* replacement $F \to FS$. The total shake-off probability is more sensitive to this form, as can be seen from Tables I and II. The formally correct way of including shape factors in the model is as yet unavailable, though a tentative step was taken in this direction by Mord[14] for the first unique decays. In our calculations, we have included S where data are available and assumed $S = 1$ for all other cases.

E. Theoretical P_K estimates

We have listed in Table I the $P_K = P_K(\mathrm{SO}) + \mathrm{SU})$ values from different models. DC corrections have been included. P_K(FM) is the Feinberg-Migdal[1,3] model using unshielded relativistic hydrogenic wave functions (URHWF). P_K(C) is from Carlson *et al.*,[11] who used self-consistent field relativistic and nonrelativistic wave functions. Comparison of P_K(FM) and P_K(C) thus indicates the relative importance of shielding within a model where the nuclear decay mechanism and the nuclear electron are neglected. P_K(SC) is a recalculation using URHWF of the Stephas-Crasemann[12] model (ignoring the uncertain Ξ factor). This model essentially accounts for phase space. A comparison between P_K(FM) and P_K(SC) shows the importance of phase space in several cases where E_0 is small. Although P_K(SC) does include the details of the nuclear decay mechanism, the antisymmetrization between the nuclear electron and the atomic electron (the Pauli principle) is neglected. Our results are listed under columns P_K(LC), P_K(+DC), P_K(SO), and P_K(SU), where the nuclear decay mechanism and antisymmetrization with the nuclear electron are taken into account also using URHWF. P_K(LC) is the sum of the P_K(SO) and P_K(SU). The column P_K(expt.) gives the mean experimental values. P_K(+DC) includes the *additive* estimate of direct collision of Eq. (19) to P_K(LC). Further comments on the P_K(expt.) and P_K(+DC) columns will be deferred to Sec. V. A comparison between P_K(SC) and P_K(LC) shows the importance of this antisymmetrization, especially in the cases where $B_K/E_0 \to 0$. In the opposite limit of $B_K/E_0 \to 1$, one would expect the Pauli principle to be less important since the K-shell electron is originally tightly bound as compared to the available energy. This is again borne out by comparisons on Sm, Hg, and Pd.

Mord's[14] shake-off results are included under column P_K(MSO). The discrepancies between our P_K(SO) and that of Mord's can be traced to his approximate numerical treatment in evaluating the hypergeometric function which arises in the matrix element. Mord also incorporated antisymmetrization into the treatment of Stephas and Crasemann.[12]

The effect of shielding is harder to disentangle. We cannot simply compare P_K(C) with P_K(LC), as our model (even with neglect of phase space) cannot be recast by using the completeness relation into the form used by Carlson *et al.*, i.e., Eq. (1), owing to the presence of the interference term. One could attempt to include shielding by the use of the *ad hoc* recipe of replacing Z by $Z - \sigma$ where $\sigma \sim 0.3$ to 0.5. This replacement assumes that the continuum state electrons after the decay see a nuclear charge of $Z + 1 - \sigma$. This is far from satisfactory as is evident from the work on Auger transitions.[22] Using $\sigma = 0.5$, P_K(LC) increases from 2.91×10^{-4} to 2.96×10^{-4} for ^{143}Pr, and from 0.023×10^{-4} to 0.024×10^{-4} for ^{151}Sm. The screening correction would be more significant, however, for L

shake-off and we have presented experimental evidence elsewhere.[13] A more sophisticated approach to screening must await better experimental data for the L shell than presently available. For the L shell, DC effects should be even smaller (based on the Feinberg[1,2] estimate) and P_L measurements for allowed decays would essentially be tests of the screening correction adapted.

Because of the effect of the Pauli principle which tends to enhance the P_K values for those decays for which $B_K/E_0 \to 0$, Isozumi, Mukoyama, and Shimizu[23] claim that our results are incorrect by a factor of 2 for P_K(SO). We have refuted this claim elsewhere.[24]

III. EXPERIMENTAL MEASUREMENTS

It is useful at this point to be explicit about what is measured experimentally in the context of a theory that draws no distinction between nuclear β particles and ejected atomic electrons.

First the total ionization probability P_K can be measured by determining the (fluorescence yield corrected) K x-ray intensity per decay. Thus

$$P_K = \frac{V}{\Lambda} = \frac{N(2e, \nu, V) + N(e, \nu, V)}{N(e, \nu)} , \tag{22}$$

where $N(e, \nu)$ is the number of β-decay events, $N(e, \nu, V)$ is the number of shake-up events, and $N(2e, \nu, V)$ is the number of shake-off events. (The latter includes direct-collision events intrinsically.)

Measurements have been reported of the β-energy dependence of x electron coincidence rates[12]; their interpretation required some assumptions, based on theory, to separate the electron spectrum into its two equal-intensity components. In the present theoretical context these experiments may be viewed simply as a direct measurement of the shape of the electron spectrum, and in this role they have been superseded by high-resolution measurements reviewed in Sec. IV.

In x-ray electron coincidence measurements, it follows from Eqs. (7) and (9) (in which factors of 2 were used to convert from the one electron model to a real two electron atom) that the momentum spectrum per β decay is

$$N(p) = \frac{N^{SO}(p) + N^{SU}(p)}{\Lambda} = \frac{2\lambda^{SO}(p) + 2\lambda^{SU}(p)}{\Lambda} . \tag{23}$$

If ionization is by shake-up then one event yields one detectable electron. But if shake-off occurs, then each recorded K x ray affords the opportunity to detect either of two emitted electrons (assuming no correlation between them). Hence, the experiment records

$$N_{\exp}(p) = \frac{4\lambda^{SO}(p) + 2\lambda^{SU}(p)}{\Lambda} \tag{24}$$

and so

$$\frac{1}{2}\int_0^{p_0} N_{\exp}(p)\,dp = P_K(\mathrm{SO}) + \tfrac{1}{2}P_K(\mathrm{SU}) . \tag{25}$$

Thus the integral of the spectrum does not yield exactly P_K. This implies that in principle, comparison of direct P_K measurements and coincident electron spectrum measurements could separate out the shake-up contribution.

IV. EXPERIMENTAL DATA ON P_K

In this section we discuss the various recent measurements of P_K and of electron spectrum shapes that may be used for comparison with the theory. Only high-resolution measurements are reviewed; this includes work involving electron detection with magnetic spectrometers and photon detection with Si(Li) or Ge(Li) spectrometers. We have excluded older measurements employing NaI(Tl) and proportional counters; these are collected in our earlier paper,[7] and a comparison with the present Table I reveals much larger scatter among the older measurements than among the new ones; for example the values previously listed for ^{147}Pm have a scatter of ±60% relative to their median, while the four new measurements have a scatter of only ~8% relative to a mean that is a factor of 2 lower. Certain types of coincidence measurements are also excluded because they do not afford a direct test of the theory; these are mentioned at the end of the section. Measurements that have not been published in the open literature are also excluded.

A. X/γ ratio measurements with semiconductor detectors

For most β emitters, the x rays of the daughter atom that signify autoionization (~10^{-4} per decay) are swamped by those arising from K internal conversion transitions that deexcite the daughter nucleus. But there are a few cases where there is only one transition in the daughter nucleus, and it has insufficient energy to convert in the K shell. The γ intensity then gives, via known decay scheme parameters the over-all decay rate Λ. The K x-ray intensity gives V. The method can be extended to cases where one γ transition in the daughter is very weakly converted, if the β branching ratio, the K and the total-conversion coefficients are all known with sufficient accuracy. There is of course some loss in precision in the second variation.

This approach was used by the present authors[5,7,13] employing high-resolution Ge(Li) x-

ray detectors to measure P_K in ^{151}Sm, ^{147}Pm, ^{169}Er, ^{185}W, and ^{210}Bi. The ^{151}Sm result in Table I is, however, a revised value. New determinations of the β branching ratio B to the 21.5 keV level in the ^{151}Sm → ^{151}Eu and of the total-conversion coefficient α of the 21.5 keV transition have been performed by Freedman and Berry.[25] When their values of $B = 0.9\%$ and $\alpha = 26.8$ are used in conjunction with our experimental data,[5] our P_K value becomes 0.023×10^{-4}. A variation was used by Howard[6] and by Ljubicic *et al.*,[26] to study ^{204}Tl. This has in addition to the prominent β branch, a weak (2.1%) electron capture branch of accurately known relative intensity. The Hg K x rays emitted following K capture yield the decay rate and the Pb K x rays give the autoionization rate. The ^{210}Bi and ^{204}Tl results have recently been confirmed independently by Pathak.[27]

B. Crystal spectrometer measurements

Van Eijk and his colleagues[28,29] have used a curved-crystal spectrometer to study nuclides disintegrating by two successive β decays, one of which involves only negligible feeding of nuclear excited states. One can distinguish in the spectrum $K_{\alpha 1}$ x rays of element Z due to autoionization accompanying the ground state to ground state decay and $K_{\alpha 1}$ x rays of $Z \pm 1$, resulting from K conversion of electromagnetic transitions in the other decay. Using half-life and decay scheme information, P_K can be deduced from the ratio of intensities of these two $K_{\alpha 1}$ x-ray lines.

This method has been applied to the two sequences ^{143}Ce → ^{143}Pr → ^{143}Nd and ^{114}In^m → ^{114}In → ^{114}Sn. The measured intensity ratios of $K_{\alpha 1}$ x rays are $10^{-3} \sim 10^{-4}$, making the 20 eV resolution (full width at half-maximum) mandatory.

C. Separate determination of activity and x-ray intensity

Hansen and Parthasaradhi[30,31] have reported nine P_K measurements based on absolute intensity determinations of β particles and K x rays in separate counting arrangements. A Si(Li) detector, calibrated with photon intensity standards, was used to record K x-ray spectra. The decay rates were determined by β counting with a calibrated end-window counter and by 4π liquid scintillation counting. An independent check of the β activity results was afforded by bremsstrahlung counting with a calibrated NaI(Tl) detector.

In several cases the Si(Li) photon spectrum contained characteristic K x rays of the parent nuclide, but the high resolution afforded sufficient separation of these β-induced x rays from the daughter characteristic x rays attributed to autoionization. This observation underlines the danger of accepting uncritically older data taken with NaI(Tl) detectors.

Legrand, Blondel, and Breton[32] performed similar studies on sources of ^{90}Sr-^{90}Y and ^{95}Nb. In the first case a 4π β-γ coincidence method was used to determine the absolute activity and in the second a NaI(Tl) detector was employed. Another study of the mixed ^{90}Sr -^{90}Y emitter was reported by der Mateosian,[33] using a variety of sources.

Watson and Chulik[34] performed an ingenious measurement of P_K for the decay of ^{99}Tc. As in the above methods, the x-ray spectrum was recorded with a Si(Li) detector. The new departure lay in the determination of absolute activity, which involved x-ray excitation by 60 MeV α particles. Several ^{99}Tc sources were made; in each case the source material was deposited on a tin layer which had already been evaporated on the plastic backing. These composite sources were bombarded by 60 MeV α particles and the Tc mass (and hence activity) in each deduced from the intensity ratio of the excited Sn and Tc K x rays.

D. X-γ coincidences

Bond, Gupta, and Zide[35] and Walen[36] have reported independent studies of the decay of ^{203}Hg. This decay feeds almost entirely the first excited state of ^{203}Tl, which decays to the ground state via the well known 279 keV γ ray. K x rays recorded in coincidence with unconverted 279 keV γ rays can be due only to autoionization. The ratio of coincidence intensity to singles K x-ray intensities then yields P_K very simply. Both groups used a NaI(Tl) detector for counting 279 keV γ rays and a Ge(Li) x-ray detector for Tl K x rays. Since P_K is small, the random x-γ coincidence rate is high in an experiment of this type, and the final uncertainty in P_K is determined essentially by the resultant statistical errors.

We note in passing that the approach was first suggested by Smith[37] who performed early NaI(Tl) -NaI(Tl) coincidence measurements on ^{203}Hg; these are omitted here because of our restriction to high-resolution experiments.

E. X-e coincidences

Freedman and his colleagues[4,25] have carried out a series of precision experiments using the Argonne double-lens iron-free β-ray spectrometer. This instrument records the electron spectrum in coincidence with K x rays counted in either a thin NaI(Tl) or a large-area Ge(Li) detector. The salient feature is the use of a very high transmission (~ 5%) electron spectrometer; without this high value the very weak electron spectrum could not be accumulated in a reasonable length of time.

TABLE III. Experimental and theoretical comparison of P'_K. The data are obtained from integrating the e-x coincidence spectrum (Ref. 25).

Nuclide	Expt. P'_K ($\times 10^{-4}$)	Theory P'_K(SO+½SU) ($\times 10^{-4}$)	Theory P'_K(SO+½SU+DC) ($\times 10^{-4}$)
^{89}Sr	7.1 ± 1.5	8.42	8.52
^{143}Pr	2.95 ± 0.32	2.86	2.99
^{147}Pm	0.81 ± 0.08	0.74	0.89
^{151}Sm	0.021 ± 0.003	0.020	0.033
^{210}Bi	1.18 ± 0.10	1.45	1.57

This technique gives negligible spectrum distortion from source, spectrometer, or detector scattering. The primary objective here is to measure the electron spectrum shape. Electron spectra have been measured down to about 7 keV for ^{143}Pr, ^{147}Pm, ^{151}Sm, ^{89}Sr, and ^{210}Bi so that the contribution of the terms in the matrix element in Eq. (4) which dominate the shake-off probability at low energy can be seen.

The absolute rate of autoionization events is obtained by taking half (see below) of the integrated intensity under the coincident electron spectrum, corrected for the efficiency of the spectrometer. The over-all rate is obtained separately either from the singles β spectrum or from an auxiliary measurement. The use of the integrated intensity under the singles β spectrum essentially allows for cancellation of uncertainties in spectrometer efficiency etc., and can be done conveniently via a linearized Kurie plot. Various auxiliary measurements have been used as checks; for ^{210}Bi, the α-decay rate of the ^{210}Po daughter was used.

The P_K values quoted for ^{147}Pm, ^{151}Sm, ^{89}Sr, and ^{210}Bi were kindly supplied to us by Freedman.[25] As we noted in Sec. III, the quantity obtained by integrating the coincident electron spectrum is

$$P'_K = P_K(\mathrm{SO}) + \tfrac{1}{2}\,P_K(\mathrm{SU}) + P_K(\mathrm{DC})$$

$$= P_K - \tfrac{1}{2}\,P_K(\mathrm{SU}). \qquad (26)$$

The approach taken by Freedman is to utilize our predicted SO/SU ratio in deriving a slight adjustment to the factor ½ that multiplies the experimental spectrum; this affords him P_K values (see Table II) which may be compared with the total theoretical ionization probability. However, the presence of a significant DC component would complicate this approach. We have therefore obtained P'_K from Freedman; the values are compared with theory in Table III.

F. Other experiments

Data that do not meet the criteria of high-resolution spectroscopy set here have been summarized by us earlier.[7] We have excluded one other type of measurement, viz. determination of K vacancy creation probability as a function of coincident electron energy. This type of experiment was done during the period when both theory and experiment attempted to distinguish between the two emitted electrons, calling one the ejected atomic electron (usually taken as the lower energy particle) and the other (the higher energy one) the β particle. The older theories differed strongly in their predictions for $P_K(E_\beta)$, viz. the "β-energy dependence of P_K." In the theoretical model presented here, this older approach is no longer useful or even relevant. The most useful type of experiment is now simply a precision determination of the electron spectrum shape over the full energy range, or as much as possible of it. Practically this means magnetic rather than solid state electron spectrometry. The former can be rendered free of the influences of detector, source- or instrument-induced scattering, or distortion. It is the unavoidability of backscattering from solid state electron detectors that makes them essentially useless for measuring continuous spectrum shapes, even though their resolution may be comparable with high-transmission magnetic devices. 4π arrangements do not help in the <100 keV region which is most important here. Thus in the present context the old solid state $P_K(E_\beta)$ measurements although equivalent in principle to the spectrum shape measurements, are hardly useful tests of the theory.

G. Intercomparison of experimental results

In 11 cases, a β emitter has been studied by more than one experimenter; further, different techniques have been employed by the different groups in most of these cases.

The agreement among the different results for these cases is generally excellent; it certainly attests to the care and ingenuity of experimenters who have contributed to this field during the current surge of interest. In the most difficult case, viz. ^{203}Hg, where P_K is very small, the agreement is less dramatic than in such cases as ^{204}Tl, ^{143}Pr, and ^{151}Sm. For most cases, reliable mean values may be derived. The only disagreements occur for ^{90}Sr and ^{90}Y where in each case the Legrand results are significantly lower than two others which, however, agree well with each other. There seems therefore the likelihood that the Legrand results for ^{95}Nb may be also low.

The prediction that the e-x results should be lower than that from other methods is reasonably borne out from results in Tables II and III, except in the case of ^{143}Pr.

V. COMPARISON OF EXPERIMENTAL AND THEORETICAL RESULTS

To facilitate comparison between experimental and theoretical results we have added a column P_K(expt.) in Table I. We have excluded the results of Legrand *et al.*[33] for the reasons stated previously. The e-x data are compared separately in Table III. For each nuclide of interest, a mean P_K is taken from the experimental data, the error quoted being merely the mean of the experimenters' quoted errors. We prefer not to derive a root-mean-square error, since such a procedure is valid only for purely statistical errors, while the basic experimental errors here probably contain significant systematic components. The column P_K(+DC) contains in addition to P_K(LC), the *additive* correction estimate of direct collision using the Eq. (19).

Consider first the simplest cases, namely, allowed decays. We do not expect complicating shape factors. For the two representatives ^{45}Ca and ^{114}In the agreement between our calculated and the experimental values is excellent. While one or two further precise measurements for such cases would be useful, it is clear that in this simplest situation the theory is quite satisfactory.

The next group of nuclides has first forbidden unique shapes. The predicted P_K(LC) and P_K(+DC) are somewhat larger than experiment; however, there is no significant evidence of discrepancy. Freedman and his colleagues[25] have made electron spectrum measurements of ^{89}Sr. Over much of this spectrum they find that the inclusion of the usual theoretical first forbidden unique shape factor which fits the singles shape of ^{89}Sr improves the fit with the theory in comparison to the case where the shape factor is entirely neglected, but below 500 keV the quality of the fit is much poorer indicating that a more sophisticated treatment of the shape factor is needed. Clearly in this case, P_K is a less sensitive test of the theory than the electron spectrum shape.

For the first forbidden decays with essentially allowed shapes (for the singles), we have quite a few representatives. We will omit ^{210}Bi for the time being. Again the agreement between experiment and P_K(LC) is satisfactory. Here we see only slight discrepancies between inclusion or noninclusion of the DC correction except in ^{151}Sm, where now there is total disagreement. The implication is that the *ad hoc* addition of the DC correction as given by Eq. (19) should not be taken too seriously. Furthermore, a more careful treatment of the DC correction is needed.

This leaves us ^{210}Bi and ^{99}Tc, both of which are complicated by shape factors. One can be more definite on ^{210}Bi where the theoretical P_K disagrees with the experimental numbers. Freedman's spectrum shape measurements for ^{210}Bi again cannot be fitted by the theory well at low energies, underlining the need to include neglected corrections. With ^{99}Tc the theoretical numbers were calculated with the second forbidden shape from Daniel[21] and an assumed allowed shape. It is difficult to draw definite conclusions for this case.

Regarding DC corrections, we are forced to conclude that even after the appearance of a large set of new experimental data, there is no unshakeable evidence for DC effects even of the relative magnitude given by $\mathrm{DC}/(\mathrm{SO}+\mathrm{SU}) = B_K/E_0$. The strongest evidence that DC is much smaller than this rule predicts is the case of ^{151}Sm where the e-x data and the x/γ data indicate the DC component is less than $\frac{1}{4}$ of the prediction.

In the case of the e-x data for P_K^1, we give them in Table III. We see that except for ^{210}Bi, the agreement between theory and experiment is again satisfactory.

The generally good agreement between experiment and our model affords no support for the contention of Isozumi *et al.* [23] that our predictions are a factor of 2 too large. It also confirms the importance of phase space sharing by the final decay products and the necessity for antisymmetrization of the final electronic state.

VI. CONCLUSIONS

The theory we have introduced[7] appears to provide a satisfactory description of K shake-off and shake-up for β decays with high end point energy and no complicating shape factors. The discussion presented here indicates that the only serious weakness is the use of a shape factor for the $(2e, \nu, V)$ spectrum simply based on the (e, ν) data. There is no compelling evidence for a simply additive DC effect as given by Feinberg's recipe. If such a mechanism contributes to K electron ejection, it is certainly smaller than his estimate.

As far as future experimental work is concerned, it appears that a definitive demonstration of the DC mechanism will now be extremely difficult There is more scope for progress on the theoretical side, where three main aspects need to be incorporated in the theory. These are (1) a more realistic treatment of the nuclear decay to extract the shape factor to use in shake-off; (2) use of self-consistent field wave functions; and (3) incor-

poration of the final state interaction either perturbatively as we have indicated in Sec. II or directly in a self-consistent field formalism. If the first of these can be accomplished, bringing theory and experiment into agreement for cases like ^{210}Bi, ^{89}Sr, etc., then the field of K-shell autoionization in β decay will be in a rather satisfactory situation. It would certainly be of interest however to see if a rigorous treatment of the final state interaction would predict the unexpectedly small contribution of the DC mechanism.

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APPENDIX

We shall give details of evaluations leading to Eq. (4) and the approximations used. Again for simplicity we shall consider only the vector part of the β-decay Hamiltonian and quote results for the axial vector part (i.e., first and second terms of Eq. (3), respectively). The normalization of the wave functions, convention for γ matrices, etc. are the same as in Gasiorowicz.[19] We will then alter the final form of the result to conform to the normalization used in Law and Campbell.[7,8]

We need the amplitude

$$M_V = \frac{G_V}{\sqrt{2}} \int d^3x \langle k' | \psi_p^\dagger(x)\psi_n(x) | k\rangle \langle e_s' e_p' | \overline{\psi}_e(x) | e_K\rangle \times \gamma_0(1-\gamma_5)\langle 0 | \psi_\nu(x) | \nu\rangle . \quad \text{(A1)}$$

Since the neutrino wave function is undistorted it can be represented by a plane wave

$$\langle 0 | \psi_\nu(x) | \nu\rangle = \frac{(2m_\nu)^{1/2}}{(2\pi)^{3/2}} e^{-i\vec{p}_\nu\cdot\vec{x}} v(p_\nu), \quad \text{(A2)}$$

where the normalization is chosen such that $m_\nu \to 0$ eventually. $v(p_\nu)$ is the negative energy Dirac spinor. (Units of $\hbar = c = 1$ are used.) The electron part can be evaluated using Fock space techniques to give

$$\langle e_s' e_p' | \overline{\psi}_e(x) | e_K\rangle = \langle e_p' | e_K\rangle \delta_{Kp} \langle e_s' | \overline{\psi}_e(x) | 0\rangle - \langle e_s' | e_K\rangle \delta_{Ks} \langle e_p' | \overline{\psi}(x) | 0\rangle , \quad \text{(A3)}$$

where δ_{Kp} is the Kronecker δ for the spin variables of the state K and p. In more familiar Slater determinant form we can write

$$\langle e_s' e_p' | \overline{\psi}_e(x) | e_K\rangle = \int d^3x_1 \int d^3x_2 \langle e_s' e_p' | x_1 x_2\rangle \times \langle x_1 x_2 | \overline{\psi}_e(x) | e_K\rangle , \quad \text{(A4)}$$

with

$$\langle x_1 x_2 | e_s' e_p'\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_s'(x_1) & \phi_s'(x_2) \\ \phi_p'(x_1) & \phi_p'(x_2) \end{vmatrix} \quad \text{(A5)}$$

and

$$\langle x_1 x_2 | \overline{\psi}_e(x) | e_K\rangle = \frac{1}{\sqrt{2}} \begin{vmatrix} \delta^3(x-x_1) & \delta^3(x-x_2) \\ \phi_K(x_1) & \phi_K(x_2) \end{vmatrix} \gamma_0 , \quad \text{(A6)}$$

whence Eq. (A3) follows. Since the electron wave function is distorted by the nucleus $\langle e_s' | \overline{\psi}_e(x) | 0\rangle$ will in general be complicated. However, we can simplify our evaluation by making a crude approximation, namely

$$\langle e_s' | \overline{\psi}_e(x) | 0\rangle \approx \sqrt{F(Z', E_s)}\, e^{-i\vec{p}_s\cdot\vec{x}} \frac{\overline{u}(p_s)}{(2\pi)^{3/2}}, \quad \text{(A7)}$$

where the distortion is thrown completely into the Fermi function $F(Z', E_s)$; $\overline{u}(p_s)$ is the positive energy electron spinor. The transition amplitude thus can be written

$$M_V = \frac{G_V}{2^{1/2}(2\pi)^3} \sqrt{2m_\nu} \times [M_N(p_\nu + p_s)\langle e_p' | e_K\rangle \delta_{Kp} \sqrt{F(Z', E_s)}\, \overline{u}(p_s) - M_N(p_\nu + p)\langle e_s' | e_K\rangle \delta_{Ks} \sqrt{F(Z', E_p)}\, \overline{u}(p)] \gamma_0(1-\gamma_5) v(p_\nu) \quad \text{(A8)}$$

with

$$M_N(p) = \int d^3x e^{-i\vec{p}\cdot\vec{x}} \langle k' | \psi_p^\dagger(x)\psi_n(x) | k\rangle . \quad \text{(A9)}$$

For allowed transitions $M_N(p) = M_N = \langle 1\rangle$, i.e. we replace $e^{-i\vec{p}\cdot\vec{x}}$ by 1. To obtain the decay rate we have to

sum over the neutrino polarization $\sum_\nu$, sum over the final electron spins $\sum_{p,s}$, and average over initial electron spin $\frac{1}{2}\sum_k$. Thus

$$\overline{|M_V|^2} = G_V{}^2 \frac{\langle 1\rangle^2}{(2\pi)^6} \frac{1}{2} \sum_k \sum_{s,p} [\sqrt{F(Z',E_s)}\,\langle e_p'|e_K\rangle \delta_{Kp}\,\bar{u}(p_s) - \sqrt{F(Z',E_p)}\,\langle e_s'|e_K\rangle \delta_{Ks}\,\bar{u}(p)]$$
$$\times (1+\gamma_5)\gamma_0 \not{p}_\nu \gamma_0 [\sqrt{F(Z',E_s)}\,\langle e_K|e_p'\rangle \delta_{Kp}\,u(p_s) - \sqrt{F(Z',E_p)}\,\langle e_K|e_s'\rangle \delta_{Ks}\,u(p)], \tag{A10}$$

where we have used

$$\lim_{m_\nu \to 0} 2m_\nu \sum_\nu v(p_\nu)\,\bar{v}(p_\nu) = \gamma_\alpha p_\nu^\alpha = \not{p}_\nu . \tag{A11}$$

Using properties of the Dirac spinors and γ matrices we have (where m is the electron mass)

$$\overline{|M_V|^2} = \frac{G_V{}^2\langle 1\rangle^2}{(2\pi)^6} \Bigg[|\langle e_p'|e_K\rangle|^2 F(Z',E_s)\,\mathrm{Tr}\left(\frac{\not{p}_s \gamma_0 \not{p}_\nu \gamma_0}{2m}\right) + |\langle e_s'|e_K\rangle|^2 F(Z',E_p)$$
$$\times \mathrm{Tr}\left(\frac{\not{p}\gamma_0 \not{p}_\nu \gamma_0}{2m}\right) - |\langle e_p'|e_K\rangle\langle e_K|e_s'\rangle| \left(\frac{F(Z',E_s)F(Z',E_p)}{2m(E_s+m)2m(E_p+m)}\right)^{1/2}$$
$$\times \tfrac{1}{2}\,\mathrm{Tr}\{[(\not{p}_s+m)(1+\gamma_0)(\not{p}+m) + (\not{p}+m)(1+\gamma_0)(\not{p}_s+m)]\gamma_0 \not{p}_\nu \gamma_0\}\Bigg]. \tag{A12}$$

The traces can be evaluated in the usual manner to give

$$\overline{|M_V|^2} = \frac{G_V{}^2\langle 1\rangle^2}{(2\pi)^6} 2E_\nu \Bigg\{ |\langle e_p'|e_K\rangle|^2 F(Z',E_s)\frac{E_s}{m}\left(1+\frac{\vec{p}_s\cdot\vec{p}_\nu}{E_s E_\nu}\right) + |\langle e_s'|e_K\rangle|^2 F(Z',E_p)\frac{E_p}{m}\left(1+\frac{\vec{p}\cdot\vec{p}_\nu}{E_p E_\nu}\right)$$
$$- |\langle e_s'|e_K\rangle\langle e_K|e_p'\rangle| \left(\frac{F(Z',E_p)F(Z',E_s)}{2m(E_s+m)2m(E_p+m)}\right)^{1/2} \Bigg[mE_p\left(1+\frac{\vec{p}\cdot\vec{p}_\nu}{E_p E_\nu}\right) + mE_s\left(1+\frac{\vec{p}_s\cdot\vec{p}_\nu}{E_s E_\nu}\right)$$
$$+ m^2 + E_p E_s\left(1+\frac{\vec{p}\cdot\vec{p}_\nu}{E_p E_\nu}+\frac{\vec{p}_s\cdot\vec{p}_\nu}{E_s E_\nu}+\frac{\vec{p}\cdot\vec{p}_s}{E_p E_s}\right)\Bigg]\Bigg\}. \tag{A13}$$

We thus finally obtain from

$$\lambda = 2\pi\,\overline{|M_V|^2}\,\delta(W_K - E_s - E_p - E_\nu)\frac{m\,d^3p}{E_p}\,\frac{m\,d^3p_s}{E_s}\,\frac{d^3p_\nu}{2E_\nu}, \tag{A14}$$

that (after integrating over p_ν, p_s, and the direction of p)

$$\lambda^{so}(p)dp = \frac{G_V{}^2\langle 1\rangle^2}{2\pi^3}\,p^2 dp \int_0^{S_0(p)} \frac{p_s{}^2 dp_s}{2\pi^2}(W_K - E_p - E_s)^2 \{M^2(E_p)F(Z',E_s) + M^2(E_s)F(Z',E_p)$$
$$- M(E_p)M(E_s)[F(Z',E_p)F(Z',E_s)]^{1/2}\eta\} \tag{A15}$$

with

$$M(E_p) = (2\pi)^{3/2} m\langle e_p'|e_K\rangle / E_p;$$
$$S_0(p) = [(W_K - E_p)^2 - m^2]^{1/2};$$
$$\eta = \left[\frac{(E_p+m)(E_s+m)}{2m\,2m}\right]^{1/2};$$
$$W_K = W_0 - B_K = \text{available transition energy}.$$

The approximation we make is that $\eta \approx 1$, since E_s, E_p are not much larger than the electron mass m. If the normalization for the continuum states of Law and Campbell[7,8] is used, then $M(E_p)$ corresponds to $\langle e_p'|e_K\rangle$ in those papers.

To account for the axial vector part, the only replacement needed is

$$\langle 1\rangle^2 \to \xi = \langle 1\rangle^2 + \frac{C_A{}^2}{C_V{}^2}\langle\sigma\rangle^2 \tag{A16}$$

in Eq. (A15).

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