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Atomic effects on the *ft* value for tritium β decay

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The atomic effects on the β-decay ft value of tritium are discussed for three atomic systems: the tritium atom and the ions T^+ and T^-. The effect of exchange between bound and continuum electrons in the decay of the tritium atom is shown to lead to an increase in the phase-space integral f by 0.15% relative to the f value for T^+. This corrects an error in earlier work which suggested that the inclusion of exchange effects led to a decrease in the f value for this decay. Differences in atomic-electron screening between the T atom and the T^+ ion are shown to lead to a reduction in f for the T atom by 0.41%, significantly larger than previous estimates of screening effects on f. The combined atomic effects are shown to lead to a difference in f between T^+ and the T atom of 0.30%. The effect of these changes in f on a recent evaluation of the ratio of the weak-interaction coupling constants, G_A/G_V, is discussed.

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I. INTRODUCTION

The tritium atom is the simplest atomic system in which atomic effects enter the β-decay process. These atomic effects may modify the β-spectrum intensity, and thereby the decay constant for emission of β^- particles, by changing the energy available for the decay (the end-point-energy effect), by changing the screening of the β-particle wave function by the atomic electrons (the screening effect) or by modifying processes in which the β particle exchanges with atomic electrons (the exchange effect) [1, 2]. The atomic effects in certain regions of the tritium β spectrum have been extensively investigated in the context of experiments attempting to measure or set limits on the mass of the electron antineutrino emitted in the β-decay process. The distortion due to atomic effects must be removed before any further distortion due to antineutrino-mass effects can be inferred. Thus the region near the maximum β-particle energy (end point) has been examined in order to set limits on the antineutrino mass of the order of tens of eV [3–8] while the low energy part of the β spectrum (in the region of order 1 keV) has been examined following claims that antineutrinos of mass 17 keV may be emitted in a small fraction of decays [9, 10].

Unfortunately, the atomic effects on the ft value do not appear to be fully understood yet, even for the simple case of atomic tritium decay. A calculation of atomic effects in this decay has been reported in [11]. However, a number of approximations employed in this work merit further examination. For instance, in [11] the exchange effect was found to lead to an inhibition in the decay rate. However, we have recently shown that exchange between bound and continuum electrons necessarily leads to an enhancement of the β spectrum in the final state having the same electronic configuration as in the initial state [2]. Furthermore, the expression given in [11] for the ratio of bound to continuum decay ignores nonorthogonality effects between initial and final states as well as electron-electron interactions in these states, and also assumes a plane-wave expression for the continuum wave function. The latter approximation alone is in error by approximately 50%. Finally, as we show below, the effect of atomic electron screening of the β-particle wave function has been significantly underestimated in this earlier work. Thus, one motivation for the present study of tritium decay has been to clarify the atomic effects in this simple but important case, using a description of atomic effects developed for more general many-electron systems [1, 2].

The ft value of tritium is also of interest in connection with the extraction of the ratio of G_A/G_V, the ratio of axial-vector to vector weak interaction coupling constants, from experimental data on the tritium β spectrum. In several recent articles, Budick [11–13] has discussed the ft value for this decay and used a measurement of the end-point energy for the decay, in combination with an improved theoretical result for the Gamov-Teller matrix element, to obtain a value for the ratio G_A/G_V=1.259 ± 0.002. This method of calculating the ratio of coupling constants requires the phase-space integral, f, to be defined accurately, to within approximately 0.2%. Since the end-point energy, E_0, of this β decay is relatively low (E_0=18.6 keV), atomic effects may influence f at a level ranging from a few tenths of a percent to one percent, depending on the particular atomic state and thus, given the quoted error in the ratio G_A/G_V, these effects need to be taken account of in the calculation of f.

In this article we thus reexamine atomic effects on the

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decay rate of tritium. Three atomic systems are studied in detail: the neutral tritium atom and the ions T^+ and T^-. In each case the atomic effects on bound-state decay, screening, exchange, and the end-point energy are considered.

II. BOUND-STATE DECAY

In the process of bound-state decay, the final electronic state contains only bound electrons so that no β^- particle emerges from the atom and the antineutrino carries away all the excess decay energy. It is convenient to express the bound-state-decay contribution as a ratio of bound to continuum decays since the nuclear matrix elements cancel leaving a ratio of purely lepton factors. We have previously presented [1] a general expression for the ratio of bound to continuum decay ($\lambda_{\gamma'}/\lambda_c$) for an allowed β transition of a general N-electron initial atomic state to a final ($N+1$)-electron state γ'. If all quantities are expressed in relativistic units this ratio is given by

$$\frac{\lambda_{\gamma'}}{\lambda_c} = \frac{\pi W_{\bar{\nu}}{}^2 A_{\gamma'}}{2f}. \tag{1}$$

Here $\lambda_{\gamma'}$ is the decay constant for bound-state decay to the electronic state γ', λ_c is the continuum decay constant, f is the phase-space integral for the continuum decay of the neutral atom, and $W_{\bar{\nu}}$ is the energy of the antineutrino emitted in the bound-state decay of the ion. This energy is given by

$$W_{\bar{\nu}} = W_{\zeta} - W_{\zeta'} + W_{\gamma} - W_{\gamma'}, \tag{2}$$

where W_{ζ} and $W_{\zeta'}$ are the total energies, including rest mass contributions, of the initial and final nuclear states and W_{γ} and $W_{\gamma'}$ are similarly the total energies of the initial and final atomic states of the ion undergoing bound-state β decay. In Eq. (1), $A_{\gamma'}$ is the decay amplitude for the bound-state decay of the ion, defined explicitly in [1]. For tritium decay, creation into s orbitals only need be considered because the components of the orbital radial wave functions associated with creation into orbitals with $l \neq 0$ are negligible in comparison. For decay of the bare tritium nucleus the dominant γ' states are thus of the form $\mathrm{He}^+\ ns^1$. The decay amplitudes to these states are

$$A_{ns^1} = [P_{ns}(R)/R]^2, \tag{3}$$

where $P_{ns}(R)$ is the large component of the radial wave function for a final-state s orbital evaluated at the nuclear radius R. The calculation of the phase-space integral requires the ^{3}H-^{3}He nuclear mass difference to be defined precisely. In this work this quantity has been taken to be 18.259 eV [14], yielding a phase-space integral equal to 2.86×10^{-6}. The one-electron final-bound-state wave functions are well-known analytic functions. Substituting into Eq. (1) and summing over all ns final states yields a value for the total ratio of bound to continuum decays, λ_b/λ_c, of 1.08%, in good agreement with the value of 1.1% obtained by Tikhonov and Chukreev [15] and 1.03% obtained by Budick [11].

For decay of a neutral tritium atom with the configuration $1s^1$, the dominant final atomic states are the He $1s^2$ state and the states of the form He $1s^1ns^1$. For the He $1s^2$ state, the decay amplitude is

$$A_{1s^2} = \tfrac{1}{2}\langle \mathrm{He}\ 1s|\mathrm{T}\ 1s\rangle^2 [P_{1s}(R)/R]^2, \tag{4}$$

where the quantity $\langle \mathrm{He}\ \ 1s \mid \mathrm{T}\ \ 1s\rangle$ denotes a one-electron overlap between an initial-state $1s$ orbital and a final-state $1s$ orbital in the neutral He atom. The final-state configuration $1s^1ns^1$ defines two electron states having two possible values of the total angular momentum (J=0,1). The decay amplitude obtained by summing over the contributions from both these J states is

$$A_{1s^1ns^1} = R^{-2}\left(\langle \mathrm{He}\ 1s|\mathrm{T}\ 1s\rangle^2 P_{ns}^2(R) - \langle \mathrm{He}\ 1s|\mathrm{T}\ 1s\rangle\langle \mathrm{He}\ ns|\mathrm{T}\ 1s\rangle P_{ns}(R)P_{1s}(R) + \langle \mathrm{He}\ ns|\mathrm{T}\ 1s\rangle^2 P_{1s}^2(R)\right). \tag{5}$$

TABLE I. Radial wave functions and orbital overlaps involving $\mathrm{He}^{(0)}$ final-state bound wave functions. $P_{ns}(R)$ is the large component of the radial wave function for an orbital of $\mathrm{He}^{(0)}$, evaluated at the nuclear radius, R.

Orbital ns	$P_{ns}(R)/R$	$\langle \mathrm{He}^{(0)}\ ns \mid \mathrm{T}\ 1s\rangle$	$\langle \mathrm{He}^{(0)}\ ns \mid \mathrm{T}^-\ 1s\rangle$
$1s$	5.6167	+0.84093	+0.66150
$2s$	0.9102	-0.36557	-0.69521
$3s$	0.4674	-0.14054	-0.37489
$4s$	0.2946	-0.08204	-0.28643
$5s$	0.2069	-0.05582	-0.23626
$6s$	0.1555	-0.04125	-0.20310
$7s$	0.1222	-0.03213	-0.17925
$8s$	0.0994	-0.02596	-0.16112
$9s$	0.0828	-0.02144	-0.14642
$10s$	0.0704	-0.01825	-0.13509

In this study, the Oxford Dirac-Fock computer program, GRASP [16], has been used to compute the wave functions for the initial and final states and hence the decay amplitudes. The final states considered were He $1s^2, 1s^1 2s^1, \ldots, 1s^1 10s^1, 2s^2, 2s^1 3s^1, \ldots, 2s^1 10s^1$, and $3s^2$. Values of the radial wave functions evaluated at the nuclear radius, $P_{ns}(R)$, and the orbital overlaps $\langle \mathrm{He}^{(0)}\ ns \mid \mathrm{T}\ 1s \rangle$ are shown in Table I. For convenience in the following discussion, the first term in bold parentheses in Eq. (5) will be called the direct term while the second and third terms in bold parentheses in Eq. (5) will be referred to as exchange terms since they involve exchange of an ns electron with a $1s$ electron. It should be noted that these exchange terms which involve two bound electrons are different from the exchange terms discussed below in Sec. IV, which involve one bound and one continuum electron. Values for the direct and exchange terms together with the associated decay amplitudes and bound to continuum decay ratios are shown in Table II for the most important of these states. The $1s^2$ final state is seen to give the largest single contribution to the bound-state decay but the contribution from excited states is of comparable magnitude. Furthermore, the exchange terms in bound-state decay to excited final states are seen to make a significant contribution to the decay amplitude for these states. Such exchange terms would be zero if there was perfect orbital orthogonality between initial- and final-state orbitals. Summing over all the final states gives λ_b/λ_c=0.55%. This may be compared with two previous calculations of the bound to continuum decay ratio in tritium, one by Sherk [17] giving λ_b/λ_c=0.56% and one by Bahcall [18] giving λ_b/λ_c=0.69%. The apparent agreement with Sherk's result is due to a fortuitous cancellation of large errors in the latter work. Thus Sherk's calculation neglected the lack of orthogonality between initial and final states and also ignored decays to excited atomic states which have been shown to constitute more than 40% of all bound-state decays. Furthermore, Sherk's approach assumed a plane-wave form for the continuum electron wave function which enters the phase-space integral, leading to an underestimate of f by approximately 50%. Bahcall's calculation included orbital nonorthogonality effects and decay to excited final states, but ignored the final-state interaction between the two bound electrons so that the electron wave functions were assumed to be orbitals of the one-electron atom He^+.

TABLE II. Ratios of bound to continuum decay, $\lambda_{\gamma'}/\lambda_c$, for the most important final atomic final states, γ', produced by bound-state decay of the tritium atom in its ground state, $1s^1$. The direct and exchange terms and decay amplitudes are defined in the text. The total amplitude is obtained by summing over all the final states described in the text and thus includes small contributions from excited states not shown in the table.

State γ'	Direct term (a.u.)	Exchange term (a.u.)	Amplitude $A_{\gamma'}$ (a.u.)	$\lambda_{\gamma'}/\lambda_c$ (%)
$1s^2$	11.1553		11.1553	0.315
$1s^1 2s^1$	0.5858	5.788	6.3740	0.180
$1s^1 3s^1$	0.1544	0.9334	1.0878	0.031
$1s^1 4s^1$	0.0614	0.3264	0.3878	0.011
$1s^1 5s^1$	0.0303	0.1528	0.1831	0.005
$1s^1 6s^1$	0.0171	0.0840	0.1011	0.003
$1s^1 7s^1$	0.0106	0.0511	0.0617	0.002
$1s^1 8s^1$	0.0070	0.0334	0.0404	0.001
$1s^1 9s^1$	0.0048	0.0231	0.0279	0.001
$1s^1 10s^1$	0.0035	0.0166	0.0201	0.001
$2s^2$	0.0533		0.0553	0.002
$2s^1 3s^1$	0.0292	-0.0055	0.0237	0.001
Total			19.6	0.554

Now we consider the bound-state decay of the ion T^-. Such decay would lead to a He^- ion. No bound states, containing only s electrons, are known to exist for this ion. A metastable ion with the configuration $1s^1 2s^1 2\bar{p}^1$ has been observed experimentally [19], but the presence of the $\bar{p}$ electron means that it would be produced with extremely small probability in β decay of the T^- ion in its ground state $1s^2$. In decay of the T atom, creation into continuum $\bar{p}$ final states occurs in only approximately 0.005% of all continuum β decays. In view of this it would seem that bound-state decay of T^- to final states containing $\bar{p}$ electrons should also have a low probability compared with the bound-state decay to s states in the T atom. Therefore we conclude that $\lambda_b/\lambda_c < 0.01\%$ for T^-. This conclusion is different from that arrived at by Budick [11], who estimated λ_b/λ_c=0.47% in T^-. This latter calculation did not consider explicit wave functions for T^- final states. Instead, the bound-state decay rate in T^- was calculated from an approximate expression derived originally [17] to calculate the bound-state decay rate of the tritium atom and which would seem to have no validity for the T^- ion.

III. SCREENING

The screening effect of the atomic electrons on the β spectrum has been discussed by a number of authors [20–22, 1]. According to Rose [20] the effect of the atomic electron distribution in the final state can be taken account of by evaluating the Fermi function at a shifted energy $(W - V_s)$ where the quantity V_s, the screening potential for a final state, is equal to the magnitude of the interaction between a unit charge at the origin and the charge distribution due to the atomic electrons in a given final electronic state. This approximation for the screening effect, which is based on the WKB approximation, tends to become less valid as the nuclear charge increases. However, comparison of screening effects calculated with continuum wave functions evaluated by fitting to Hartree-Fock atomic potentials [21] with screening effects obtained using the WKB approximation indicates that, for a low-Z decay such as that of tritium, the WKB method works well and reproduces the screening effects on the phase-space integral to within the accuracy required here (approximately two significant figures). Hence in the following the Rose WKB method is used to evaluate the screening effects on the phase-space integrals.

It is convenient to consider an average final-state screening potential, obtained by weighting the screening potentials for each final state in proportion to the probability of production of each final state [23, 1, 24]. This average final-state screening potential for decay of an N-electron initial state is then given by

$$\bar{V}_s = \sum_{\bar{\gamma}} \langle N,\bar{\gamma}|N,\gamma\rangle^2 \langle N,\bar{\gamma}| \sum_{i=1}^{N} r_i^{-1} |N,\bar{\gamma}\rangle, \qquad (6)$$

where γ defines the inital state of the N atomic electrons. For decay of the tritium atom, the final $\bar{\gamma}$ states are one-electron He ns^1 states and the screening potentials are easy to compute for each state from the hydrogenic wave functions. This yields $\bar{V}_s$=41.7 eV, in agreement with the value obtained by Budick. Evaluation of the phase-space integral with this value of $\bar{V}_s$ yields the result that the effect of screening leads to a fractional change, $\Delta f/f$, in the phase-space integral of -0.41% . In this and subsequent sections the values of the fractional changes, $\Delta f/f$, are defined to be positive if the associated atomic effect increases the f value relative to that for the T^+ ion. The magnitude of this result for the T atom is significantly larger than the value of $\Delta f/f$=-0.22% obtained by Budick [11]. The latter result was based on a numerical result $\frac{1}{f}\frac{\partial f}{\partial \bar{V}_s} = -0.0055\%$ per eV obtained previously by Bergkvist [23]. It would thus seem that Bergkvist's partial differential with respect to $\bar{V}_s$ implies screening effects which are too low by a factor of about 2. This conclusion is supported by a calculation by Alder, Bauer, and Raff [25], who obtained a result of $\Delta f/f$=-0.275% based on a final-state screening potential of 27.21 eV. Scaling this result for $\bar{V}_s$=41.7 eV yields a screening effect of $\Delta f/f$=-0.42% in reasonable agreement with the result obtained above.

For decay of the ion T^-, the dominant $\bar{\gamma}$ states are states of the neutral He atom with configurations $1s^2$ and $1s^1ns^1$. Values of the screening potentials, $V_s(\bar{\gamma})$, for various final states, calculated using wave functions obtained with the Oxford Dirac-Fock program are shown in Table III, together with values of the squared overlaps $\langle$He $\bar{\gamma}|$ T $1s\rangle^2$. The ground final state $1s^2$ gives the largest single contribution to the sum over $\bar{\gamma}$ in Eq. (6). However, contributions from the $1s^12s^1$ and $2s^2$ states are non-negligible. The average final-state screening potential is found to be 37.8 eV. Evaluating the phase-space integral with this value of $\bar{V}_s$ yields $\Delta f/f = -0.45\%$ for T^-, close to the value for the T atom. By considering just one final state and assuming a simple product of hydrogenic wave functions to describe the helium orbitals, Budick [11] obtained a value of 63 eV for $\bar{V}_s$ and $\Delta f/f = -0.35\%$. This latter result again assumed the numerical relation given in [23] involving the partial differential of f with respect to $\bar{V}_s$ which has been shown to give results which are a factor of 2 too low.

TABLE III. Screening potentials $V_s(\bar{\gamma})$ for the dominant final states produced in continuum β decay of the T^- ion. Each atomic state, $\bar{\gamma}$, is a two-electron state of $\mathrm{He}^{(0)}$ and is produced with a probability given by the squared overlap $\langle N,\bar{\gamma}|N,\gamma\rangle^2$.

Final state $\bar{\gamma}$	$\langle N\bar{\gamma}\|N\gamma\rangle^2$	$V_s(\bar{\gamma})$ (eV)	$\langle N\bar{\gamma}\|N\gamma\rangle^2 V_s(\bar{\gamma})$ (eV)
$1s^2$	0.19147	108.07	20.692
$1s^12s^1$	0.21149	61.837	13.078
$1s^13s^1$	0.00227	57.349	0.130
$1s^14s^1$	0.00143	55.856	0.080
$1s^15s^1$	0.00070	55.188	0.039
$1s^16s^1$	0.00039	54.826	0.021
$1s^17s^1$	0.00024	54.612	0.013
$1s^18s^1$	0.00016	54.474	0.008
$1s^19s^1$	0.00011	54.380	0.006
$1s^110s^1$	0.00008	54.314	0.004
$2s^2$	0.23359	15.605	3.645
$2s^13s^1$	0.00250	11.117	0.028
$2s^14s^1$	0.00158	9.625	0.015
$2s^15s^1$	0.00077	8.953	0.007
$3s^2$	0.00003	6.629	0.000

IV. EXCHANGE

The nonorthogonality of initial- and final-state wave functions allows electrons to be shaken off in the decay process. It is thus possible for a final state containing a continuum electron to arise by creation of the electron in a bound orbital with simultaneous shakeoff of a bound electron into the continuum. Such a process is termed exchange decay in contrast to the direct decay process in which a β^- electron is created directly into a continuum orbital. In the T^+ ion, such exchange effects are absent since there are no atomic electrons. For the tritium atom, the intensity of the β spectrum at an energy E, including exchange, can be written [2]

$$\frac{dI}{dE} = K\frac{W}{p}[\bar{E}_0 - E]^2 \sum\!\!\!\!\!\!\int_A [\langle \mathrm{He}\ A|\mathrm{T}\ 1s\rangle^2 P_{Es}^2(R) - \langle \mathrm{He}\ A|\mathrm{T}\ 1s\rangle\langle \mathrm{He}\ Es|\mathrm{T}\ 1s\rangle P_{Es}(R)P_A(R) + \langle \mathrm{He}\ Es|\mathrm{T}\ 1s\rangle^2 P_A^2(R)], \qquad (7)$$

where $W = E+mc^2$ is the total β-particle energy, p is the β momentum, $\bar{E}_0$ is the average end-point energy, and K is a constant. The contribution from final states containing an $E\bar{p}$ electron is of the order of 0.005% of the total intensity and has been neglected for convenience. The summation integration in Eq. (7) arises from considering the contributions to the β-decay rate from all possible two-electron final states of the form AEs. Thus the summation includes terms in which A is a bound ns orbital (n=1,2,...) and also terms where A is a continuum orbital, in which case the integration is over the energy of this second continuum electron. In the following, these two contributions will be considered separately. In Eq. (7) $\langle \text{He } A | \text{T } 1s\rangle$ is an overlap integral between a $1s$ orbital of tritium and an orbital A of the helium atom in a final state having the configuration A^1Es^1. Exchange in final states $A^1E\bar{p}^1$ is ignored since these final states give only a very minor contribution to the total decay rate for tritium decay.

If exchange effects are ignored then the terms in Eq. (7) which involve the quantity $P_A(R)$ vanish. Then using orbital closure [1] yields the standard result for the β intensity calculated ignoring exchange effects (indicated by the superscript NE)

$$\frac{dI^{\rm NE}}{dE} = K P^2_{Es}(R)\frac{W}{p}[\bar{E}_0 - E]^2. \tag{8}$$

Combining Eqs. (7) and (8), the phase-space integral including exchange can be written

$$f = \int_{E=0}^{\bar{E}_0} \frac{dI^{\rm NE}}{dE}\left(\sum_{n=1}^{\infty} \eta^{ns}_{\rm ex}(E) + \chi^{\rm cont}_{\rm ex}(E)\right) dE. \tag{9}$$

Here $\eta^{ns}_{\rm ex}(E)$ represents the distortion of the β spectrum at the energy E due to exchange in the ns final state and is given by

$$\eta^{ns}_{\rm ex}(E) = -\,\langle \text{He } Es|\text{T } 1s\rangle\langle \text{He } ns|\text{T } 1s\rangle \frac{P_{ns}(R)}{P_{Es}(R)} + \langle \text{He } Es|\text{T } 1s\rangle^2 \left[\frac{P_{ns}(R)}{P_{Es}(R)}\right]^2. \tag{10}$$

In Eq. (9) $\chi^{\rm cont}_{\rm ex}(E)$ yields the modification to the phase-space integral due to the presence of a second continuum electron in final states of the form $E'sEs$ in which there are two continuum electrons with energies E and E'. From Eq. (7), $\chi^{\rm cont}_{\rm ex}(E)$ is given by

$$\chi^{\rm cont}_{\rm ex}(E) = \int_{E'=0}^{E_{\rm max}} \phi(E,E')\, dE', \tag{11}$$

with $\phi(E,E')$ given by

$$\phi(E,E') = \left(-\langle \text{He } Es|\text{T } 1s\rangle\langle \text{He } E's|\text{T } 1s\rangle \frac{P_{E's}(R)}{P_{Es}(R)} + \langle \text{He } E's|\text{T } 1s\rangle^2 \left[\frac{P_{E's}(R)}{P_{Es}(R)}\right]^2\right)\frac{W'}{c^2p'}. \tag{12}$$

The factor of W'/c^2p' arises from the density of states of the continuum electron with total energy $W' = E' + mc^2$ and momentum p'. In Eq. (11) the quantity $E_{\rm max}$, the upper limit on the E' integration, arises from the need to avoid double counting of the states with two continuum electrons and is given by $E_{\rm max} = E$ if $E < \frac{1}{2}\bar{E}_0$ and $E_{\rm max} = \bar{E}_0 - E$ if $E \geq \frac{1}{2}\bar{E}_0$. Thus $\chi^{\rm cont}_{\rm ex}(E)$ does not represent the modification to the β intensity at the energy E due to exchange effects in states with two continuum electrons since, in the latter case, final states with continuum electrons with energies E and E' may contribute to the β intensity at both energies, whereas such states make only a single contribution to the final-state summation in f.

It should be noted that Eq. (10) differs from the subshell exchange factors discussed in [2] since in the latter work the focus was on exchange in medium- and high-Z decays in which only one final state of the s and $\bar{p}$ electrons dominates. This state has the same s and $\bar{p}$ occupation numbers as in the initial state and is produced with greater than 99.9% probability in decays of medium- and high-Z atoms, and thus exchange in final states with excited s and $\bar{p}$ electrons is negligible. However, this single configuration of the s and $\bar{p}$ electrons gives rise to a number of nonzero exchange terms involving different s (or $\bar{p}$) subshells since, for medium- and high-Z atoms, there will, in general, be a number of such subshells which are occupied in the initial state. In the present case of tritium decay, in which the nuclear charge is low, the final $\bar{\gamma}$ states which contain an excited s electron are produced in approximately 30% of decays and it is therefore necessary to explicitly take into account exchange effects in these excited states. However, there is only one ($1s$) electron in the initial state and thus for each excited state there is only a single exchange term.

It is convenient to define exchange contributions to the phase-space integral, $f^{ns}_{\rm ex}$ and $f^{\rm cont}_{\rm ex}$, through

$$f^{ns}_{\rm ex} = \int_{E=0}^{\bar{E}_0} \frac{dI^{\rm NE}}{dE}\eta^{ns}_{\rm ex}(E)\, dE \left(\int_{E=0}^{\bar{E}_0} \frac{dI^{\rm NE}}{dE}\, dE\right)^{-1} \tag{13}$$

and

$$f^{\rm cont}_{\rm ex} = \int_{E=0}^{\bar{E}_0} \frac{dI^{\rm NE}}{dE}\chi^{\rm cont}_{\rm ex}(E)\, dE \left(\int_{E=0}^{\bar{E}_0} \frac{dI^{\rm NE}}{dE}\, dE\right)^{-1}. \tag{14}$$

The quantity $f^{ns}_{\rm ex}$ represents the fractional change in the phase-space integral for the decay as a result of inclusion of exchange effects in the final states ns^1Es^1. The quantity $f^{\rm cont}_{\rm ex}$ represents the fractional change in the phase-space integral as a result of inclusion of exchange effects in all final states of the kind $E's^1Es^1$ containing two continuum electrons.

In this work we have used hydrogenic wave functions to compute the radial wave functions and overlaps in Eqs. (10) and (12). In this case the overlaps can be expressed in a simple analytic form as described in [2]. Figure 1 shows the quantities $\eta^{ns}_{\rm ex}(E)$ (for n = 1, 2, and 3) and $\chi^{\rm ex}_{\rm cont}(E)$ in the range 0.5–3 keV, together with the sum of all these factors, $\chi^{T}_{\rm ex}(E)$, given by

$$\chi^{T}_{\rm ex}(E) = \sum_{ns} \eta^{ns}_{\rm ex}(E) + \chi^{\rm cont}_{\rm ex}(E). \tag{15}$$

The $1s$ state exchange factor is positive over the whole spectrum, whereas all the excited bound states give negative exchange factors. The values for the 1s, 2s, and 3s exchange factors and continuum exchange factors at 1 keV are +0.174%, −0.036%, −0.005%, and −0.011% and may be compared with the values of +0.19%, −0.04%, 0.00%, and −0.04% implied in Table I of [9]. Figure 2 shows the quantity $\chi^{T}_{\rm ex}(E)$ for the whole energy range from zero to the end-point energy. Integrating over the β spectrum

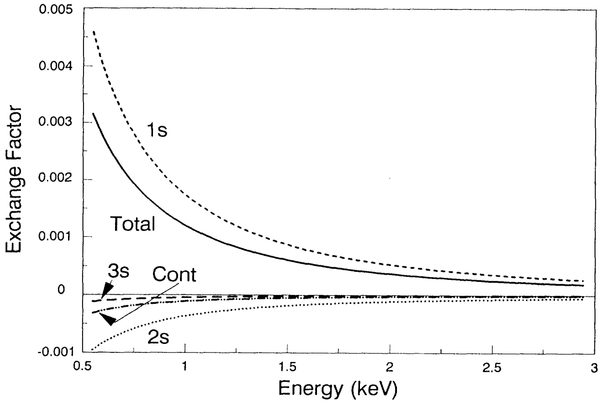

FIG. 1. Energy dependence of the exchange factors $\eta_{\rm ex}^{ns}(E)$ (n=1,2,3), $\chi_{\rm ex}^{\rm cont}(E)$, and $\chi_{\rm ex}^{T}(E)$ in the energy range 0.5–3 keV for decay of $\mathrm{T}^{(0)}$.

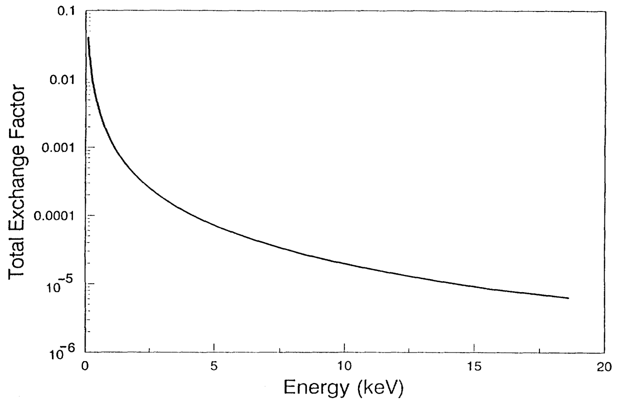

FIG. 2. Energy dependence of the total exchange factor $\chi_{\rm ex}^{T}(E)$ for decay of $\mathrm{T}^{(0)}$.

according to Eqs. (13) and (14) yields the exchange contributions shown in Table IV. The contribution from exchange in the 1s final state dominates but exchange in other final states, including states with two continuum electrons, is non-negligible. Summing over all final states yields a total exchange contribution of 0.153%, indicating that the inclusion of exchange enhances the overall β-decay rate.

Budick [11] has previously calculated the exchange effect in tritium decay and reported a value of −0.15% implying that the inclusion of exchange decreases the β^--decay rate. This latter result was based on an expression for exchange effects given by Bahcall [26] that contains an inconsistency in the evaluation of the overlap between bound and continuum wave functions [2] which leads to the exchange factors being negative at all energies. We have shown previously [2] in the general case that the exchange terms must interfere constructively in the final state having the same configuration as the initial state, which in the case of tritium decay corresponds to the 1s final state. Since this final state gives the dominant contribution to the exchange effect, it follows that the total effect of exchange leads to an enhancement of the β decay rate. In the case of tritium decay, although the sign is incorrect, the magnitude of the exchange effect calculated by Bahcall's method appears to agree reasonably closely with the result obtained here, though it should be noted that in the general case, the magnitudes of the exchange effects calculated by the former method are significantly in error [2].

The calculation of exchange effects in the T^- ion is somewhat more complicated than that in the T atom since there are a number of three-electron final states possible in the case of T^- decay. It is shown in the Appendix that the total exchange factor for T^- decay can be written in the form of Eq. (9) with the exchange factor $\eta_{\rm ex}^{ns}(E)$ given by

$$\eta_{\rm ex}^{ns}(E) = -2\langle \mathrm{He}\ Es|\mathrm{T}\ 1s\rangle\langle \mathrm{He}\ ns|\mathrm{T}\ 1s\rangle\frac{P_{ns}(R)}{P_{Es}(R)} + \langle \mathrm{He}\ Es|\mathrm{T}\ 1s\rangle^2\left[\frac{P_{ns}(R)}{P_{Es}(R)}\right]^2 . \tag{16}$$

The exchange factor, $\chi_{\rm ex}^{\rm cont}(E)$, is given similarly by Eq. (11) with

$$\phi(E,E') = \left(-2\langle \mathrm{He}\ Es|\mathrm{T}\ 1s\rangle\langle \mathrm{He}\ E's|\mathrm{T}\ 1s\rangle\frac{P_{E's}(R)}{P_{Es}(R)} + \langle \mathrm{He}\ E's|\mathrm{T}\ 1s\rangle^2\left[\frac{P_{E's}(R)}{P_{Es}(R)}\right]^2\right)\frac{W'}{c^2p'} . \tag{17}$$

These expressions are seen to be similar to those given in Eqs. (10) and (12) for decay of the T atom except that there is an extra factor of 2 in the first term in the T^- exchange factors. The factor of 2 arises because of the presence of two electrons in the T^- atom, both of which may participate in exchange processes as compared with the single electron in the T atom. It should be noted that although Eqs. (16) and (17) have a similar form to Eqs. (10) and (12), the initial and final orbital sets are necessarily different in T and T^- decay.

In this work we have used unscreened hydrogenic wave functions to evaluate the quantities $\langle \mathrm{He}\ Es|\mathrm{T}\ 1s\rangle$, $\langle \mathrm{He}\ E's|\mathrm{T}\ 1s\rangle$, and $P_{Es}(R)$, which involve the continuum electron wave functions, and used values of $\langle \mathrm{He}\ ns|\mathrm{T}\ 1s\rangle$ and $P_{ns}(R)$ calculated with the GRASP code. We have previously shown in the case of exchange effects in decays of medium- and high-Z decays [2] that the evaluation of the bound-continuum orbital overlaps with the full nuclear charge is a reasonable approximation and this approach should be valid for tritium decay where the screening effects are even less. The bound helium orbitals used in the evaluation of the orbital overlaps $\langle \mathrm{He}\ ns|\mathrm{T}\ 1s\rangle$, between a 1$s$ orbital in T^- and an ns orbital in the $\mathrm{He}^{(0)}$ atom, were evaluated for neutral helium in an extended

TABLE IV. Summary of the exchange contributions, f_{ex}^{ns} and $f_{\text{ex}}^{\text{cont}}$, to the phase-space integral for bound ns orbitals and continuum orbitals involved in the exchange process in the decay of the T atom and T^- ion.

Orbital	Exchange contribution f_{ex}^{ns} or $f_{\text{ex}}^{\text{cont}}$ (%)	
	T	T^-
1*s*	+0.202	+0.301
2*s*	-0.035	-0.047
3*s*	-0.004	-0.008
4*s*	-0.001	-0.004
Continuum	-0.009	-0.022
Total	+0.153	+0.220

average level calculation and were the same set used in the calculation of the bound-state decay rate of the tritium atom. The orbital overlaps, calculated in this way, are shown in Table I. This procedure attempts to provide the best possible description of the chemically sensitive bound orbitals while at the same time allowing the computation of the orbital overlaps using a final-state orbital set in which orthogonality between final-state orbitals is preserved. The motivation for this approach has been discussed in more detail in [2].

The exchange contributions for T^- decay, calculated using the above procedure, are shown in the third column of Table IV, from which it can be seen that the qualitative pattern of the exchange contributions is the same as in the T atom. The total exchange contribution for T^- is +0.22%, which is somewhat larger than for the T atom. Although the dominant exchange term for T^- decay contains an extra factor of 2 as compared to that in the decay of the T atom, the exchange contributions for T^- are less than twice those for the T atom, principally because of a nonorthogonality effect which leads to the magnitude of the overlap $\langle \text{He } 1s | \text{ T } 1s \rangle$ for T^- decay being less than that of the equivalent overlap for decay of the tritium atom, thereby reducing the magnitude of the dominant 1*s* exchange factor in T^- compared to that in $\text{T}^{(0)}$.

V. END-POINT-ENERGY EFFECT

Each β^- transition between nuclear states is split into a number of branches as a result of excitation of atomic electrons which leads to a distribution in final atomic states, each of which has a slightly different end-point energy. It is convenient to evaluate the effect of the shake-up of the atomic electrons by defining an average end-point energy, $\bar{E}_0$, by weighting the end-point energies for decay to each final state in proportion to the probability of decay to that atomic state [23]. Then it can be shown that the average electronic contribution to $\bar{E}_0$ is given by the total mean inverse radius for the initial atomic state [1]. Using the standard expression for the phase-space integral, the fractional change in the integral due to a change $\Delta\bar{E}_0$ in atomic electron binding energy can be conveniently evaluated using the relation

$$\frac{1}{f}\frac{\Delta f}{\Delta \bar{E}_0} = \frac{1}{f}\frac{\partial f}{\partial \bar{E}_0} = \frac{2}{f}\int_0^{\bar{E}_0} F(Z,E)pW(\bar{E}_0 - E)dE, \tag{18}$$

where $F(Z,E)$ is the Fermi function. Numerical evaluation yields a value for the right-hand side of 1.798×10^{-4} per eV. For tritium decay, the expectation value of the mean radius of the initial state is easily evaluated using hydrogenic wave functions, giving an electronic contribution to $\bar{E}_0$ of 27.21 eV. This yields $\Delta f/f = 0.49\%$, in good agreement with the value of 0.50% reported by Budick [11].

For the ion T^-, the total mean inverse radius of the $1s^2$ initial state is found to be 37.32 eV, yielding $\Delta f/f = 0.18\%$. These results again agree closely with those reported in [11].

VI. DISCUSSION

The atomic effects on the bound to continuum decay ratio, λ_b/λ_c, and on the phase-space integral, f, for continuum decay of tritium are summarized in Table V and compared with the previous calculation by Budick [11]. These quantities are related to the half-life, t, for a particular atomic state of tritium by

$$\frac{\ln(2)}{t} = \frac{G_V^2}{2\pi^3}\left(\langle 1\rangle^2 + R_e^2\langle\sigma\rangle^2\right) f_t, \tag{19}$$

where f_t is given by

$$f_t = f\left(1 + \frac{\lambda_b}{\lambda_c}\right), \tag{20}$$

and $\langle 1\rangle$ and $\langle\sigma\rangle$ are the Fermi and Gamow-Teller matrix elements for the decay. It should be noted that when "ft values" are commonly discussed in the context of weak interaction coupling constants, strictly speaking it is the product $f_t t$ which is meant rather than the quantity which is the product of the phase-space integral for the continuum decay, f, and the half-life, t. In most cases the bound-state decay contribution is very small and f_t equals f to a very good approximation. The case of tritium decay is one decay in which the difference between f_t and f (of order 1%) may be significant and should be taken account of in the extraction of estimates of weak interaction coupling constants from data on the half-life.

For atomic T, the results presented here for the screening and exchange effects differ significantly from the results reported in [11]. Summing all the atomic effects gives a total difference in f_t between T and T^+ of 0.30% and between T^- and T^+ of 0.64% compared to the values of 0.22% and 0.38% reported in [11].

In [13], the relationship between the $f_t t$ value and the nuclear matrix elements was used, in combination with a measurement of the half-life of molecular tritium, to obtain an estimate for the quantity $R_e\langle\sigma\rangle$ where R_e is the

TABLE V. Comparison of atomic effects on the bound to continuum decay ratio, λ_b/λ_c, and on the phase-space integral, f, for continuum decay in different chemical forms of tritium. The sign of the fractional change, $\Delta f/f$, in the phase-space integral f for continuum decay is positive if the associated atomic effect increases the phase-space integral relative to that for the T^+ ion. The quantity f_t is defined in Eq. (20). $\frac{\Delta f_t}{f_t}$ represents the fractional change in the total decay constant as a result of all the atomic effects on both bound and continuum decay.

Ion	Bound-state decay ratio $\frac{\lambda_b}{\lambda_c}$ (%)	Fractional change due to atomic effect (%)				Author
		End point $\frac{\Delta f}{f}$	Screening $\frac{\Delta f}{f}$	Exchange $\frac{\Delta f}{f}$	Total $\frac{\Delta f_t}{f_t}$	
T^+	1.08	0	0	0	1.08	This work
T	0.55	0.49	-0.41	0.15	0.78	This work
T^-	0.00	0.67	-0.45	0.22	0.44	This work
T^+	1.03	0	0	0	1.03	[11]
T	0.69	0.50	-0.22	-0.15	0.82	[11]
T^-	0.47	0.68	-0.35	-0.15	0.65	[11]

ratio of axial-vector to vector coupling constants and $\langle\sigma\rangle$ is the Gamow-Teller matrix element. The phase-space integral for the tritium ion T^+ was corrected by 0.32% for atomic effects in the molecule T_2 and this then yielded $R_e\langle\sigma\rangle = 2.098 \pm 0.003$. Using a recent theoretical estimate of $\langle\sigma\rangle = \sqrt{3}(0.962 \pm 0.002)$ yielded $R_e = 1.259 \pm 0.007$. This enabled an estimate of the neutron lifetime $\tau_n = 897 \pm 3$ s to be derived. However, the atomic correction used to obtain these latter results included a contribution from exchange effects which has been shown above to be of the wrong sign and a screening correction which is significantly underestimated. In this work we do not present results for atomic effects in the T_2 molecule since a proper treatment, including the bound-state decay process, requires development of a molecular, rather than atomic, formalism. However, as a first approximation, it may be reasonable to assume that the atomic effects in the T_2 molecule are similar to those in the T atom. If one uses the result obtained here for the atomic correction to f_t in the T atom of 0.78% as an estimate of the atomic correction to f_t in T_2, then the results obtained using the same method as used in [13] are $R_e\langle\sigma\rangle = 2.092 \pm 0.003$, $R_e = 1.255 \pm 0.002$, and $\tau_n = 901 \pm 3$ s. These results may be compared with $R_e{=}1.261 \pm 0.004$ derived from angular correlation measurements in neutron decay and $R_e = 1.267 \pm 0.007$ from measurements of the neutron lifetime [27]. The latter measurements also yield $\tau_n = 889.1 \pm 1.8$ s.

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APPENDIX: DERIVATION OF EXPRESSION FOR THE EXCHANGE CONTRIBUTION TO T^- DECAY

In the orbital approximation used throughout this paper to describe atomic electronic structures, the T^- initial state is designated $|1s^2;0,0\rangle$ where the first zero denotes that the overall total angular momentum (J) is zero while the second zero denotes that the z component (M_J) of the total angular momentum is also zero. This state is represented by a single Fock-space ket as

$$|1s^2;0,0\rangle = |1s(\tfrac{1}{2}),1s(-\tfrac{1}{2})\rangle, \tag{A1}$$

where a ket such as $|a,b\rangle$ denotes that each of the orbitals a and b is occupied by a single electron. The notation $B(m_j)$ denotes the orbital belonging to subshell B and having a z component of its total angular momentum equal to m_j. The three-electron final states containing a continuum electron with specified kinetic energy E can be constructed by vector coupling this electron onto two-electron states having a definite value of zero or one for the overall total angular momentum of these two electrons. Since only three-electron states having a J value of $\frac{1}{2}$ can be generated by allowed decays from the $|1s^2;0,0\rangle$ initial state and moreover only those in which all three electrons have $j = \frac{1}{2}$ are produced with non-negligible probability, there are only three types of final state containing a continuum electron of kinetic energy E to be considered. The first of these, $|B^2E;\frac{1}{2},M_J\rangle$, contain, besides the continuum electron of kinetic energy E, two electrons in the s subshell B. The second and third types of final states, $|(BC)_0E;\frac{1}{2},M_J\rangle$ and $|(BC)_1E;\frac{1}{2},M_J\rangle$, have a single electron in each of the subshells B and C and differ only in the angular momentum (0 or 1) of the two-electron state produced by vector coupling angular momenta, both equal to $\frac{1}{2}$, of the individual electrons in the subshells B and C.

The reduced matrix elements $\langle 1s^2;0||\hat{b}_X||\gamma';\frac{1}{2}\rangle$ entering the decay amplitudes ($A_{\gamma'}$) are related to Fock-space matrix elements $\langle 1s^2;0,0||\hat{b}_{X,\frac{1}{2}}||\gamma';\frac{1}{2},\frac{1}{2}\rangle$ through

$$\langle 1s^2;0||\hat{b}_X||\gamma';\tfrac{1}{2}\rangle = -\langle 1s^2;0,0||\hat{b}_{X,\frac{1}{2}}||\gamma';\tfrac{1}{2}\tfrac{1}{2}\rangle. \qquad \text{(A2)}$$

This allows the $A_{\gamma'}$ to be evaluated using

$$A_{\gamma'} = \frac{1}{2}\sum_X \left[\langle 1s^2;0,0||\hat{b}_{X,\frac{1}{2}}||\gamma';\tfrac{1}{2},\tfrac{1}{2}\rangle P_X(R)\right]^2, \qquad \text{(A3)}$$

where the sum over X is over the complete set of all final-state subshells having $j=\frac{1}{2}$. The three types of final state having M_J equal to $\frac{1}{2}$ can be expanded into basic Fock-space kets $|a,b,c\rangle$ according to

$$|B^2E;\tfrac{1}{2},\tfrac{1}{2}\rangle = |B(\tfrac{1}{2}),B(-\tfrac{1}{2}),E(\tfrac{1}{2})\rangle, \qquad \text{(A4)}$$

$$|(BC)_0E;\tfrac{1}{2},\tfrac{1}{2}\rangle = \frac{1}{\sqrt{2}}\left[|B(\tfrac{1}{2}),C(-\tfrac{1}{2}),E(\tfrac{1}{2})\rangle - |B(-\tfrac{1}{2}),C(\tfrac{1}{2}),E(\tfrac{1}{2})\rangle\right], \qquad \text{(A5)}$$

$$|(BC)_1E;\tfrac{1}{2},\tfrac{1}{2}\rangle = \sqrt{\tfrac{2}{3}}|B(\tfrac{1}{2}),C(\tfrac{1}{2}),E(-\tfrac{1}{2})\rangle - \frac{1}{\sqrt{6}}\left[|B(\tfrac{1}{2}),C(-\tfrac{1}{2}),E(\tfrac{1}{2})\rangle + |B(-\tfrac{1}{2}),C(\tfrac{1}{2}),E(\tfrac{1}{2})\rangle\right]. \qquad \text{(A6)}$$

Only states in which the label C appears after the label B in the standard ordering of orbitals need to be considered.

Substitution of the states given in Eqs. (A4), (A5), and (A6) into Eq. (A3) followed by standard Fock-space manipulations in which the creation operators are acted backwards onto the bra shows that the decay amplitudes for the three types of final γ' state are

$$A_{B^2E} = \tfrac{1}{2}\left[\langle B|1s\rangle^2 P_E(R) - \langle B|1s\rangle\langle E|1s\rangle P_B(R)\right]^2, \qquad \text{(A7)}$$

$$A_{(BC)_0E;\frac{1}{2}} = \frac{1}{2}\left(\sqrt{2}\langle B|1s\rangle\langle C|1s\rangle P_E(R) - \frac{1}{\sqrt{2}}\left[\langle B|1s\rangle\langle E|1s\rangle P_C(R) + \langle C|1s\rangle\langle E|1s\rangle P_B(R)\right]\right)^2, \qquad \text{(A8)}$$

$$A_{(BC)_1E;\frac{1}{2}} = \tfrac{3}{4}\langle E|1s\rangle^2\left[\langle B|1s\rangle P_C(R) - \langle C|1s\rangle P_B(R)\right]^2. \qquad \text{(A9)}$$

It is convenient here to sum the last two decay amplitudes to give

$$\begin{aligned} A_{(BC)_0E;\frac{1}{2}} + A_{(BC)_1E;\frac{1}{2}} = \tfrac{1}{2}\big(\, & 2\langle B|1s\rangle^2\langle C|1s\rangle^2 P_E^2(R) - 2\langle B|1s\rangle\langle C|1s\rangle\langle E|1s\rangle\left[\langle B|1s\rangle P_C(R) + \langle C|1s\rangle P_B(R)\right] P_E(R) \\ & + 2\langle E|1s\rangle^2\left[\langle B|1s\rangle^2 P_C^2(R) + \langle C|1s\rangle^2 P_B^2(R) - \langle B|1s\rangle\langle C|1s\rangle P_B(R) P_C(R)\right]\big). \qquad \text{(A10)} \end{aligned}$$

The result of Eq. (2) of [2] shows that the total intensity (dI) of the β spectrum for particles emitted with kinetic energies between E and $E+dE$ is given by summing over all possible final states γ' containing such a β particle so that

$$\frac{dI}{dE} = K'\frac{W}{p}\sum_{\gamma'}\left[E_0(\bar{\gamma}) - E\right]^2 A_{\gamma'}. \qquad \text{(A11)}$$

Here K' is a constant while $E_0(\bar{\gamma})$ is the end-point energy for decays generating two electrons in subshells B and C in the final state γ'. The sum over γ' is generated as a single sum over B to include all final states of the type $|B^2E;\frac{1}{2},\frac{1}{2}\rangle$ plus a double sum over B and C (greater than B) to include just once all the final states of the types $|(BC)_0E;\frac{1}{2},\frac{1}{2}\rangle$ and $|(BC)_1E;\frac{1}{2},\frac{1}{2}\rangle$. The sums over B and C include not only those over all bound orbitals but also integrations over the appropriate portion of the continuum thus including all those final states having two or three continuum electrons. Those terms in Eqs. (A7) and (A10) which involve only the value $P_E(R)$ of the continuum wave function and not the quantities $P_B(R)$ and $P_C(R)$ constitute the direct terms since they correspond to the direct creation of the β particle in the continuum orbital of energy E with the two T$^-$ 1s electrons originally present passing either both into the final-state subshell B or one passing into B and the second into C. All the remaining terms in Eqs. (A7) and (A10) involve the quantities $P_B(R)$ or $P_C(R)$ and constitute the exchange contribution to the β spectrum. Substituting the decay amplitudes in Eqs. (A7) and (A10) into Eq. (A11) and then replacing the end-point energies $E_0(\bar{\gamma})$ by an average value $\bar{E}_0$ shows that the direct portion of the spectrum, denoted NE (no-exchange), is given by

$$\frac{dI^{\mathrm{NE}}}{dE} = \frac{K'}{2}\frac{W}{p}(\bar{E}_0 - E)^2\left(\sum_B\langle B|1s\rangle^4 P_E^2(R) + 2\sum_B\sum_{C\,(>B)}\langle B|1s\rangle^2\langle C|1s\rangle^2 P_E^2(R)\right). \qquad \text{(A12)}$$

Rearrangement of the summations simplifies this into

$$\frac{dI^{\rm NE}}{dE}=\frac{K'}{2}\frac{W}{p}(\bar{E}_0-E)^2\sum_B\sum_C\langle B|1s\rangle^2\langle C|1s\rangle^2P_E^2(R). \tag{A13}$$

The sums over B and C are, in principle, restricted by energy conservation to include only those states having energies less than the end-point energy. However, since only a minute fraction of potential final states in Eqs. (A4), (A5), and (A6) are excluded by this condition, the sums over both B and C in Eq. (A13) can be performed using orbital closure to produce

$$\frac{dI^{\rm NE}}{dE}=\frac{K'}{2}\frac{W}{p}(\bar{E}_0-E)^2P_E^2(R), \tag{A14}$$

whose structure is identical to the result in Eq. (8).

The portion, denoted $dI^{\rm ex}$, of the spectrum arising from exchange is found from Eqs. (A7), (A10), and (A11) to be given by

$$\begin{aligned}\frac{dI^{\rm ex}}{dE}=\frac{K'}{2}\frac{W}{p}(\bar{E}_0-E)^2\Bigg(&-2\langle E|1s\rangle P_E(R)\Bigg[\sum_B\langle B|1s\rangle^3P_B(R)\\&+\sum_B\sum_{C\,(>B)}\langle B|1s\rangle\langle C|1s\rangle\,[\langle B|1s\rangle P_C(R)+\langle C|1s\rangle P_B(R)]\Bigg]\\&+\langle E|1s\rangle^2\Bigg[\sum_B\langle B|1s\rangle^2P_B^2(R)+2\sum_B\sum_{C\,(>B)}\langle B|1s\rangle^2P_C^2(R)\\&+\langle C|1s\rangle^2P_B^2(R)-\langle B|1s\rangle\langle C|1s\rangle P_B(R)P_C(R)\Bigg]\Bigg),\end{aligned} \tag{A15}$$

which can be rearranged into the form

$$\begin{aligned}\frac{dI^{\rm ex}}{dE}=\frac{K'}{2}\frac{W}{p}(\bar{E}_0-E)^2\Bigg(&-2\langle E|1s\rangle P_E(R)\sum_B\sum_C\langle B|1s\rangle^2\langle C|1s\rangle P_C(R)\\&+\langle E|1s\rangle^2\sum_B\sum_C\langle B|1s\rangle^2P_C^2(R)+\sum_B\sum_{C\,(>B)}[\langle B|1s\rangle P_C(R)-\langle C|1s\rangle P_B(R)]^2\Bigg).\end{aligned} \tag{A16}$$

After using orbital closure to remove the unrestricted sums over B, the exchange contribution to the β intensity reduces to

$$\begin{aligned}\frac{dI^{\rm ex}}{dE}=\frac{K'}{2}\frac{W}{p}(\bar{E}_0-E)^2\Bigg(&\langle E|1s\rangle\sum_C P_C(R)\,[-2\langle C|1s\rangle P_E(R)+\langle E|1s\rangle P_C(R)]\\&+\langle E|1s\rangle^2\sum_B\sum_{C\,(>B)}[\langle B|1s\rangle P_C(R)-\langle C|1s\rangle P_B(R)]^2\Bigg).\end{aligned} \tag{A17}$$

It then follows by combining this result with Eq. (A14) that the total β intensity dI/dE can be expressed in the form of Eqs. (9) and (15) with the factor $\chi^T_{\rm ex}(E)$ given by

$$\begin{aligned}\chi^T_{\rm ex}(E)=\sum_C&-2\langle E|1s\rangle\langle C|1s\rangle\left[\frac{P_C(R)}{P_E(R)}\right]+\langle E|1s\rangle^2\left[\frac{P_C(R)}{P_E(R)}\right]^2\\&+\langle E|1s\rangle^2\sum_B\sum_{C\,(>B)}\left(\langle B|1s\rangle\left[\frac{P_C(R)}{P_E(R)}\right]-\langle C|1s\rangle\left[\frac{P_B(R)}{P_E(R)}\right]\right)^2.\end{aligned} \tag{A18}$$

The first term in Eq. (A18) gives the dominant contribution since it contains only the first power of the overlap $\langle E|1s\rangle$ which is small over almost all the spectrum, only becoming significant at extremely low energies. The two terms in the double summation over B and C are very small because they contain the second power of $\langle E|1s\rangle$ as well as a product of two overlaps of the kind $\langle B|1s\rangle$ or $\langle C|1s\rangle$. In addition, the terms in this double summation tend to cancel one another. Hence in the following these terms will be neglected. The quantity $\chi^T_{\rm ex}(E)$ can then be written

$$\chi^T_{\rm ex}(E)=\sum_C\eta^C_{\rm ex}(E), \tag{A19}$$

where the subshell exchange factor, $\eta_{\rm ex}^{C}(E)$, is given by

$$\eta_{\rm ex}^{C}(E) = -2\langle E|1s\rangle\langle C|1s\rangle \left[\frac{P_C(R)}{P_E(R)}\right] + \langle E|1s\rangle^2 \left[\frac{P_C(R)}{P_E(R)}\right]^2 . \tag{A20}$$

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