PHYSICAL REVIEW C VOLUME 27, NUMBER 4 APRIL 1983

Atomic final-state interactions in tritium decay

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(Received 8 November 1982)

We calculate the effect of the Coulomb interaction of the ejected β ray with the bound atomic electron in the β decay of a tritium atom. The excited state probabilities of the residual helium ion are changed by at most 0.17% from the usual sudden approximation.

[RADIOACTIVITY ^{3}H; atomic final states, neutrino mass.]

In a recent experiment, Lubimov *et al.*[1] attemped to determine the mass of the electron antineutrino from the β-decay spectrum of a tritiated valine source, and obtained a value between 14 and 46 eV. Since this mass is comparable with atomic binding energies, one expects atomic effects on the spectrum to be important. Bergkvist[2] calculated several such atomic and molecular effects in the usual sudden approximation, and obtained an effective decrease in his detector resolution. Law[3] calculated these effects more exactly, including continuum states (total ionization of the He atom), while Fukugita and Kubodera[4] treated the continuum states with Coulomb effects. In this paper, we further refine the calculation of atomic state probabilities by including the Coulomb interaction of the β ray with the bound electron. This interaction has been studied for other nuclei,[5,6] where effects are expected to be more pronounced, but not, to our knowledge, for tritium.

The interaction of the atomic electron with the β ray is small because the β ray wavelength $2\pi/k$ is small compared to the Bohr radius $a=(me^2)^{-1}$, where m is the electron mass and e the charge (we use units where $\hbar=c=1$, so that $e^2\approx\frac{1}{137}$). At the tritium end-point energy, 18.57 keV, the usual Sommerfeld parameter $\eta\equiv -me^2/k=-1/ka=-0.0271$ is small, so that our results need only be calculated to leading order in η.

We will consider a process in which a tritium atom with its atomic electron in the ground ($1s$) orbital decays by emitting a β ray (momentum k), leaving the atomic electron in an excited He atomic orbital η_f. To first order in the weak interaction V_W, the amplitude for this process is

$$T_{fi}=\langle\Psi_f^{(-)}|V_W|\Phi_i\rangle \ ,$$

where Φ_i is the initial tritium $1s$ wave function, and $\Psi_f^{(-)}$ is the full solution to the interacting two-electron problem, specified by k and n_f and by incoming-wave boundary conditions. This latter scattering wave function is a solution to the Hamiltonian describing two electrons in the presence of a He nucleus,

$$(E-H)\Psi_f^{(-)}=0 \ ,$$

$$E=\epsilon_f+k^2/2m \ ,$$

$$H=\frac{p^2}{2m}+\frac{p'^2}{2m}-\frac{2e^2}{r}-\frac{2e^2}{r'}+\frac{e^2}{|r-r'|} \ ,$$

where (r,p) describe the atomic electron with final energy ϵ_f and (r',p') describe the β ray, whose final energy is $k^2/2m$ using nonrelativistic kinematics.

A perturbative approximation to $\Psi_f^{(-)}$ accurate to the order required can be obtained by iterating the Lippmann-Schwinger equation. We partition H as

$$H=H_0+V \ ,$$

$$H_0=\frac{p^2}{2m}+\frac{p'^2}{2m}-\frac{2e^2}{r}-\frac{e^2}{r'} \ ,$$

$$V=-\frac{e^2}{r'}+\frac{e^2}{|r-r'|} \ ,$$

where we will treat the interelectron repulsion as a perturbation, and we have split the β-nucleus attraction $(-2e^2/r')$ between H_0 and V such that $V\approx r'^{-2}$ as $r'\rightarrow\infty$. The Lippmann-Schwinger equation is

$$\langle\Psi_f^{(-)}|=\langle\Phi_f^{(-)}|+\langle\Psi_f^{(-)}|VG_0^{(+)}$$
$$\approx\langle\Phi_f^{(-)}|+\langle\Phi_f^{(-)}|VG_0^{(+)} \ ,$$

where the Green's function is

$$G_0^{(+)}=\lim_{\zeta\rightarrow 0^+}(E-H_0+i\zeta)^{-1}$$

and $\langle\Phi_f^{(-)}|$ is the solution to H_0 with energy E and the required boundary conditions. Specifically,

$$\langle rr'|\Phi_f^{(-)}\rangle=\chi_{n_f}(r)u_k^{(-)}(r') \ ,$$

where χ_{n_f} is the final $Z=2$ atomic orbital, bound or continuum, and $u_k^{(-)}$ is the Coulomb-distorted plane wave with incoming spherical waves,

$$u_k^{(-)}(r')=4\pi\sum_{lm}i^l e^{-i\sigma_l}\frac{F_l(kr')}{kr'}Y_{lm}^*(k)Y_{lm}(r') \ .$$

Here, F_l are the usual Coulomb wave functions[7] for charge $Z=1$, and σ_l are the related Coulomb phase shifts. We thus approximate the decay amplitude as

$$T_{fi}=T_{fi}^{(0)}+T_{fi}^{(1)} \ ,$$
$$T_{fi}^{(0)}=\langle\Phi_f^{(-)}|V_W|\Phi_i\rangle \ ,$$
$$T_{fi}^{(1)}=\langle\Phi_f^{(-)}|VG_0^{(+)}V_W|\Phi_i\rangle \ .$$

For the allowed decay considered here, we may safely take V_W to create the β ray at the nucleus with zero angular momentum. Thus, apart from an overall constant, $V_W=\delta(r')$, and so, in an obvious notation,

$$T_{fi}^{(0)}=u_k^{(-)*}(0)\int d^3r\,\chi_{n_f}^*(r)\chi_i(r) \ ,$$
$$T_{fi}^{(1)}=\int d^3r\,d^3r'\,u_k^{(-)*}(r')\chi_{n_f}^*(r) \times V(r,r')\langle rr'|G_0^{(+)}|\chi_i;0\rangle \ .$$

Upon identifying $u_k^{(-)*}(0)=e^{i\sigma_0}C_0(\eta)$, with C_0 the usual Gamow factor,[5] we see that

$$T_{fi}^{(0)}=e^{i\sigma_0}C_0(\eta)\int d^3r\,\chi_{n_f}^*\chi_i$$

is the usual sudden approximation amplitude, corrected for $Z=1$ Coulomb distortion. To treat $T_{fi}^{(1)}$, we use a spectral representationof $G_0^{(+)}$ in terms of the $Z=2$ atomic states χ_n to obtain

$$\langle rr'|G_0^{(+)}|\chi_i;0\rangle=\sum_n\chi_n(r)g_{E-\epsilon_n}^{(+)}(r',0)\langle\chi_n|\chi_i\rangle \ ,$$

where $g_E^{(+)}$ is the $Z=1$ single-particle Coulomb Green's function. Since the atomic energies ϵ_n are small compared to the total energy, $E\approx 18$ keV, we may set $E-\epsilon_n\approx E$, independent of n, and employ closure to obtain

$$\langle rr'|G_0^{(+)}|\chi_i;0\rangle=g_E^{(+)}(r',0)\chi_i(r) \ ,$$

which gives for the first order amplitude,

$$T_{fi}^{(1)}=\int d^3r\,d^3r'u_k^{(-)*}(r')\chi_{n_f}^*(r) \times\left[\frac{e^2}{|r-r'|}-\frac{e^2}{r'}\right]g_E^{(+)}(r',0)\chi_i(r) \ .$$

Since the β ray has zero angular momentum,

$$u_k^{(-)*}(r')=e^{i\sigma_0}\frac{F_0(kr')}{kr'} \ ,$$
$$g_E^{(+)}(r',0)=-\frac{\eta k}{2\pi e^2}\frac{(G_0+iF_0)(kr')}{kr'} \ ,$$

where G_0 is the irregular Coulomb function. We can safely discard the $l\neq 0$ atomic final states, which have only order η^2 changes in their probabilities, since $T_{fi}^{(0)}$ is zero.[8] By using the asymptotic expressions for the Coulomb functions,[5] to order η, we can write

$$T_{fi}^{(1)}=e^{i\sigma_0}C_0(\eta)\langle\chi_{n_f}(r)|Q(kr)|\chi_i(r)\rangle \ ,$$

$$Q(x)=2\eta\int_0^x dx'\sin x' e^{ix'}\left[\frac{1}{x}-\frac{1}{x'}\right]$$
$$=-\eta\left[-\frac{1}{2x}+\frac{\pi}{2}+i(\ln 2x+\gamma-1)\right] \ ,$$

where $\gamma=0.5772$ is Euler's constant. Note that $-\eta\pi/2-i\eta\gamma$ is x independent. It therefore gives a contribution proportional to $T_{fi}^{(0)}$ and, indeed, reflects the change in $e^{i\sigma_0}C_0(\eta)$ going from $Z=1$ to $Z=2$.

The required matrix elements of Q can be found analytically for the bound states; those of $1/r$ can also be found analytically for the continuum final states. However, for the $\ln r$ continuum matrix element we

TABLE I. Matrix elements and decay probabilities to various He^+ states.

State	$\left\langle f\left\|\frac{a}{r}\right\|i\right\rangle$	$\left\langle f\left\|\ln\frac{r}{a}\right\|i\right\rangle$	$\|T_{fi}^{(0)}\|^2$	$\|T_{fi}^{(0)}+T_{fi}^{(1)}\|^2$
1s	1.257 08	−0.147 35	70.23%	70.06%
2s	0.	0.614 82	25.00%	25.17%
3s	−0.031 35	0.096 66	1.27%	1.28%
4s	−0.023 28	0.052 81	0.38%	0.39%
5s	−0.017 42	0.035 29	0.17%	0.17%
Continuum			2.63%	2.62%
Total			99.69%	99.69%

used the approximation

$$\langle F_0(kr)/kr|\ln r|1s\rangle=\langle F_0(kr)/kr|1s\rangle \times\frac{\langle j_0(kr)/kr|\ln r|1s\rangle}{\langle j_0(kr)/kr|1s\rangle}\ .$$

We have also estimated the exchange contributions to the decay amplitudes (β ray emitted into a $Z=2$ atomic orbital and original atomic electron ejected) to be lower by a factor η^2 than the direct contributions calculated above, and thus negligible.

Table I shows matrix elements of a/r and $\ln r/a$ between the $Z=1$ 1s state and the $Z=2$ ns states, for $n=1$ to 5, and the probabilities of the ns states and the probability for ionization, normalized so that the sum of the probabilities in each column is the same. This sum is not exactly unity since bound s states with $n\geqslant 6$ have been neglected.

The corrections are of order 0.2% for the 1s and 2s states and much smaller thereafter. In the analysis of the Lubimov experiment,[1] a change in the He^+ 2s probability from zero to 0.3 changes the inferred antineutrino mass by 15 eV, so that the effects of the electron-electron interaction are negligible until the antineutrino mass is known to within 0.1 eV, which seems far beyond present experimental capabilities.

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[8]Intemann, in Ref. 6, states that higher partial waves are important below $l_{\max}=1/ka=-\eta=0.0271$, which is further support for this approximation. We find the probability of exciting the 2p state to be 0.01%.