Atomic Effects in Low-Energy Beta Decay: The Case of Tritium

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In a recent experiment, Simpson found an excess intensity in the measured tritium beta spectrum below 1.5 keV. A detailed account of the decay energy and Coulomb-screening effects raises the theoretical curve in precisely this energy range, so that little, if any, of the excess remains. This correction is shown to be approximately given by a simple analytical expression.

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Simpson[1] observed a surplus of electrons below 1.5 keV in the beta spectrum of tritium (see Fig. 1 of Ref. 1) and interpreted this as evidence for mixing of neutrino flavors and for the existence of a second neutrino with mass 17.1 keV. The belief in this interpretation is waning since experiments[2] on ^{35}S have failed to reproduce the corresponding effect. In the following we shall demonstrate that the surplus may be accounted for by corrections arising from atomic effects going beyond those considered in Ref. 1 and in recent papers[3-5] on the same subject.

The qualitative basis for our correction to Simpson's theoretical beta spectrum is as follows. The familiar unscreened Coulomb enhancement in β decay contains a factor $1/[1-\exp(-\xi)]$, where $\xi = 4\pi e^2/\hbar v$ in tritium decay, v being the velocity of the emitted electron. This factor behaves approximately as $1/\xi$ when $\xi < 1$; but it becomes ≈ 1 and nearly independent of ξ, if $\xi > 1$. The value $\xi = 1$ corresponds to an electron energy of 2 keV. For this reason, a neglect of minor modifications of ξ can cause a spurious shift in the β spectrum in the neighborhood of the energy where the surplus of electrons was recorded. We shall therefore carefully look into the effects of both Coulomb screening and small corrections in the detailed account of decay energy.

One notable circumstance in Simpson's experiment is that the beta spectrum was measured with a total-absorption spectrometer instead of with a magnetic spectrometer. The tritium was imbedded by ion implantation into the sensitive region of a Si(Li) detector which registered the number of ionizations and hence the total energy release $E = Q - E_\nu$ within the detector for the process $^3\mathrm{H} \rightarrow {}^3\mathrm{He} + e^- + \nu$. The quantity Q ($= 18.6$ keV) is the energy difference between the ground states of mother and daughter atoms, including their chemical bindings. For simplicity, we disregard the chemical bindings for the present; they constitute only a minor correction.

Not all of the energy E is available to the outgoing electron when the transition takes place at the nucleus. In order to see this, it is convenient to introduce a more basic Q value, Q^*, as that available in the β decay of a nucleus stripped of electrons,

$$Q^* = Q + \epsilon_{Z+1}^{Z+1}(0) - \epsilon_Z^Z(0), \tag{1}$$

where $\epsilon_Z^n(0)$ is the (negative) total atomic energy of the ground state of an atom with n electrons and nuclear charge Z, chemical bindings being disregarded. Similarly the available electron energy is

$$E^* = E + \epsilon_{Z+1}^{Z+1}(0) - \epsilon_Z^Z(0), \tag{2}$$

or, for tritium, a reduction by 65.4 eV.

For a nucleus stripped of electrons, the beta transition probability is known accurately, involving a product of phase-space factors and a Coulomb correction. From this result let us make a preliminary evaluation of the beta transition probability in the atomic decay. As the energy of the outgoing beta particle is high, it seems reasonable to identify the total energy and electron kinetic energy with Q^* and E^*, respectively. This means that we replace the actual spectrum of final states by an average. Since $Q^* - E^* = Q - E$, the beta spectrum can then be estimated from the expression

$$N(E)\,dE = \mathrm{const} \times F(Z+1, W^*) \times p^* W^* (Q-E)^2 dE, \tag{3}$$

where $W^* = mc^2 + E^*$, p^* is the corresponding momentum, and F the usual Fermi function. Figure 1 shows the ratio of the expression (3) relative to the shape assumed by Simpson.[1] It will be seen that the modification accounts for most of the upward bend below 2 keV, if one allows a normalization at 2.5 keV, which corresponds to the maximum intensity of the spectrum.

At this point it is useful to examine in more detail the validity of Eq. (3). Consider the general nonrelativistic atomic Hamiltonian for an n-electron atom or ion,

$$H_Z^n = \sum_{i=1}^{n} \left[\frac{p_i^2}{2m} - \frac{Ze^2}{r_i} + \sum_{j<i} \frac{e^2}{r_{ij}} \right], \tag{4}$$

and note that a β particle at the origin would be in a

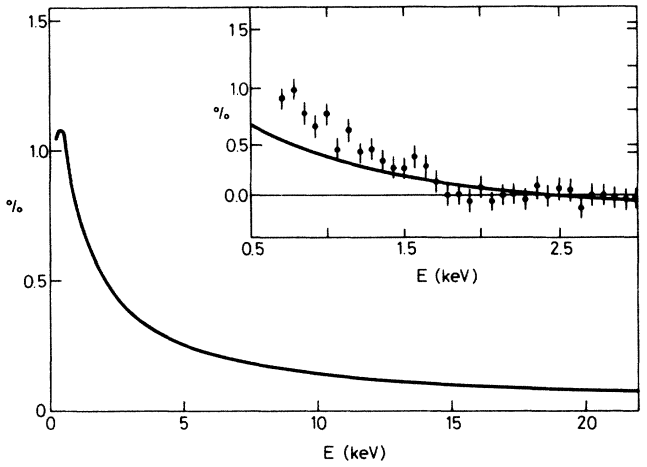

FIG. 1. Deviation in percent of the expression (3) relative to the theoretical shape assumed by Simpson. An explanation of this deviation is given in connection with a simple approximate formula, Eq. (9). The curve in the inset shows the same calculation, now normalized at 2.5 keV corresponding to the maximum of the tritium beta spectrum. A change in the normalization point by ± 0.5 keV corresponds to a vertical displacement of the curve by $\pm 0.065\%$.

potential V_e^n from the electron cloud, where

$$V_e^n = \sum_{i=1}^{n} \frac{e^2}{r_i} = -\frac{\partial H_Z^n}{\partial Z} = H_Z^n - H_{Z+1}^n. \tag{5}$$

The eigenvalues and eigenfunctions of the Hamiltonian H_Z^n are denoted $\epsilon_Z^n(s)$ and $|s_Z^n\rangle$, where s labels the quantum state in question. For the decay of a neutral atom with nuclear charge Z and for the beta-decay energies of interest here, the sudden approximation can be assumed to be valid. Consequently, the wave function for the final atomic state, which is not an energy eigenstate, can be approximated by that of the initial state $|O_Z^Z\rangle$. We shall now show how the successive physical processes during and after the beta decay contribute to the shifted energy Eq. (2).

(i) *Screening correction.*—In his classical paper, Rose[6] summarized his analysis to the effect that in beta decay "the electron distribution is always such as though the nucleus were not conscious of the screening and as though it emitted electrons into its immediate vicinity always in the same way; the only effect of the screening is then to accelerate the electrons . . . ." The correction is made simply by evaluating the electron phase-space factor and Coulomb correction with the energy shifted back by a constant value taken to be the electronic potential at the origin, Eq. (5). The expectation value is

$$\langle V_e \rangle = \langle O_Z^Z | V_e^Z | O_Z^Z \rangle = -\left. \frac{\partial \epsilon_Z^n(0)}{\partial Z} \right|_{n=Z}. \tag{6}$$

As follows from the WKB arguments of Rose and from the Hulthén solutions to be discussed presently, the quantity $\langle V_e \rangle$ determines the screening correction to beta decay when only the energy of the beta particle is detected.

(ii) *Mean excitation energy.*—After the beta decay the ion is deexcited. The mean energy release is, in the sudden approximation,

$$\begin{aligned} \langle \Delta\epsilon \rangle &= \langle O_Z^Z | H_{Z+1}^Z | O_Z^Z \rangle - \epsilon_{Z+1}^Z(0) \\ &= \epsilon_Z^Z(0) - \langle O_Z^Z | V_e^Z | O_Z^Z \rangle - \epsilon_{Z+1}^Z(0) \\ &\approx -\tfrac{1}{2}[\partial^2 \epsilon_Z^n(0)/\partial Z^2]_{n=Z}, \end{aligned} \tag{7}$$

where the last expression is a good approximation for large Z and is exact for $Z=1$. This is the result obtained by Serber and Snyder.[7]

(iii) *Neutralization energy.*—The final energy release occurs when the ion is neutralized to the ground state

$$I = \epsilon_{Z+1}^Z(0) - \epsilon_{Z+1}^{Z+1}(0), \tag{8}$$

where we have neglected chemical binding as in Eq. (2) and also the original binding of the captured electron. In this approximation the energy release (8) is identical to the ionization potential.

When the three contributions Eqs. (6)–(8) are subtracted from E one obtains exactly the definition [Eq. (2)] of E^*, leading to the previous tentative result, Eq. (3). In the case of the tritium decay, the three terms are comparable in magnitude: $\langle V_e \rangle = 27.2$ eV, $\langle \Delta\epsilon \rangle = 13.6$ eV, and $I = 24.6$ eV.

Even though we are here primarily concerned with the hydrogen decay, it may be worthwhile to note the order of magnitude of the effects for a heavy atom, for which the energy of the ground state may be represented by the Thomas-Fermi estimate $\epsilon_Z^Z(0) = -CZ^{7/3}$, where C is 16–20 eV. One finds for $Z=70$ that $I \approx 5$–10 eV, $\langle \Delta\epsilon \rangle \approx 120$ eV, and $\langle V_e \rangle \approx 12\,400$ eV. Thus for heavy atoms the screening correction dominates completely. The screening correction of 99.4 eV used by Simpson stems from the use of a Thomas-Fermi estimate for a neutral atom with $Z=2$.

Rose's screening correction, mentioned in (i), was based on a WKB estimate of the wave function for the emitted electron in a Coulomb potential with static screening. The justification for use of a static potential is that the velocity of the beta particle is high, so that the distribution of the electron cloud remains essentially unchanged during the passage of the beta particle, and so that other dynamic interaction effects remain relatively small. Let us show that the same screening correction is obtained in an exactly soluble case of Coulomb screening,[5,8] the Hulthén potential.[9]

This potential is defined as

$$V(r) = -Z'e^2q/(e^{qr}-1),$$

where q^{-1} represents an effective range of the screening potential. The function $V(r)$ has the property that for small qr it approaches a pure Coulomb potential minus a constant, $Z'qe^2/2$, which quantity represents simply $\langle V_e \rangle$ of the electronic charge distribution in question. For large qr the function $V(r)$ goes rapidly to zero, thus representing a neutral atom. In the application to beta decay we put $Z' = Z+1$ and choose $\frac{1}{2}Z'e^2q = \langle V_e \rangle$, which gives the correct potential energy at the origin. For heavier atoms ($Z > 10$), a good approximation is $e^2q = \frac{14}{3}CZ^{1/3}$. Approximate solutions of the Dirac equation with the Hulthén potential appropriate for high Z have been discussed by Bühring.[10]

The fact that this potential has analytic solutions for s waves has been used by Lindhard and Winther[8] for deriving a closed expression for χ, the Coulomb enhancement at the origin. Following their calculation with wave vector k and definitions $\lambda = k/q$, $b = 2Z'/a_0q$, $\beta_1 = (\lambda^2 - b)^{1/2}$, $\xi = \pi b/\lambda = 2\pi Z'v_0/v$, and

$$\xi_1 = 2\pi(\lambda - \beta_1) \approx \xi(1 + \langle V_e \rangle / mv^2),$$

we obtain $\chi = \xi/[1-\exp(-\xi_1)]$. Because of the phase-space factor $v\,dE_{\rm kin}$, the effect of the screening is to replace $E_{\rm kin}$ by $E_{\rm kin} - \langle V_e \rangle$ in the formula for the β spectrum, in agreement with Rose's result. If we consider the above solution at low β energies, we can conclude that one must demand $\lambda^2 >> b$ in order that Rose's result remains valid, or $E_{\rm kin} >> 2\langle V_e \rangle$. This condition is fulfilled at all energies in Simpson's measurements.

When we describe the process in terms of the total energy release, we have to add the energy in Eqs. (7) and (8), and arrive precisely at the formula (3).

If we can consider the displacement $E^* - E$ as small, we obtain a useful approximate formula for the relative correction to the spectrum, by expansion of the Hulthén solution or by taking the logarithmic derivative of (3),

$$\frac{\Delta N(E)}{N(E)} \cong \frac{E^*-E}{2E}\,\frac{\xi}{\exp(\xi)-1}, \qquad (9)$$

where $\xi = 2\pi(Z+1)v_0/v$. Likewise, if we want to consider the present correction to Simpson's theoretical curve, we replace $E^* - E$ in (9) by $\delta(E^* - E)$ $= 99.4 - 65.4$ eV $= 34$ eV, and this gives a quite accurate representation of the curve in Fig. 1.

In conclusion then, the atomic effects considered so far shift the energy scale of Simpson by 34 eV, thereby accounting for perhaps two thirds of the upward bend. An additional shift may arise from chemical bindings. If a hydrogen atom is bound more strongly in Si than a He atom, the shift is increased, and the same trend obtains when the electron neutralizing the He atom is originally bound in Si by the work function. In all, these two effects may amount to 5–10 eV. It may be mentioned that Haxton[3] suggests that exchange corrections can account for 15% of the total upward bend. It should further be noted that the uncertainty in conversion from detector response to total energy can be important. Silicon detectors are not proven[11] to be linear to better than 1% at these energies. There may also be a separate deficiency in the conversion into charge carrier pairs of the 13.6 + 24.6 eV available as atomic excitation energy in helium. In total, there seems to be no clear evidence of an upward bend in the tritium spectrum.

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