Atomic overlap correction to the statistical rate function

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In nuclear β decay, the transition rate depends on the statistical rate function, *f*, an integral over phase space,

$$f = \int_1^{W_0} pW(W_0 - W)^2 F(Z,W) S(Z,W)\ dW, \tag{1}$$

where W is the total energy of the electron in electron-rest-mass units; W_0 is the maximum value of W; $p = (W^2 - 1)^{1/2}$ is the momentum of the electron; Z is the atomic number of the daughter nucleus; $F(Z,W)$ is the Fermi function and $S(Z,W)$ is the shape-correction function. What we address here is the inclusion of an additional factor in Eq. (1) to account for the mismatch in the initial and final *atomic* states in the β decay. Since the nucleus changes charge by one unit in beta decay, the final atomic state does not overlap perfectly with the initial atomic state, an effect that leads to a slight inhibition in the beta-decay rate. In the past, this effect has justifiably been considered too small to be of practical concern but, with the advent of Penning-trap mass measurements, the experimental uncertainties in transition *Q*-values have been reduced so much that they are now comparable to the effects of the imperfect atomic overlap.

We begin by writing

$$f = \int_1^{W_0} pW(W_0 - W)^2 F(Z,W) S(Z,W) r(Z,W)\ dW, \tag{2}$$

where $r(Z,W)$ is the atomic overlap correction we are seeking. We then follow the method of Bahcall [1] by expressing *f* as a double integral with an energy-conserving delta function:

$$f = \int\int pWq^2 F(Z,W) S(Z,W) \sum_{A'} |\langle A'|G\rangle|^2 \delta(E_f - E_i)\ dW dq, \tag{3}$$

where q is the neutrino momentum. We have introduced into this equation an overlap of the initial and final atomic electron configurations: $|G\rangle$ is the state vector for the initial neutral atom with $(Z+1)$ electrons, and $|A'\rangle$ is the state vector for the final *ionized* atom with $(Z+1)$ electrons but only charge Z in the nucleus. There are many such possible final states, so a sum over A' is included.

The energy difference in the delta function is

$$E_f - E_i = q + W - W_0 + [B(G') - B(A')], \tag{4}$$

where $B(G')$ is the total electron binding energy for the *neutral* atom of charge Z in the atomic ground-state configuration. For the energy-conserving delta function we now make a Taylor series expansion about the value $q + W - W_0$:

$$\delta(E_f - E_i) = \delta(q + W - W_0) + \delta'(q + W - W_0)[B(G') - B(A')] + \ldots \tag{5}$$

If the first term in this expansion is inserted into the double integral, Eq. (3), then the expression for f reduces to the original form Eq. (1) since the atomic overlap factor is unity under the assumption that the sum over electronic configurations A' can be completed by closure: *i.e* $\sum_{A'} \left|\langle A'|G\rangle\right|^2 = \sum_{A'} \langle G|A'\rangle\langle A'|G\rangle = \langle G|G\rangle = 1$. The second term in Eq. (5) involves a derivative of a delta function. This is handled by an integration by parts, in which the rest of the integrand is differentiated with respect to q. No boundary terms survive as the integrand vanishes at the boundaries. Thus the atomic overlap correction becomes

$$r(Z,W) = 1 - \frac{2}{W_0 - W} \sum_{A'} \left|\langle A'|G\rangle\right|^2 \left[B(G') - B(A')\right]$$
$$= 1 - \frac{1}{W_0 - W} \frac{\partial^2}{\partial Z^2} B(G). \qquad (6)$$

A derivation of this latter expression is given in our recent survey [2].

TABLE I. Comparison of statistical rate functions calculated without the atomic overlap correction, $f_{without}$, those calculated with it included, f_{with}. The change in the Q_{EC} value that would lead to the same change in f is given in the last column.

Parent	$f_{without}$	f_{with}	*df/f(%)*	*dQ/Q(%)*	*dQ(eV)*
^{10}C	2.30089	2.30039	0.02178	0.00436	83
^{14}O	42.7779	42.7724	0.01277	0.00255	72
^{22}Mg	418.423	418.386	0.00877	0.00175	72
^{26m}Al	478.279	478.237	0.00880	0.00176	75
^{34}Ar	3414.68	3414.46	0.00647	0.00129	78
^{34}Cl	1996.10	1995.96	0.00711	0.00142	78
^{38m}K	3298.10	3297.88	0.00663	0.00133	80
^{42}Sc	4472.52	4472.24	0.00643	0.00129	83
^{46}V	7211.63	7211.20	0.00598	0.00120	84
^{50}Mn	10746.6	10746.0	0.00565	0.00113	86
^{54}Co	15767.5	15766.6	0.00537	0.00107	89
^{62}Ga	26401.6	26400.2	0.00557	0.00111	102
^{74}Rb	47296.9	47294.5	0.00523	0.00105	109

It remains to estimate the second derivative of the electronic binding energy of neutral atoms in their ground-state configuration. For this we use binding-energy values from the tables of Carlson *et al.* [3], which were obtained from self-consistent Hartree-Fock calculations and have been demonstrated to agree with experimental values to within 5%. We performed a fit to these tabulated values using a fitting function, aZ^b, in three ranges of Z values, with the following results:

$$B(G) = \begin{cases} 13.080\, Z_i^{2.42}\ \mathrm{eV}, & 6 \le Z_i \le 10 \\ 14.945\, Z_i^{2.37}\ \mathrm{eV}, & 11 \le Z_i \le 30 \\ 11.435\, Z_i^{2.45}\ \mathrm{eV}, & 31 \le Z_i \le 39, \end{cases} \tag{7}$$

where Z_i is the charge of the parent atom in the beta-decay process. It is conventional to use Z as the charge of the daughter nucleus in beta decay; thus for positron decay $Z_i = Z+1$. The second derivative is easily obtained from these expressions.

We have re-computed the statistical rate function f, and some sample results are listed in Table I. Those results obtained without the atomic overlap correction, Eq. (1), are given under the heading $f_{without}$, while those with the correction, Eqs. (2) and (6), are labelled f_{with}. The fractional difference between f_{with} and $f_{without}$ in percent is given in column 4 and is of order 0.01%, decreasing with increasing mass value. This is a very small correction. Furthermore, the statistical rate function depends on the Q-value to the fifth power, so the fractional change in Q that would lead to a change in f of the same size as that induced by the atomic overlap correction is even smaller: $1/5 \times df/f$. This percentage change is given in column 5 of Table I. As small as this effect is, it can be seen from the last column of the table that the equivalent change in Q-value ranges from 70 to 110 eV, an amount that is similar to the experimental uncertainties on the most precisely measured Q-values.

[1] J. N. Bahcall, Phys. Rev. **129**, 2683 (1963).
[2] J. C. Hardy and I. S. Towner, Phys, Rev. C **79**, 055502 (2009).
[3] T. A. Carlson, C. W. Nestor, N. Wasserman, and J. D. McDowell, At. Data **2**, 63 (1970).