New Hartree-Fock calculations for isospin-symmetry breaking correction in nuclear beta decay

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For accurate work, an isospin-symmetry breaking correction of between 0.5% and 1.5% is applied to *ft* values of nuclear beta decay. The correction is nucleus dependent and its evaluation dependent on nuclear-structure models. Conveniently the correction is divided into two components: $\delta_C = \delta_{C1} + \delta_{C2}$, where δ_{C1} arises from inserting charge-dependent terms into the Hamiltonian employed in a shell-model calculation, while δ_{C2} depends on radial-function differences between the initial-state proton and final-state neutron involved in the beta transition. These radial functions are taken to be eigenfunctions of either a Saxon-Woods (SW) or a mean-field Hartree-Fock (HF) potential with adjustments to ensure the radial functions have the appropriate asymptotic behaviour. It has been found in the past that the results for δ_{C2} obtained with SW were systematically larger than those of HF and this difference is included in the error analysis.

Until now, the HF calculations were all performed by Ormand and Brown [1-3]. This past year, we decided to examine the HF method and came upon an inconsistency, which when fixed considerably reduced the difference between the HF and SW δ_{C2} values. To be clear about the procedure, we illustrate it for the specific case of the decay of ^{34}Cl to ^{34}S. The decaying nucleus has $Z + 1 = 17$ protons; the daughter nucleus has $Z = 16$ protons. In the SW approach, the proton radial wave functions are taken to be eigenfunctions of a potential defined for a nucleus of mass A and charge Z+1 as follows:

$$V(r) = -V_0 f(r) - V_s g(r) \mathbf{l}.\boldsymbol{\sigma} + V_C(r), \qquad (1)$$

where V_0 and V_s are strengths of the central and spin-orbit terms, $f(r)$ is a Saxon-Woods radial function, $g(r)$ is its derivative, and $V_C(r)$ is a Coulomb term, whose asymptotic form is $V_C(r) \rightarrow Ze^2/r$ for large r. In our calculations [4] most of the parameters were fixed at standard values, with the well depth V_0 being adjusted case by case so that the binding energy of the eigenfunction being computed matched the separation energy to the corresponding parent state – in ^{33}S, for our example. Likewise the neutron radial functions were taken to be eigenfunctions of an similar potential but with the Coulomb term omitted.

The HF procedure is similar. For our illustrative example, a HF calculation is first mounted for ^{34}Cl, which would yield a mean field with central, spin-orbit and Coulomb terms. The required proton radial functions would then be taken as eigenfunctions of this mean field with the strength of the central term readjusted case by case so that the computed binding energy matched the appropriate separation energy. A second HF calculation is then mounted for ^{34}S, from which the neutron radial functions would be similarly determined in the mean field, but without the Coulomb term. However, under these circumstances, if the Coulomb terms in the HF mean-field potential were to be compared with those in the SW potential, a very significant difference would emerge. In the HF case, the Coulomb term is

$$V_C(\mathbf{r}) = \int d^3\mathbf{r}' \, \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\rho_p(\mathbf{r}') - \frac{3e^2}{2}\left[\frac{3}{\pi}\rho_p(\mathbf{r})\right]^{1/3}, \qquad (2)$$

which depends on the proton density (of ^{34}Cl in our example) that is generated as part of the HF procedure. The two terms in Eq. (2) are called the direct and exchange terms respectively. If we take the asymptotic limit of the direct term for large *r*, we obtain

$$V_C^{\rm dir}(\mathbf{r}) = \int d^3\mathbf{r}' \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}\rho_p(\mathbf{r}') \stackrel{r\to\infty}{\longrightarrow} \frac{e^2}{r}\int d^3\mathbf{r}'\rho_p(\mathbf{r}') = \frac{(Z+1)e^2}{r}. \qquad (3)$$

Since the HF proton density is normalized to *(Z+1)* protons in ^{34}Cl, the asymptotic form of the Coulomb potential tends to $(Z+1)e^2/r$. However, this disagrees with the equivalent SW calculation, which has the form Ze^2/r.

This discrepancy is important and constitutes a flaw in the HF calculations of the radial-mismatch factors. Since a proton removed from a nucleus of charge *Z+1* leaves behind *Z* protons, its asymptotic interaction is with charge *Z* -- as described by the SW potential -- and not with charge *Z+1*. This deficiency in HF would be cured in principle by the Coulomb exchange term. However, in Skyrme-Hartree-Fock calculations it is not possible to compute the exchange term exactly without sacrificing the simplicities that come with use of zero-range Skyrme interactions. The exchange term appearing in Eq. (2) is a commonly used local approximation, which might well be appropriate for the nuclear interior and for the computation of bulk properties such as binding energies and radii, but it does not do the job asymptotically, which is the region of greatest importance to our calculations.

To circumvent this difficulty, we have chosen to alter the HF protocol. Instead of mounting two HF calculations -- for ^{34}Cl and ^{34}S -- as just described, we mount a *single* calculation for the nucleus with *(A-1)* nucleons and *Z* protons -- ^{33}S in our example. We then use the proton mean field from this calculation to generate the proton eigenfunctions and the neutron mean field from the same calculation to generate the neutron eigenfunctions. In this procedure, the Coulomb interaction automatically has the correct asymptotic form. Calculations of δ_{C2} with this new HF protocol yields results larger than those obtained with the conventional protocol by between 10% and 40% depending on the Skyrme interaction used and the nucleus under study. This change of protocol goes a long way in reducing the systematic error between SW and HF calculations.

The results from our HF calculations for δ_{C2} are listed in column 3 of Table I. For each transition, the central value is an average of the results obtained with the three choices of Skyrme interactions. To assign an uncertainty, we have examined the spread in results obtained with the different Skyrme interactions and with different shell-model effective interactions and model spaces. Observe that these new results of ours are systematically larger than those computed by Ormand and Brown (given in column 2) and are much closer to the SW values (column 4).

TABLE I. Isospin-symmetry-breaking corrections, δ_{C2} in percent units, and their assigned uncertainties obtained from HF calculations. Also listed are earlier results obtained with HF (column 2) and SW (column 4) eigenfunctions.

	Hartree-Fock		Saxon-Woods
Nucleus	OB95[a]	This work	TH08[b]
^{10}C	0.11	0.215(35)	0.165(15)
^{14}O	0.14	0.255(30)	0.275(15)
^{22}Mg	0.19	0.250(55)	0.370(20)
^{26}Al	0.29	0.410(50)	0.280(15)
^{34}Ar	0.37	0.510(60)	0.635(55)
^{34}Cl	0.51	0.595(55)	0.550(45)
^{38}K	0.48	0.640(60)	0.550(55)
^{42}Sc	0.31	0.620(55)	0.645(55)
^{46}V	0.29	0.525(55)	0.545(55)
^{50}Mn	0.33	0.575(55)	0.610(50)
^{54}Co	0.40	0.635(55)	0.720(60)
^{62}Ga	0.89	0.93(16)	1.20(20)
^{74}Rb	0.83	1.29(16)	1.50(30)

[a]Ref. [3]
[b]Ref. [4]

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[4] I. S. Towner and J. C. Hardy, Phys. Rev. C **77**, 025501 (2008).