Skyrme-Hartree-Fock calculations of the isospin-symmetry breaking correction in superallowed beta decay

I. S. Towner and J. C. Hardy

Over the past few years we have performed Hartree-Fock calculations of the isospin-symmetry breaking correction in superallowed beta decay, δ_{c2} , using many different parameter sets for the input Skyrme nucleon-nucleon interaction. For each set, we have applied a test [1] to the results: they should satisfy the requirements of the Conserved Vector Current (CVC) hypothesis. A figure of merit for this test is the chi-square per degree of freedom, χ^2/n_d . When Saxon-Woods eigenfunctions are used to calculate δ_{c2} , the test is passed with flying colours – the figure of merit is χ^2/n_d = 1.2 . With Hartree-Fock eigenfunctions, the figure of merit ranges from 5 to 16 depending on the Skyrme interaction used. To date, we have tried 20 different Skyrme interactions and none give an acceptable result for the test. The general flaw is too small a δ_{c2} correction in the high-Z cases, ^{62}Ga and ^{74}Rb, and too large a correction in ^{26}Al. There is another curious result from the Hartree-Fock calculations. If one considers a pair of mirror superallowed transitions, such as the decay of the $T_z = -1$ nucleus ^{26}Si→^{26}Al compared to the decay of a $T_z = 0$ nucleus ^{26}Al→^{26}Mg, one would intuitively expect the difference

$$\Delta\delta_{C2} = \delta_{C2}(T_z = -1) - \delta_{C2}(T_z = 0) \quad (1)$$

to be positive. This is simply a statement that there are more protons in the $T_z = -1$ nucleus and the Coulomb interaction between the protons is primarily responsible for the isospin-symmetry breaking. Certainly the Saxon-Woods calculations yield positive values for $\Delta\delta_{c2}$, while Hartree-Fock calculations typically give negative values.

These imperfections in the Hartree-Fock calculations seem to be suggesting there is a flaw in the way the Hartree-Fock procedure is being implemented. Certainly it is well known that the Hartree-Fock iteration scheme when applied to a nucleus with $N \neq Z$, will *not* conserve isospin even though the input Skyrme nucleon-nucleon interaction is isoscalar and the Coulomb potential has been turned off. Since we perform the Hartree-Fock calculation on the odd-mass nucleus with (A-1) nucleons, (see the discussion in the appendix of Ref. [2],) our results will suffer from some measure of spuriosity.

In the Saxon-Woods calculation, the central and spin-orbit potentials used for protons and neutrons are initially identical. Then the well-depth of the central potential is readjusted separately for protons and neutrons so that the experimental proton and neutron separation energies are reproduced as eigenvalues of the potential. A Coulomb potential is also included in the proton potential. If the Coulomb potential is turned off and the separation energies for protons and neutrons are made equal, then the isospin-symmetry correction δ_{c2} calculated with the Saxon-Woods code goes to zero, as it should. Thus, there is no spuriosity in the Saxon-Woods computation.

By contrast, if the same analysis is performed on the mean-field potentials produced by the Hartree-Fock procedure, namely turning the Coulomb force off and setting the proton and neutron separation energies equal, the calculated δ_{c2} correction does not go to zero. The reason is that the central

and spin-orbit potentials coming out of the Hartree-Fock code are not initially identical. To illustrate this consider just the first term in the Skyrme nucleon-nucleon interaction

$$V(\boldsymbol{r_1}, \boldsymbol{r_2}) = t_0(1 + x_0 P_\sigma)\delta(r_1 - r_2) + \ldots \tag{2}$$

and the mean-field potentials for protons and neutrons that this term produces:

$$U_p = \frac{1}{2} t_0 \left[(2 + x_0)(\rho_p + \rho_n) - (1 + 2x_0)\rho_p \right] + \ \ldots$$
$$U_n = \frac{1}{2} t_0 \left[(2 + x_0)(\rho_p + \rho_n) - (1 + 2x_0)\rho_n \right] + \ \ldots \tag{3}$$

Here ρ_p and ρ_n are proton and neutron densities constructed from the sum of the squares of the single-particle wave functions of the occupied states. Notice the structure of Eq. (3). The first term is isoscalar, while the second is an isovector/isoscalar equal mix. All the other pieces of the Skyrme interaction lead to terms in U_p and U_n with the same isospin structure. It is now obvious that if $N \neq Z$, then $U_p \neq U_n$ because the densities ρ_p and ρ_n are not the same, being separately normalized to the number of protons and neutrons respectively. Only when $N = Z$ can one produce mean-field potentials that are equal for protons and neutrons (in the absence of the Coulomb potential, of course).

To proceed, we will alter our protocol established in [2] and now insist the central and spin-orbit potentials for protons will equal that for neutrons at the end of the Hartree-Fock iterations. There are a number of ways to implement this, but it turns out the final values for δ_{c2} are rather insensitive to how this is accomplished. So we will average the proton and neutron densities and in Eq. (3) put $\rho_p \rightarrow (\rho_p + \rho_n)/2$ and $\rho_n \rightarrow (\rho_p + \rho_n)/2$ to obtain

$$U_p = U_n = \tfrac{3}{4} t_0 (\rho_p \ + \ \rho_n) + \ \ldots \tag{4}$$

With the new protocol, we have computed isospin-symmetry-breaking corrections for 20 nuclei for 12 Skyrme interactions. The unweighted average for each nucleus is recorded in the last column of Table I. The assigned error is compounded from two sources: half the spread between the highest and lowest result obtained with the different Skyrme interactions, and the spread among the different shell-model effective interactions used to compute the spectroscopic factors needed in the δ_{c2} computation. This latter error is also included in the error budget for the Saxon-Woods computations. Also in Table I are the previous Hartree-Fock results with the old protocol, as published in [2], and the Saxon-Woods values from [3]. Immediately one can see the new protocol has effected some improvements:

- The values of δ_{c2} in the high-Z cases of ^{62}Ga and ^{74}Rb are much larger and, within the stated errors, agreeing with the Saxon-Woods result.
- The mirror-transitions comparisons, $\Delta\delta_{c2}$ of Eq. (1), are firmly positive, as expected intuitively.

But there is a downside: the results for low-Z cases are also increased. To assess the impact of this we have subjected the sets of δ_{C2} values for each Skyrme interaction to the CVC test mentioned above. The figure of merit, χ^2/n_d , ranged from 2.7 to 5.7, much better than the range reported under the old protocol of 5 to 16, but still worse than1.4 obtained with Saxon-Woods radial functions. So the nucleus-to-nucleus variations in the δ_{c2} values required by the CVC hypothesis are still not being achieved in the Hartree-Fock computations.

TABLE I. δ_{C2} values (in percent units) calculated with Saxon-Woods eigenfunctions (as published in TH08 [3]), with Hartree-Fock eigenfunctions with the old protocol (as published in HT09 [2]), and with Hartree-Fock eigenfunctions with the new protocol. Also listed are the δ_{C2} differences for mirror transitions, $\Delta\delta_{C2}$ of Eq. (1), and the figure of merit, χ^2/n_d, from the CVC test (see [1]).

	TH08 SW	HT09 HF	new HF
^{10}C	0.165(15)	0.215(35)	0.32(3)
^{14}O	0.275(15)	0.255(30)	0.39(3)
^{18}Ne	0.411(25)	0.205(55)	0.36(4)
^{22}Mg	0.370(20)	0.250(55)	0.38(3)
^{26}Si	0.405(25)	0.335(55)	0.47(5)
^{30}S	0.700(20)	0.540(55)	0.76(7)
^{34}Ar	0.635(55)	0.510(60)	0.75(7)
^{38}Ca	0.745(70)	0.600(60)	0.87(9)
^{42}Ti	0.835(75)	0.535(60)	0.78(10)
^{26}Al	0.280(15)	0.410(50)	0.36(7)
^{34}Cl	0.550(45)	0.595(55)	0.61(10)
^{38}K	0.550(55)	0.640(60)	0.71(11)
^{42}Sc	0.645(55)	0.620(55)	0.64(10)
^{46}V	0.545(55)	0.525(55)	0.57(9)
^{50}Mn	0.610(50)	0.575(55)	0.65(10)
^{54}Co	0.720(60)	0.635(55)	0.72(11)
^{62}Ga	1.20(20)	0.93(16)	1.23(25)
^{66}As	1.35(40)	1.11(35)	1.41(40)
^{70}Br	1.25(25)	1.14(25)	1.49(25)
^{74}Rb	1.50(30)	1.29(16)	1.75(25)
$\Delta\delta_{C2}(A=26)$	0.126	−0.075	0.11
$\Delta\delta_{C2}(A=34)$	0.086	−0.085	0.14
$\Delta\delta_{C2}(A=38)$	0.194	−0.040	0.16
$\Delta\delta_{C2}(A=42)$	0.192	−0.085	0.15
χ^2/n_d	1.2	8.3	3.3

[1] I.S. Towner and J.C. Hardy, Phys. Rev. C**82**, 065501 (2010).
[2] J.C. Hardy and I.S. Towner, Phys. Rev. C**79**, 055502 (2009).
[3] I.S. Towner and J.C. Hardy, Phys. Rev. C**77**, 025501 (2008).