Influence of $2p-2h$ Excitations in the $^{41}\text{Sc}-^{41}\text{Ca}$ Coulomb Energy Shift

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The influence of $2p-2h$ core excitations on the $^{41}\text{Sc}-^{41}\text{Ca}$ Coulomb energy difference is studied. A simple parametrization of the main wave function components shows that the calculated energy shift could only agree with experiment for rather unrealistic values of the amplitudes. Using an effective interaction appropriate for this region, we find that when this kind of excitations is included, the calculated Coulomb energy shift is increased by 105 keV.

1. Introduction

In calculations of the Coulomb energy shift of mirror nuclei with one particle outside closed shells, it is generally assumed that the single particle wave function coupled to an inert core is sufficient in describing the nuclei to a good first approximation [1, 2]. Qualitative estimates of corrections due to configuration mixing effects were given by Nolen and Schiffer [1] and Auerbach et al. [3]. Auerbach, Kahana and Weneser [4] (AKW) were the first to consider the isovector mode of the core polarization induced by an extra nucleon. In terms of the shell-model, this effect is essentially a mixing of $1p-1h$ excitations of the core. With the first quantitative calculations [4, 5] of the AKW effect it was hoped that the Coulomb energy anomaly would be solved. However, detailed calculations [6-8], some of them using the Hartree-Fock theory, have shown that the AKW effect was too small to resolve the anomaly. The purpose of this paper is to study the influence of $2p-2h$ excitations in the Coulomb energy shift of $^{41}\text{Sc}-^{41}\text{Ca}$, since, as we shall see, they play an important role in the ground state of these nuclei. Some preliminary results of the present work are given in [9]. Sato [10] also has considered this problem, although the cross terms in the expectation value of the Coulomb interaction and the charge distribution due to core excitations were not considered in his calculations. The latter shortcoming appears also in a very recent paper by Barroso [11], where the Kallio-Kollveit residual interaction is treated in first order perturbation theory in an attempt to describe the effect of $2p-2h$ excitations on Coulomb displacement energies. Our approach to this problem is different in several aspects and being more complete, it avoids the shortcomings mentioned above, as will become clear later on.

We have selected this mirror pair as a typical example in which calculations of many other correction terms are now available. Looking at a summary table (see, for example, Negele's [6] or Shlomo's [2]) one immediately realizes that corrections such as the finite size of protons, isospin impurities in the core, short range correlations, etc., are all, at the most, of the order of 1% of the Coulomb energy shift, and their signs are so randomly distributed that the final calculated value is quite close to what one obtains considering only the pure Coulomb interaction of point protons.

First, we shall study in detail the influence of configuration mixing on the main term, i.e., the Coulomb interaction of point protons, and later we shall consider how other corrections can be affected.

2. The Coulomb Term

Shell-model calculations for the $A=41$ nuclei have shown that the ground state contains important
We shall use the harmonic oscillator (HO) well for the from the experimental nuclear charge radius. Taking the oscillator size parameter \( b \) will be determined wave functions have an excellent overlap with Hartree-Fock wave functions (see, for example, Negele [6]).

For the centre of mass motion, the mean square charge

Coulomb two-body matrix elements. For the \( A=41 \)

decomposing the operator \( V_c = e^2/r \) in the isoscalar, isovector and isotensor parts. Actually, since we are interested in the energy difference of \( T=1/2 \) states, only the isovector part needs to be calculated. The reduction from the many-nucleon to the two-body matrix elements has been achieved following the explicit expressions for the shell-model matrix elements of two-body tensor operators of any rank given in [14].

The results of our calculation, including the correct adjustment of the oscillator parameter in each case, are shown in Figure 1 as a function of the amplitude parameters \( a \) and \( b \) of the wave function (1). Then \( c \) is, of course, fixed by normalization, except for its sign. The figure corresponds to \( c \geq 0 \), but very similar curves are obtained for \( c \leq 0 \). The Coulomb energy shift should be compared with the experimental value \( \Delta E = 7.28 \text{ MeV} \). The calculated value for the pure \( f_{7/2} \) single particle state coupled to an inert core (point \( a=1 \) in the figure) is \( \Delta E = 6.69 \text{ MeV} \).

Several calculations [1-7] of the \( ^{41}\text{Sc} - ^{41}\text{Ca} \) Coulomb energy shift, including various corrections to the pure Coulomb term, but not including the kind of core excitations that we are considering, give theoretical values for the corrections ranging approximately between 0 and 200 keV. Thus, if this kind of configuration mixing were to be able to explain the remaining discrepancy, we would have to obtain a value of about 7.1-7.3 MeV for the Coulomb term (exchange included). Figure 1 shows that these values can be achieved for adequate amplitudes, roughly \( a \lesssim 0.7 \) and a very small value of \( |c| \). This would mean at least 50\% of the \( 3p-2h \) configuration.

In an attempt to get a reasonable estimate for amplitudes \( a \), \( b \) and \( c \), we have used the effective nuclear interaction fitted by Zuker [12,15] for these shell-model orbits. With this interaction we diagonalize the Hamiltonian in the subspace of (1) and the wave function becomes

\[ \Psi(J=7/2, T=1/2) = a |d^6(00)f^3(7/2 1/2)\rangle + b |d^6(01)f^3(7/2 1/2, v=1)\rangle + c |d^6(01)f^3(7/2 3/2, v=1)\rangle. \]  

We shall use the harmonic oscillator (HO) well for the single particle wave functions in the calculation of the Coulomb two-body matrix elements. For the \( A=41 \) nuclei it is a good approximation, since the required wave functions have an excellent overlap with Hartree-Fock wave functions (see, for example, Negele [6]). The oscillator size parameter \( b \) will be determined from the experimental nuclear charge radius. Taking into account the finite proton size and the correction for the centre of mass motion, the mean square charge radius of the nucleus becomes

\[ \langle r^2 \rangle_{\text{ch}} = \langle r^2 \rangle_{\text{proton}} + \langle r^2 \rangle_{\text{point}} \frac{3 b^2}{2 A} \]  

where \( \langle r^2 \rangle_{\text{proton}} = 0.65 \text{ fm}^2 \).

Unfortunately, the radius of \( ^{41}\text{Ca} \) is not known. The rms radius of the charge distribution of \( ^{42}\text{Ca} \) is 0.03 fm greater [13] than that of \( ^{40}\text{Ca} \), and a simple interpolation is not reliable. But while the accurate knowledge of the experimental charge radii of the mirror nuclei considered would be of primary importance in determining the magnitude of the Coulomb energy shift, it is not significant for an estimation of the configuration mixing correction. So we shall assume that the charge radius of \( ^{41}\text{Ca} \) is equal to the experimental value of \( ^{40}\text{Ca} \), \( \langle r^2 \rangle_{\text{ch}}^{1/2} = 3.49 \text{ fm} \) [13].

However, it is very important to modify the single particle wave functions in order to keep constant the radius of the charge distribution when using wave functions with different amounts of configuration mixing. For example, using a closed shell configuration for \( ^{40}\text{Ca} \) and HO wave functions, one gets \( \langle r^2 \rangle_{\text{point}} = 3.0 b^2 \), but by using Zuker's [12] wave function, which contains 30\% of the excited component \( d^6(01)f^2(01) \), we get \( \langle r^2 \rangle_{\text{point}} = 3.014 b^2 \). Thus, to be consistent with the implications of configuration mixing, we shall fit the oscillator parameter to the "experimental" charge radius of \( ^{41}\text{Ca} \) using a wave function with mixing.

The \( ^{41}\text{Sc} - ^{41}\text{Ca} \) Coulomb energy shift is given, in first order perturbation theory, by the difference of expectation values of the Coulomb interaction calculated in the \( T_s = -1/2 \) and \( T_s = 1/2 \) states. The calculation has been carried out in isospin formalism decomposing the operator \( V_c = e^2/r \) in the isoscalar, isovector and isotensor parts. Actually, since we are interested in the energy difference of \( T=1/2 \) states, only the isovector part needs to be calculated. The reduction from the many-nucleon to the two-body matrix elements has been achieved following the explicit expressions for the shell-model matrix elements of two-body tensor operators of any rank given in [14].

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\[ ^{41}\text{Sc}, \quad ^{41}\text{Ca}, \quad a=0.876, \quad b=-0.348, \quad c=-0.334. \]

This wave function gives an oscillator parameter \( b = 1.967 \text{ fm} \) and a Coulomb energy shift of 6.76 MeV, which is 70 keV larger than the value obtained without mixing. To check the stability of our results, the calculations have been repeated including the basis components of the type \( |d^6(01)f^3(7/2 1/2, v=3)\rangle \).

There are two different components with these quantum numbers. Let us represent their amplitudes