Shell Model Description of Isotope Shifts in Calcium

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Isotope shifts in the nuclear charge radius of even and odd calcium isotopes are calculated within the nuclear shell model. The model space includes all configurations of nucleons in the 2s, 1d₃/₂, 1f₇/₂, and 2p₃/₂ orbits. The shell model describes well the energies of the intruder states in Sc and Ca, as well as the energies of the low-lying 2⁺ and 3⁻ states in the even Ca isotopes. The characteristic features of the isotope shifts, the parabolic dependence on A and the prominent odd-even staggering, are well reproduced by the model. These features are related to the partial breakdown of the Z = 20 shell closure caused by promotion, due to the neutron-proton interaction, of the ds shell protons into the fp shell.

21.10.Ft, 21.60.Cs, 21.60.-n

Introduction The appearance of shell gaps associated with magic nucleon numbers is one of the cornerstones in nuclear structure. However, it has been increasingly evident in recent years that these magic numbers, and the corresponding shell closures, might get eroded with increasing neutron excess. To understand the origin of this erosion and to identify whether this trend applies to increasing neutron excess. To understand the origin of this erosion and explanation of the nuclear charge radii, argue in this Letter. Our argument is based on the un-

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Due to the configuration mixing across the $Z = 20$ shell boundary, protons are lifted from the $sd$ to the $fp$ shell, resulting in the increase of $\langle r_z^2 \rangle$ equal to

$$\delta r_z^2(A) = \frac{1}{2 Z} \langle n_{fp}(A) \rangle b^2,$$

where $Z = 20$, $b$ is the oscillator parameter which we assume remains constant for $A = 40 - 48$, and the number of protons in the $fp$ shell, $n_{fp}(A)$, is the calculated quantity. Below we show how it is calculated and how one can relate it to other manifestations of breaching of the $Z = 20$ shell boundary.

**Shell model** Progress in the application of modern nuclear shell model has been facilitated by the development of numerical codes (the $m$-code ANTOINE and the $J$-coupled code NATHAN) that can be used with relatively large valence spaces. The selection of the appropriate single-particle space, and the corresponding effective interaction (in particular the choice of its uncertain monopole part) is the most important starting point of any shell model application.

Since here we are interested in the description of calcium isotopes, it is imperative to include states in the vicinity of the $N = Z = 20$ shell boundary. Therefore, the chosen valence space consists of the $d_{3/2}, s_{1/2}, f_{7/2}$ and $p_{3/2}$ subshells for both protons and neutrons. (Thus $^{28}$Si represents the inert core.) This valence space, first used in Ref. [13], has the advantage that the existing codes make it possible to describe all Ca isotopes without truncation. (The largest dimension, 34,274,564 in the $m$-scheme basis, is encountered for the ground state of $^{43}$Ca.) The other advantage is the essential absence of the spurious center-of-mass motion (no attempt to suppress it has been made).

For this valence space we start with the two-body matrix elements (TBME) of Ref. [14], which are defined with respect to the $^{16}$O core. The single particle energies are now modified to reproduce the $^{29}$Si spectrum. The interaction of Ref. [14] was built in blocks ($sd−sd, sd−fp$ and $fp−fp$), which incorporate the higher-order excitations (core polarization, $2p2h$ excitations etc...). In particular, the $2p2h$ effects consist mainly in pairing renormalizations. As we will include explicitly such mixing, and to avoid double counting, a schematic pairing hamiltonian was subtracted from the interaction. Finally, the cross $sd−fp$ monopoles of Ref. [14] were adjusted to the masses of neutron-rich isotopic chains. They were here retuned to reproduce the gap at $^{40}$Ca and the spectra of $^{39}$K and $^{41}$Ca.

**Results** As indicated in Eq. (1) above, we assume that the main cause of variation of the charge radius with changing neutron number is the lifting of protons from the $sd$ shell into the larger $fp$ shell. This feature then suggests that there should be a correlation between the isotope shifts and other manifestations of the incomplete $Z = 20$ shell closure, e.g. the appearance of low-lying intruder states. In Fig. 1 the experimental excitation energies of the intruder $3/2^+$ states in odd-$A$ Sc isotopes are compared with the calculated ones. The agreement is very satisfactory, and in particular the lowering of these states in $^{43}$Sc and $^{45}$Sc is properly described.

![FIG. 1. Excitation energies of intruder states in Sc and in even Ca isotopes. The experimental (circles) and calculated (squares) energies of the $3/2^+$ states in Sc and the experimental (stars) and calculated (crosses) energies of the excited $0^+_2$ states in Ca are shown.](image-url)
to achieve saturation. This means that the “lifting” is a complicated process, involving substantial rearrangement of many nucleons. This can be seen also in the fact that approximately equal numbers of protons and neutrons are lifted from the $ds$ shell. It is therefore difficult to identify a simple cause, or a definite component of the hamiltonian, as the driving force of this effect.

In the full space the quantity $n_{fp}(A)$ is 1.10 in $^{40}$Ca, reaches its maximum of 1.97 in $^{44}$Ca, and then decreases again to 0.78 in $^{48}$Ca.

Knowing the quantities $n_{fp}$ one can calculate the isotope shifts from Eq. (1) by subtracting the corresponding $\delta r^2(A = 40)$ from $\delta r^2(A)$. (Nucleon form factors contribute negligibly to the isotope shift and thus are neglected.) The results, calculated with a constant $b = 1.974$ fm as in [1], are shown in Fig. 2 and compared with the experimental values. The trends, i.e. the properties (i) - (iii) are clearly well reproduced, but the magnitude of the calculated shifts is smaller than the experiment suggests.

This cannot be attributed to our choice of the oscillator parameter $b$. Neither it can be cured by replacing the harmonic oscillator wave functions by the Woods-Saxon single-particle wave functions, which changes the isotope shifts shown in Fig. 2 only very little, provided the core $(r^2)$ is assumed to be independent of $A$. (Although assuming a very slight increase of $b(A)$, i.e. a gradual increase of the core $(r^2)$ from $A = 40$ to $A = 48$, might “straighten” the curve a bit.) Moreover, choosing the recommended average dependence of $b$ on the mass number $A$ and isospin $T$ [13] $(b^2 = 1.074^{1/3}(1 - (2T/A)^2)\exp(3.5/A)\text{ fm}^2)$ would make the radius of $^{48}$Ca considerably larger than the radius of $^{40}$Ca. The $b(A, T)$ dependence, which on average follows [14], clearly is subject to local shell effects. Most likely, the calculated amplitude of the isotope shift might be modified if the so far neglected effects of the filled $d_{5/2}$ and empty $f_{5/2}$ orbits are added.

Collective states When considering isotope shifts, one also has to take into account the effect of the zero-point motion associated with the surface vibrational modes (see [15] for a systematic approach to this question). There it is stressed that only the low-lying low-multipolarity surface vibrational states contribute significantly. The collective states increase the mean square radius by

$$\delta r^2 = R_0^2 \sum_\lambda \beta^2_\lambda,$$

where $R_0$ is the equivalent sharp nuclear radius, and $\beta_\lambda$ is the vibrational amplitude of the mode $\lambda$, related to the corresponding $B(E\lambda, 0 \rightarrow J = \lambda)$ value. What matters for the isotope shifts, naturally, is not the absolute value of the amplitudes $\beta_\lambda$, but their variation with $A$.

Formula (2) was derived as a correction to the mean square radius calculated using the mean-field methods. On the other hand, since the shell model includes all correlations of nucleons in the valence shells, blind use of it would amount to at least partial double counting.

The energies of the lowest lying $2^+$ and $3^-$ states are compared to the shell model in Fig. 3. The good agreement there shows not only that the chosen interaction describes this important spectroscopic data well, but that the zero-point motion effect on the nuclear radius is (at least most of it) automatically included.

In addition, in Fig. 3 we compare the experimental and shell model $B(E2, 2 \rightarrow 0)$ values. (The calculations were performed with the usual effective charges $e_p = 1.5, e_n = 0.5$.) Again, the agreement is quite good, strengthening
our belief that most of the effect of the collective states is already contained in our calculation.

**Discussion** The present calculation shows that the $Z = 20$ and $N = 20$ shell boundaries are clearly not absolute, and that substantial configuration mixing involving nucleons from the $ds$ shell is present even in the Ca isotopes.

This finding is in line with the previously recognized and perhaps more dramatic “islands of inversion” related to the configuration mixing involving the $N = 20$ shell boundary in neutron rich nuclei (see Ref. [16,17]). Here we are encountering a similar situation, now however in stable nuclei near or at $N = Z$.

Is there any other evidence for the incomplete shell closure in $^{40}$Ca? Indeed, the study of the $(n, p)$ and $(p, n)$ reactions [18–20] on $^{40}$Ca revealed that the integrated Gamow-Teller strength $B(GT) = 1.6 \pm 0.1$ below 15 MeV. Obviously, if the $ds$ shell in $^{40}$Ca were really closed, the $B(GT)$ would vanish. Note, that without the full inclusion of the $f_{5/2}$ and $d_{5/2}$ orbit we can only estimate the total Gamow-Teller strength in $^{40}$Ca. Without these orbits we obtain the total $B(GT) = 0.53$ using the usual quenching of 0.744 [2]. When we allow the $t = 1$ (i.e. one particle or one hole) excitations involving the $f_{5/2}$ and $d_{5/2}$ orbits, we obtain $B(GT) = 2.75$ with quenching, in fair agreement with the experiment. Clearly, some of the strength associated with these orbits will be above 15 MeV, and should not be counted.

In conclusion, the present calculation shows that the isotope shifts, and the position of the intruder states in Ca isotopes, can be well described by large scale shell model calculations. The judicious choice of the valence space and the corresponding effective hamiltonian is the key ingredient to this success. Thus, the challenge to the nuclear structure theory, described in the introduction to this work, has been largely met. No new forces or parameters are needed to describe the dependence of the nuclear radius in the odd and even Ca isotopes on the mass number $A$.

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