Mirror displacement energies and neutron skins

J. Duflo[1] and A. P. Zuker[2]

[1]*Centre de Spectrométrie Nucléaire et de Spectrométrie de Masse (IN2P3-CNRS), F-91405 Orsay Campus, France*
[2]*IReS, Bât27, IN2P3-CNRS/Université Louis Pasteur, BP 28, F-67037 Strasbourg Cedex 2, France*
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A gross estimate of the neutron skin $[0.80(5)(N-Z)/A$ fm] is extracted from experimental proton radii, represented by a four parameter fit, and observed mirror displacement energies (CDE). The calculation of the latter relies on an accurately derived Coulomb energy and smooth averages of the charge symmetry breaking potentials constrained to state of the art values. The only free parameter is the neutron skin itself. The Nolen Schiffer anomaly is reduced to small deviations (rms = 127 keV) that exhibit a secular trend. It is argued that with state of the art shell model calculations the anomaly should disappear. Highly accurate fits to proton radii emerge as a fringe benefit.

Recent experiments [1,2] have considerably added to our knowledge of neutron radii, the most elusive of the fundamental properties of nuclear ground states. The two sets of measures are consistent with one another, and a recognizable pattern emerges ([1] Fig. 4), leading to an estimate for the neutron skin ($\nu \equiv$ neutrons, $\pi \equiv$ protons, $t = N - Z$)

$$\Delta_{r_{\nu\pi}} = \sqrt{\langle r_\nu^2 \rangle} - \sqrt{\langle r_\pi^2 \rangle} = -0.04(3) + 1.01(15)\frac{t}{A}\text{fm.} \quad (1)$$

A third—totally different—experiment [3] adds weight to this estimate: it deals with the sodium isotopes, lighter and far more exotic than the species studied in [1,2]. Nonetheless, their $\Delta_{r_{\nu\pi}}$ behavior is very much the same, as seen in Fig. 1.

On the theory side, we have an elegant analysis of $\Delta_{r_{\nu\pi}}$ [4], and many mean-field calculations. Some of them are close to estimate (1), others not so close [5], though in the Na isotopes several Skyrme forces seem to give equally good results [6]. As was pointed out in [7], the neutron skins could be easily varied in such forces, without perturbing other observables, but the criteria to fix them were not obvious. The problem has been tackled head on recently [8,9] by constraining agreement with realistic calculations of the equation of state for neutron matter but no systematic study has appeared so far.

The idea that started this investigation is that—assuming isospin conservation—a complete knowledge of *proton* radii would determine $\Delta_{r_{\nu\pi}}$. As the available experimental data turn out to be consistent with a wide range of possible values of $\Delta_{r_{\nu\pi}}$, we resort to the Coulomb displacement energies (CDE) *which are very sensitive to this quantity*. The originality of our approach rests on the derivation, for all the observables, of smooth—Bethe Weizsäcker type—forms that depend only on N and Z. The differences between these averages and the experimental values—i.e., the shell effects—will be found to exhibit secular behavior that leads to high quality phenomenological fits for the radii. For the CDE, they lead to an optimistic assessment of the present status of a famous problem, the Nolen Schiffer anomaly [10].

To relate neutron and proton radii we start by noting that $r_\pi^2 = [\Sigma_{i<j}(1/2 - t_z^i)(1/2 - t_z^j)r_{ij}^2]/A^2$ has the same form as

the Coulomb energy (interchange r_{ij}^2 by r_{ij}^{-1}). It follows that $\langle r_\pi^2 \rangle = \alpha(A,T) + \beta(A,T)T_z + \gamma(A,T)T_z^2$. This result relies on the same arguments that lead to the isobaric multiplet mass equation ([11], p. 302). As $\langle r_\pi^2 \rangle$ is a functional of the state occupancies, α, β, and γ may vary rapidly. To obtain a smooth form we assume some continuous occupancies, which make it possible to obtain a four-parameter expression based only on dimensional considerations. Since we are interested only in mirror nuclei with $T_z = 2t$, we propose

$$\sqrt{\langle r_\pi^2 \rangle} \approx \rho_\pi = A^{1/3}\left(\rho_0 - \frac{\zeta}{2}\frac{t}{A^\sigma} - \frac{\upsilon}{2}\left(\frac{t}{A}\right)^2\right)e^{(g/A)}. \quad (2)$$

The overall $A^{1/3}$ dependence is a general asymptotic result for self-bound systems. The $\exp(g/A)$ correction accounts for the larger radii for small A. The terms in υ and ζ must be *at most* of the same order as ρ_0 for large t/A and the only remaining uncertainty is in the scaling σ in t/A^σ.

Obviously, we can derive a similar expression for ρ_ν with $t \Rightarrow -t$. Therefore $\upsilon > 0$ represents a uniform contraction of the two fluids, while $\zeta > 0$ implies a π contraction and ν dilation, which gives the neutron skin

$$\Delta_{r_{\nu\pi}} \equiv \Delta(\zeta) = (\rho_\nu - \rho_\pi) = \frac{\zeta t}{A^{\sigma-1/3}}e^{(g/A)}. \quad (3)$$
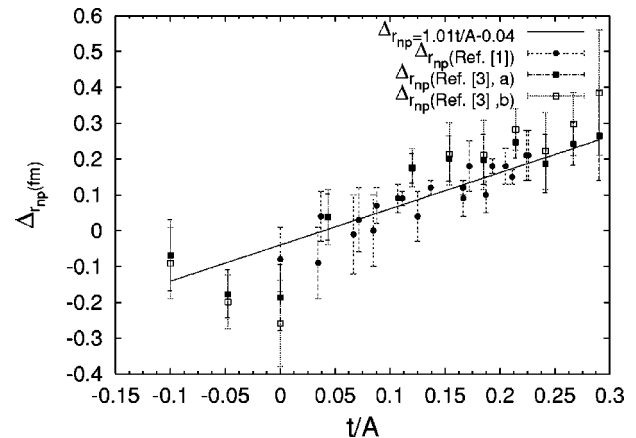

FIG. 1. $\Delta_{r_{\nu\pi}}$ from [1], (Fig. 4) (circles), the two approximations of Ref. [3] (Table I) (squares), and Eq. (1).

TABLE I. Root mean square deviations from observed CDE for three sets of coefficients in Eq. (7) with $A_0 = 16$. V_C from Eq. (12). All energies in keV. See text.

		V^d_{Cm}	V^{st}	$V^d_{Cm} + V_B$		
ζ	ν	rmsd	rmsd	B_ν	B_s	rmsd
1.0	0.51	**540**	**272**	540	350	**127**
0.9	0.57	**434**	**184**	431	281	**127**
0.8	0.62	**320**	**127**	306	199	**127**
0.7	0.68	**213**	**170**	181	119	**127**
0.6	0.73	**136**	**268**	56	39	**127**

If $\sigma = 1$ the volumes occupied by the two fluids may differ by a quantity of order A, and we have a "volume" skin.

If $\sigma = 4/3$ we have a "surface" skin, since the difference in volumes is at most of order $A^{2/3}$.

The volume option would be the correct one for strong attraction between like particles. In nuclei, the $\nu\pi$ force is by far the strongest, and we adopt a surface skin. (A volume skin also leads to excellent radii, but it will be ruled out by the CDE.)

To determine the coefficients in Eq. (2) we shall fit the experimental values of charge radii (full references are given in [12]), reduced to point radii through the standard prescription $\rho^{exp}_\pi = [\langle r^2_\pi \rangle^{exp}_{charge} - 0.64]^{1/2}$ (used in [1], full form in [8]).

A fit is made to 82 experimental values for nuclei with N or $Z = 6, 14, 28, 50, 82, 126$ (the classical closures which we call EI, for extruder-intruder), for which shell effects can be assumed to be minimal. The results are altogether remarkable: for $0.4 \leqslant \zeta \leqslant 1.2$ the root mean square deviations (rmsd) are below 10 mf. We find nearly common parameters $\rho_0 = 0.943(2)$, $g = 1.04(3)$, for different (ν, ζ) pairs, given in Table I for $0.6 \leqslant \zeta \leqslant 1.0$.

To decide which is the favored (ν, ζ), we compare 63 experimental [13] displacements, CDE$=BE(Z_>,N_<)-BE(Z_<,N_>)$—where $Z_> = N_> = \max(Z,N)$ [24]—with calculations. (We have followed [14] where, out of 78 values, those involving proton-unbound states are discarded.) In the next paragraphs we define one by one the ingredients and then examine their effect column by column in Table I.

The Coulomb potential V_C will be written in an oscillator representation. To conform to standard use we introduce $R_\pi = (5/3)^{1/2}\rho_\pi$. One of the many advantages of the oscillator basis is that one can separate trivially an adimensional two-body $\widehat{(1/r)}$ operator through the first equality below:

$$V_C = e^2 \sqrt{\frac{M\omega_\pi}{\hbar}} \widehat{\left(\frac{1}{r}\right)} = \frac{1.934}{R_\pi} Z^{1/6} \widehat{\left(\frac{1}{r}\right)} \text{MeV}. \quad (4)$$

The second equality provides the connection between CDE and radii. It follows from a famous estimate ([15], Eq. (2-157)), which we apply separately to neutrons and protons (MeV units):

$$\frac{\hbar\omega_\pi}{(2Z)^{1/3}} = \frac{35.59}{\langle r^2_\pi \rangle}; \quad \frac{\hbar\omega_\nu}{(2N)^{1/3}} = \frac{35.59}{\langle r^2_\nu \rangle}. \quad (5)$$

The $\widehat{(1/r)}$ operator will be evaluated in detail later, and it will be shown that Eq. (4) leads to a "smooth average of the diagonal monopole part,"

$$\langle V^d_{Cm} \rangle \approx \frac{0.864(Z(Z-1)-Z)}{R^c_\pi} \text{ MeV}, \quad (6)$$

identical—within a small exchange term—to the classical expression for the charged sphere. [R^c_π is the charge, not the point radius, as explained after Eq. (12).]

The column labeled $\langle V^d_{Cm} \rangle$ in Table I gives the rms deviations when only this term is included. The preferred value is at $\zeta \leqslant 0.6$.

The Bethe Weizsäcker form for the charge symmetry breaking (CSB) potentials is

$$V_B = -\frac{t}{2}\left[B_\nu - B_s\left(\frac{A_0}{A}\right)^{1/3} \right]\text{keV}. \quad (7)$$

The parameters B_ν and B_s *cannot* be chosen arbitrarily. They are not known experimentally, but enormous theoretical work has been devoted to CSB potentials, extensively described in Ref. [16], from which we take the V_B contribution to be ≈ 100 keV around $A = 16$, and ≈ 300 keV in nuclear matter. Accordingly, we set $A_0 = 16$ and define a standard V^{st}_B at $B_\nu = 300$ keV and $B_s = 200$ keV. Calling $V^{st} = V^d_{Cm} + V^{st}_B$, the corresponding column shows that the preferred value moves to $\zeta = 0.8$, with a slight gain in rmsd.

In the last three columns B_ν and B_s are allowed to vary simultaneously to give an idea of the range of plausible V_B parameters. (Note the advantage of introducing A_0 in Eq. (7): $B_\nu - B_s$ equals the contribution at $A = 16$.) The constancy of the rmsd indicates the absolute need of constraints on V_B. Conversely, the rapid variation of V_B constrains the skin to a narrow range of plausible values for B_ν and B_s. We propose [25] $\Delta_{r_{\nu\pi}} = 0.80(5)\ t/A$, (nearly) compatible with Eq. (1) [26] and (perfectly) compatible with the estimate for ^{208}Pb in [9].

The results depend on the validity of Eq. (2) which was derived assuming isospin purity for the wave functions. The assumption is likely to hold near stability, but approaching the proton drip line it becomes more questionable. This is why we followed Ref. [14] in rejecting data from 15 pairs with proton-unbound $Z_>$. If they are reincorporated, the numbers are telling: the preferred ζ moves slightly up at 0.85 but the rmsd doubles at 254 keV. Some of the rejected pairs do fairly well, but for eight of them the error is above 500 keV. (In the restricted sample no error is larger than 300 keV.) These findings are consistent with good T near stability and deteriorating away from it. At stability, the $T \approx 0$ nuclei raise the problem of a negative skin, small for $A \lesssim 60$ and quickly dissappearing as T increases (see for example [17]). Our calculation should detect it as a slight deterioration for $T = 1/2$ with respect to $T = 3/2$ or higher. If anything, what is seen is the opposite. This observation does not contradict the results of Ref. [17]; it simply suggests that the hitherto neglected shell effects are stronger than those induced by T violation.

Let us examine now the smooth forms we have introduced. The radii enter only through the oscillator frequencies in Eq. (5), which define the basis in which we should work.
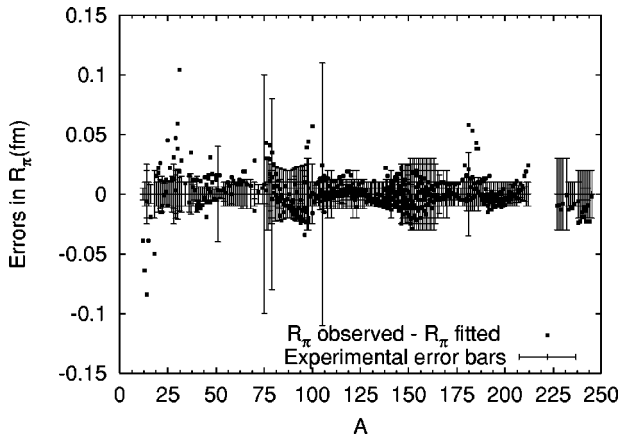
FIG. 2. Comparison between experimental errors and differences between observed and calculated radii $R_\pi = (5/3)^{1/2}\rho_\pi$ ($\zeta = 0.8$, undistinguishable from other choices).

For magic nuclei the basis reduces to a single state, and the observed radii can be assumed to be given by ρ_π. When moving away from closed shells, configuration mixing will increase the size of the system: moderately for nearly spherical nuclei, and radically for deformed ones. The crucial point is that *ρ_π is not supposed to produce good radii, but a good basis*. To check whether this is the case we propose the following test: Try to fit all the available data through a shell corrected radius $\rho_\pi^{sc} = \rho_\pi + \mathcal{D}$, fixing ρ_π to the values we have obtained. The test is passed if the fit is good and nothing is gained by refitting ρ_π.

The definition of $\mathcal{D}$ is suggested by previous work on shell corrections [12,18,19]. We have

$$\rho_\pi^{sc} = \rho_\pi + \mathcal{D}, \quad \mathcal{D} = \lambda S_\pi S_\nu + \mu Q_\pi Q_\nu. \quad (8)$$

S stands for spherical, Q for deformed. The correction $\mathcal{D}$ is a functional of the orbital occupancies in the EI (extruder-intruder) valence spaces. They consist in the orbits of harmonic oscillator shell p, except the largest (extruder), plus the largest (intruder) orbit from shell $p + 1$. For protons, say, the EI degeneracy is $D_\pi = (p_\pi + 1)(p_\pi + 2) + 2$ (e.g., $p_\pi = 3$ between $Z = 28$ and $Z = 50$). The degeneracy of the non-intruder orbits is $D_{r\pi} = p_\pi(p_\pi + 1)$. Now call z the number of valence protons, and define $S_\pi = z(D_\pi - z)/D_\pi^2$, $Q_\pi = z(D_{r\pi} - z)/D_\pi^2$; and similarly for neutrons. By construction, $\mathcal{D}$ vanishes at the EI closures.

Fits of ρ_π^{sc} to 634 experimental values keeping the parameters previously obtained for ρ_π—variation leaves them unchanged—lead again to remarkable results: with $\lambda = 5.6(2)$, $\mu = 23(1)$ we obtain rmsd $\leqslant 11$ mf in all cases. Figure 2 gives an idea of the quality of the results: most of the calculated points fall within (or very close to) the experimental error bars. The exceptions are the light nuclei (where halo orbits are important), and the region around the light Pt isotopes known for shape coexistence in the ground states. The test is passed: ρ_π makes sense. It should be noted that a fit of Eq. (2) to all nuclei makes little sense.

The Bethe Weiszäker form for V_B is obvious.

The Coulomb potential is a different matter. The quality and credibility of our approach rests on an *exact* treatment of V_{Cm}^d.

Following Ref. [20] we separate the Hamiltonian $H = H_m + H_M$. The monopole part H_m contains all terms in scalar products of fermion operators $(a_r^+ \cdot a_s)$ for subshells r and s. We consider the *diagonal* part involving the number operators $m_r = a_r^+ \cdot a_r$. The nondiagonal one—responsible for isospin impurities—will be ignored, as will the multipole H_M which contributes to shell effects [18,20–23].

Calling $V_{iki'k'}$ the matrix elements of $\widehat{1/r}$, the diagonal monopole part is

$$\left(\widehat{\frac{1}{r}}\right)_m^d = \sum_{i \leqslant k} \frac{z_i(z_k - \delta_{ik})}{1 + \delta_{ik}} V_{ik}, \quad V_{ik} = \frac{\sum_J V_{ikik}^J[J]}{\sum_J [J]}, \quad (9)$$

$[J] = 2J + 1$, $z_k =$ number of protons in orbit k, where $k \equiv plj$ stands for the quantum numbers specifying a given harmonic oscillator (ho) orbit (p is the principal quantum number). The sum over the first κ major shells containing τ orbits can be reduced to a sum of factorable terms by diagonalizing the matrix $\frac{1}{2}\{V_{ik}\}$. This technique is extensively described in [20]. As the highest eigenvalue E_τ overwhelms all others, when combined with the corresponding eigenvector U_k and the single particle counter term in Eq. (9) it determines the largest contribution by far (z_k is the number operator for orbit k):

$$\left(\widehat{\frac{1}{r}}\right)_m^d = \frac{1}{2}\left[E_\tau\left(\sum_k z_k U_k\right)^2 - \sum_k z_k V_{kk}\right], \quad (10)$$

which amounts to a basically exact representation in Fock space: E_τ is 30 times bigger than the second biggest eigenvalue, and 100 times bigger than the third. Furthermore—as we shall see—U_k leads to an extremely coherent operator, while the other eigenvectors do not. We have treated the $\kappa = 8$, $\tau = 36$ case, but the results are independent of the number of orbits.

Figure 3 shows the forms of U_k and $V_{kk} \equiv V_k$. To deal with quantities of order 1, we have rescaled $U_k \Rightarrow \sqrt{(\tau} U_k$ and accordingly $E_\tau \Rightarrow \tau E_\tau = 0.383$. The $(2j + 1)$-weighted averages over j orbits within a major shell p are also shown (U_p and V_p). By referring the $l(l + 1)$ term to its centroid we have to good approximation

$$U_k = U_p - 0.01[l(l + 1) - p(p + 3)/2]/(p + 3/2). \quad (11)$$

For V_k the j dependence is more complicated. To leading order in a $(p + x)^{-y}$ expansion the averages are $U_p \approx 1.522(p + 1.4)^{-1/4}$, and $V_p \approx 0.93(p + 3/2)^{-1/2}$.

To extract a smooth form, we fit separately the two terms of Eq. (10) at the p closures (i.e., replacing the sum over k by a sum over p, with $z_k \equiv (p + 1)(p + 2) = D_p$, $U_k \equiv U_p$, and $V_k \equiv V_p$) to forms $a(Z - b)^c$. Exact values for U_p, and V_p are kept. Then we insert the factor in Eq. (4), to obtain (MeV units)

$$\langle V_{Cm}^d \rangle \approx \frac{0.858 Z^{1/6}[(Z - 1/2)^{2 - 1/6} - Z^{1 - 1/6}]}{R_\pi}. \quad (12)$$
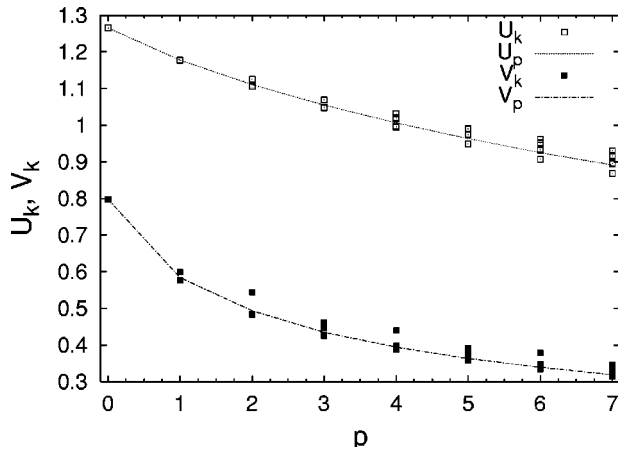
FIG. 3. The terms in Eq. (10). See text.

The numerical uncertainties of the fit ($\approx 0.1\%$) allow the choice of the round numbers shown. This is the form used in the calculations. For clarity, in Eq. (6) it has been very slightly (and innocuously) simplified and the point radius parameter $R_0 = \sqrt{5/3}\rho_0 = 1.219$ replaced by its charged value $R_0^c = 1.226$, so as to change the overall coefficient, which becomes the one for the classical charged sphere: $3e^2 Z^2/5R^c \approx 0.864 Z^2/R^c \approx 0.7 Z^2/A^{1/3}$. A pleasing result.

The form of averaging we have used eliminates all shell effects, which show cleanly in the first panel of Fig. 4 the difference between experimental and calculated values. For clarity only $t = 1$ and 2 cases are kept. They are sufficient to indicate the secular nature of the deviations.

Smooth filling can be replaced by *orderly* filling, which, using exact values for U_k and V_k in Eq. (10), should be close to a Hartree Fock (HF) result, since Coulomb matrix elements are quite unsensitive to details of the single particle wave functions, except in the case of halo orbits.

The difference between smooth and HF approximations is mostly due to the $l(l+1)$ term in Eq. (11), whose influence can be understood by noting that above a closed shell with $Z = Z_{cs}$ it produces a single particle field

$$\varepsilon_{Cl} = \frac{-4.5 Z_{cs}^{13/12}[2l(l+1) - p(p+3)]}{A^{1/3}(p + 3/2)} \text{ keV}, \quad (13)$$

obtained from Eqs. (4) and (10), using $E_\tau = 0.383$, and the coefficient in $U_p \approx 1.522(p+1.4)^{-1/4}$, mentioned after Eq. (10).
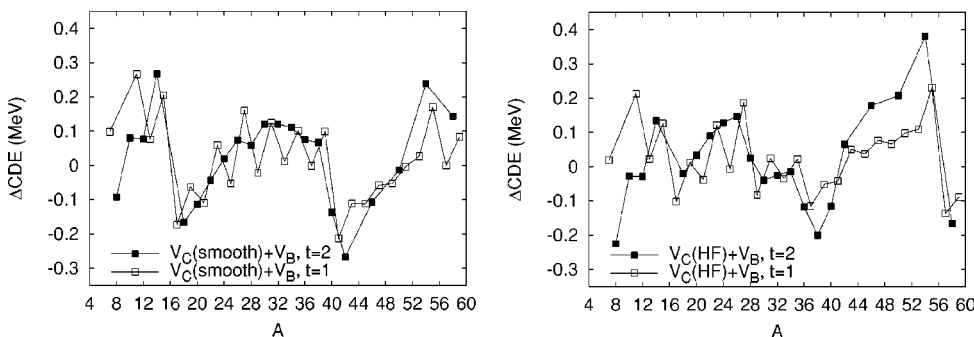
The HF displacements in the second panel of Fig. 4 indicate that the $l(l+1)$ effect leads to a dramatic improvement for the $A = 15$–17 and $A = 39$–41 pairs, the two test cases most extensively studied in the literature ([10,16,22] and references therein). This gain is upset by a loss of regularity in the shell-effect patterns and the (apparent) need for a too strong V_B. If we keep V_B^{st} (and $\zeta = 0.8$) the rmsd becomes large (330 keV). The figure corresponds to a fit (rmsd = 150 keV) that leads to a huge change in V_B, at $B_v - B_s = 425 - 180 = 245$ keV.

The situation is in all respects similar to that in Ref. [14], where a full HF description with the SKXcsb force also demands a too large V_B contribution (355 keV at $A = 17$). The agreement between ([14] bottom Fig. 2c), and the second panel of Fig. 4 is quite good, to within an overall shift of some 100 keV for the latter [27]. A convincing indication that our approximation to a full HF result is sound. However, it casts doubts on the very use of the HF approach: Near closed shells it is likely to be valid, and the improvement it brings about is very beneficial. Elsewhere, HF produces misleading patterns through shell effects that should be treated in conjunction with those of multipole and CSB origin. Unless this is done, it is clearly better to keep the smooth approximation.

To conclude, we examine what can be said about the Nolen Schiffer anomaly (NSA), which we define as a systematic failure to obtain good CDE without *ad hoc* adjustable parameters. The historical origin of the problem is clear from column V_{Cm}^d in Table I, showing that the Coulomb potential leads to large discrepancies for acceptable values of the neutron skin [28]. It is also clear that the V_B potentials though small (of the order of the Coulomb exchange), are crucial in moving the skin to a reasonable range. As a consequence, the remaining discrepancies are the shell effects in the left panel of Fig. 4.

As we have seen, for the classical test cases—at $A = 15$, 17 and $A = 39$, 41—the $l(l+1)$ term reduces the errors (to some 100 keV for the former and 50 keV for the latter). To achieve greater precision, good quality shell model calculations are necessary, a difficult task, not undertaken so far for the CDE. Therefore, at present, we cannot decide whether there subsists an anomaly or not.

However, for nuclei with several particles in a major shell, high quality configuration mixing is possible, and the task has been undertaken, not for the CDE, but for the differences in excitation energies between mirror yrast bands (CED or MED) [23]: Shell effects play a major role, and the CSB contribution is at least as important as the Coulomb

FIG. 4. Left panel: Experimental-calculated CDE for $t = 1$ and 2 with smooth occupancies ($\zeta = 0.8$). Right panel: As above for Hartree Fock occupancies.

one. The results achieve an accuracy of ≈ 10 keV on differences of up to 100 keV. This is the order of magnitude of the discrepancies we want to correct. Furthermore, the CDE are unlikely to demand better control of the wave functions and the interactions than the MED do. As a consequence—though we cannot decide whether there remains a problem

until the CDE calculations are done—a fairly safe bet is that the Nolen Schiffer anomaly will disappear.

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[24] We shall use throughout $Z_>$ ($Z_<$) for ''the proton (neutron) excess mirror partner.''

[25] The error bars are probably too large. R. Machleidt considers $B_v = 300$ keV to be an upper limit (private communication).

[26] It is often argued that measures are model dependent and sensitive to an ''interaction'' radius rather than to $\Delta_{r_{\nu\pi}}$ proper. Our answer to this objection is threefold. (A) We are unaware of estimates indicating that uncertainties are larger than the—large—quoted errors. (B) If anything, the effect would lead to smaller $\Delta_{r_{\nu\pi}}$, as our calculations do indeed. (C) We compare with experimental results but make no use whatsoever of them.

[27] In ([14], bottom Fig. 2c), crosses and squares should be interchanged. Then it only takes good eyes to check the agreement.

[28] This description of the NSA is compact and accurate but nonstandard. In the late 1970's some experiments appeared to be consistent with vanishing neutron skin, and it was pointed out that under this assumption the NSA would disappear [S. Shlomo and E. Friedman, Phys. Rev. Lett. **39**, 1180 (1977)]. After this proposal turned out to be unrealistic, little emphasis was put on the strong correlation between CDE and neutron skin, with few exceptions (such as [7]).