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Shell corrections to a liquid-drop description of nuclear masses and radii

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Abstract. It is shown that a consistent treatment of nuclear bulk and surface effects leads to an improved version of the liquid-drop mass formula with modified symmetry and Coulomb terms. If in addition shell effects are modelled through the counting of the number of valence nucleons, a very simple mass formula is obtained with an rms deviation from the 2003 database of atomic masses of about 800 keV. As an application, the volume and surface symmetry energy for $A \to \infty$ are determined. A similar description of nuclear radii is suggested with specific reference to the neutron skin.

PACS. 21.10.Dr Binding energies and masses – 21.10.Ft Charge distribution – 21.10.Gv Nucleon distributions and halo features

1 Introduction

The systematics of binding energies and radii of nuclei can be addressed straightforwardly in terms of the liquid-drop model (LDM). This approach provides valuable information on global properties of nuclei and one can get a handle on separate parts of the nuclear interaction, such as the surface, pairing, or symmetry energies. In many cases it is of interest to extrapolate either to exotic nuclei that can be studied with radioactive beams or to infinite nuclear (neutron) matter. This requires an accurate treatment of corrections to the standard liquid-drop approach, most notably shell effects.

The information thus obtained can be applied in related fields, *e.g.*, the symmetry energy plays a crucial role in the equation of state of neutron stars, and charge and neutron radii are needed as an input to interprete the results of atomic parity violation experiments.

Several complementary approaches exist to calculate masses and radii of nuclei [1]. Fully microscopic approaches starting from first principles require many-body approximations, based in general on the notion of a mean field and in particular on Hartree-Fock-Bogolyubov (HFB). This method exists in different versions, the latest of which is reported in ref. [2]. In a second class of models the nucleus is viewed as a liquid drop to which shell and deformation corrections are applied. This was first proposed by Myers and Swiatecki [3] and subsequently evolved into a global macroscopic-microscopic model leading to the finite-range liquid-drop model (FRLDM) [4]. The third type of approach, based on the shell model and developed by Duflo and Zuker [5–7], yields the most accurate results in terms of root-mean-square deviation from the measured nuclear masses. Of course, hybrid methods have been developed such as, for example, in refs. [8,9].

Although all these approaches certainly have merits, they also have drawbacks for the particular phenomenon we wish to point out here, namely the existence of correlations between shell corrections in nuclear masses and radii. This requires reasonably accurate mass and radius formulas with a well-defined macroscopic part to which a simple shell correction is applied. In HFB there is no clear separation between macroscopic and microscopic parts while FRLDM requires rather complicated shell corrections. The approach followed in this paper is closest to the one of Duflo and Zuker [5–7] but care is taken to retain only the most important shell corrections which therefore remain of a rather simple character. In addition, for the macroscopic part the more recent refined approach of Danielewicz [10] is followed which separates bulk and surface effects explicitly and consistently. Note that in ref. [10] shell effects, which are crucial to our analysis, have not been included.

One would expect that certain correlations exist between the ways in which masses and radii vary with N and Z. For example, it has been pointed out that there is a strong correlation between the size of the neutron skin and the (surface) symmetry energy. Also, closed-shell

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nuclei are more strongly bound and have a smaller radius than their neighbors. Deformation will in general increase the binding energy as well as the radius when compared to the spherical case. Therefore it seems of interest to investigate whether the prescriptions for including shell effects in masses can also be used to improve the description of radii.

In this paper the starting point is a generalized liquid-drop approach, in which bulk and surface effects are treated consistently. We consider simple shell corrections both for masses and radii based upon counting the number of valence nucleons. As an application the volume and surface symmetry energy for nuclear matter are determined. Using the latter, neutron skins for heavy nuclei are predicted in terms of empirical isovector separation energies and of the surface symmetry energy.

The content of this paper is as follows. In sect. 2 various terms which are present in the modified LDM are reviewed, namely the symmetry and Coulomb energies, and shell corrections are introduced. As illustrations two-nucleon separation energies are displayed and the extraction of the volume and surface symmetry energy is discussed. In sect. 3 the charge and neutron radii in the modified LDM are addressed in terms of the parameters of the symmetry energy, and shell corrections are discussed; as an application results for isotope shifts and for the neutron skin of heavy isotopes are presented. Section 4 contains a summary and concluding remarks.

2 Masses

Our starting point is a generalized LDM mass formula which includes a systematic separation of volume (v) and surface (s) effects. The general philosophy [10,11] is to separate the neutrons and protons into two sets each, pertaining to the volume and surface of the nucleus, respectively. In this way the binding energy of the nucleus in principle depends on the separate numbers N_v, N_s, Z_v and Z_s (neutrons and protons, in the volume and at the surface, respectively). This binding energy is maximized under constraint of constant neutron and proton numbers $N_\mathrm{v}+N_\mathrm{s}=N$ and $Z_\mathrm{v}+Z_\mathrm{s}=Z$, plus an additional condition that will be discussed below. As we will see, this procedure yields a modified LDM mass formula with an N, Z-dependence that is different from the standard Weizsäcker formula. We begin with the discussion of the symmetry energy for which the procedure is simplest.

2.1 Symmetry energy

Following Danielewicz [10], the symmetry energy takes the form

$$E_\mathrm{S}=-a_\mathrm{v}A+S_\mathrm{v}\frac{(N_\mathrm{v}-Z_\mathrm{v})^2}{A}+a_\mathrm{s}A^{2/3}+S_\mathrm{s}\frac{(N_\mathrm{s}-Z_\mathrm{s})^2}{A^{2/3}}\,, \tag{1}$$

where the first (last) two terms refer to the volume (surface) contributions. Since the differences $\delta_\mathrm{v}\equiv N_\mathrm{v}-Z_\mathrm{v}$ and $\delta_\mathrm{s}\equiv N_\mathrm{s}-Z_\mathrm{s}$ are related through $\delta_\mathrm{v}+\delta_\mathrm{s}=\delta\equiv N-Z$, the symmetry energy E_S depends, under constant N and Z, on a single combination which can be chosen as δ_s. The minimization of E_S with respect to δ_s,

$$\frac{\partial E_\mathrm{S}}{\partial\delta_\mathrm{s}}=0, \tag{2}$$

leads to the condition

$$\frac{\delta_\mathrm{v}}{\delta}=\frac{1}{1+yA^{-1/3}}\,,\qquad\frac{\delta_\mathrm{s}}{\delta}=\frac{yA^{-1/3}}{1+yA^{-1/3}}\,, \tag{3}$$

where the notation $y\equiv S_\mathrm{v}/S_\mathrm{s}$ is introduced. Insertion of these conditions into the expression (1) leads to

$$E_\mathrm{S}=-a_\mathrm{v}A+a_\mathrm{s}A^{2/3}+S_\mathrm{v}\frac{(N-Z)^2}{A(1+yA^{-1/3})}\,. \tag{4}$$

Note that this result is exact and independent of any additional constraint on $\{N_\mathrm{v},N_\mathrm{s},Z_\mathrm{v},Z_\mathrm{s}\}$ besides $N_\mathrm{v}+N_\mathrm{s}=N$ and $Z_\mathrm{v}+Z_\mathrm{s}=Z$. This no longer is the case if in addition the Coulomb energy is considered as is shown in the next subsection.

2.2 Coulomb energy

From elementary considerations the Coulomb energy of a volume-plus-surface system can be evaluated as [10]

$$\begin{aligned}E_\mathrm{C}&=\frac{a_\mathrm{c}}{A^{1/3}}\left(Z_\mathrm{v}^2+\frac{5}{3}Z_\mathrm{v}Z_\mathrm{s}+\frac{5}{6}Z_\mathrm{s}^2\right)\\&=\frac{a_\mathrm{c}}{A^{1/3}}\left(\frac{1}{6}Z_\mathrm{v}^2+\frac{5}{6}Z^2\right),\end{aligned} \tag{5}$$

comprising a volume-volume, volume-surface, and surface-surface interaction. As before, the total energy $E_\mathrm{S}+E_\mathrm{C}$ should be minimized in the space $\{N_\mathrm{v},N_\mathrm{s},Z_\mathrm{v},Z_\mathrm{s}\}$ under the constraint of constant N and Z. If no additional constraint is imposed, this procedure leads to an unphysical result, namely all protons migrate to the surface ($Z_\mathrm{s}=Z$) leaving the volume exclusively to the neutrons. This condition is compatible with the one obtained from the minimization of E_S, eq. (3), as it is entirely decoupled from it.

We follow here the prescription of Danielewicz [10] who imposes the so-called "leptodermic" constraint $N_\mathrm{s}+Z_\mathrm{s}=0$. It should be emphasized, however, that alternative constraints are possible [11] and that further studies are needed to explore them. The minimization

$$\frac{\partial}{\partial\delta_\mathrm{s}}\left(E_\mathrm{S}+E_\mathrm{C}\right)=0, \tag{6}$$

under the constraint $N_\mathrm{s}+Z_\mathrm{s}=0$ leads to the conditions

$$\frac{\delta_\mathrm{v}}{\delta}=\frac{1+xA^{4/3}/\delta}{1+yA^{-1/3}+xA^{1/3}}\,,\qquad\frac{\delta_\mathrm{s}}{\delta}=\frac{yA^{-1/3}-2xA^{1/3}Z/\delta}{1+yA^{-1/3}+xA^{1/3}}\,, \tag{7}$$

with $x \equiv a_c/24S_s$. Insertion of these conditions into $E_S + E_C$ leads to a complicated expression which for $x \ll 1$ can be simplified to

$$E_S + E_C = -a_v A + a_s A^{2/3} + S_v \frac{(N-Z)^2}{A(1+yA^{-1/3})} + \frac{a_c Z^2}{A^{1/3}} \left(1 + \frac{N-Z}{6Z(1+y^{-1}A^{1/3})}\right). \quad (8)$$

2.3 Modified liquid-drop model

The results of the preceding subsections can be combined into the following modified LDM mass formula for the (negative) nuclear interaction energy:

$$E_{\rm LDM}(N,Z) = -a_v A + a_s A^{2/3} + S_v \frac{4T(T+1)}{A(1+yA^{-1/3})} + a_c \frac{Z(Z-1)}{(1-\Lambda)A^{1/3}} - a_p \frac{\Delta(N,Z)}{A^{1/3}}. \quad (9)$$

Concerning the pairing interaction, empirically one finds a scaling of the pairing with mass number as A^γ with γ between -0.4 and -0.5, the exact value depending whether/which shell corrections are considered. However, in all cases the dependence on γ is very shallow and $\gamma = -1/3$ gives essentially the same rms deviation. We have taken the latter since shell model calculations suggest that this is the appropriate mass dependence of the nucleon-nucleon interaction. Note also that we have taken $\Delta = 2$, 1, and 0 for even-even, odd-mass and odd-odd nuclei, respectively, whereas usually $\Delta = 1$, 0, and -1 is taken. Again, no significant difference in rms is found between the two choices but we prefer the former since it fits naturally with the idea of a strong attractive interaction between two identical nucleons coupled to spin 0^+ and essentially no interaction when they are coupled to other angular momenta.

Furthermore, in the modification Λ in the Coulomb term we include in addition to the surface asymmetry from eq. (8) a surface diffuseness correction, *i.e.*,

$$\Lambda \equiv \frac{N-Z}{6Z(1+y^{-1}A^{1/3})} - \frac{5\pi^2}{6}\frac{d^2}{r_0^2 A^{2/3}}. \quad (10)$$

It has been introduced in the denominator of the Coulomb term, suggesting that it can be viewed as a correction to the radius of the nucleus. Note also the replacement of $(N-Z)^2$ by $4T(T+1)$ to account for the Wigner energy, and of Z^2 by $Z(Z-1)$ to eliminate the Coulomb interaction of a proton with itself.

2.4 Shell corrections

A fit of the LDM mass formula (9) to the 2149 nuclei with $N, Z \geq 8$ in the compilation of Audi *et al.* [12] leads to a root-mean-square (rms) deviation of 2.39 MeV. The bulk of this deviation is due to the neglect of shell effects in the LDM mass formula. In the literature many different ways of implementing shell corrections to the LDM can be found; in general, these methods are rather laborious. A simple method was proposed in refs. [13,14] based on counting the number of valence nucleons, as suggested by the interacting boson model (IBM) [15]. This "shell" correction is linear and quadratic in the total number of valence nucleons,

$$E'_{\rm shell}(N,Z) = b_1(n_v + z_v) + b_2(n_v + z_v)^2, \quad (11)$$

where n_v and z_v are the numbers of valence neutrons and protons (particle- or hole-like, following the counting rule of the IBM) and b_i are parameters. Inclusion of these two terms in the LDM mass formula (9) reduces the rms deviation from 2.39 to 1.05 MeV.

Although simple and successful, refinements of the correction (11) are needed, in particular to cure its discontinuity at mid-shell (see also ref. [16]). An upgraded version of the terms (11) is suggested by the microscopic mass formula of Duflo and Zuker [5–7]:

$$E_{\rm shell}(N,Z) = a_1 S_2 + a_2 (S_2)^2 + a_3 S_3 + a_{np} S_{np}, \quad (12)$$

where

$$S_2 = \frac{n_v \bar{n}_v}{D_n} + \frac{z_v \bar{z}_v}{D_z},$$
$$S_3 = \frac{n_v \bar{n}_v (n_v - \bar{n}_v)}{D_n} + \frac{z_v \bar{z}_v (z_v - \bar{z}_v)}{D_z},$$
$$S_{np} = \frac{n_v \bar{n}_v z_v \bar{z}_v}{D_n D_z}, \quad (13)$$

with $\bar{n}_v \equiv D_n - n_v$ and $\bar{z}_v \equiv D_z - z_v$ where D_n (D_z) is the degeneracy of the neutron (proton) valence shell, *e.g.*, $D = 32$ for the 50–82 shell.

The dependence on the valence particle number and on the shell size of the various terms (13) is suggested by seniority reduction formula in the shell model [17]. The form of the S_2 term is reminiscent of the energy dependence of the pairing interaction for a seniority-zero state, $E(n) = Gn(D-n+2)$ [17]; however, a realistic pairing force is attractive ($G < 0$), whereas use of S_2 leads to a repulsive correction to the LDM energy. The attraction comes from the $(S_2)^2$ term. The S_3 term (also referred to as a "monopole drift" [6]) changes sign at mid-shell and thus introduces an asymmetry between particles and holes.

The use of the shell correction (12) leads to a reduction of the rms deviation to 0.84 MeV, to be compared, *e.g.*, with 0.65 MeV for the much more sophisticated microscopic model of Koura *et al.* [8] and about 0.60 MeV for the mass formula of Royer [9]. The following values are obtained for the parameters: those in the LDM mass formula (9) are $a_v = 15.78$, $a_s = 18.56$, $S_v = 31.51$, $y = 2.75$, $a_p = 5.4$ and $a_c = 0.71$, while those for the shell corrections (defined with magic numbers 2, 8, 14, 28, 50, 82, 126, and 184) are $a_1 = -1.39$, $a_2 = 0.020$, $a_3 = 0.003$ and $a_{np} = 0.075$, all in MeV except y which is dimensionless.

More accurate shell corrections can be applied to the LDM mass formula but the terms (13) suffice for the present purpose of establishing a correlation between masses and radii. One additional effect could be of importance for this correlation, namely deformation. Duflo and Zuker [7] parametrize its effect (somewhat *ad hoc*) by adding a term S_{def} which is identical to (12) but with n replaced by $n-4$ to simulate the occupation of high-spin intruder orbitals in the Nilsson model. In the present work the effect of deformation, which can be of the order of one MeV or more, is effectively included through the presence of the neutron-proton term S_{np} at the r.h.s. of eq. (13). The latter is reminiscent (for small n/D) of the so-called "promiscuity" term [18].

It is worth noting that there are large differences between the shell correction energy in the various approaches. For example, in ref. [8] this energy ranges from -15 MeV (closed-shell nuclei) to $+3$ MeV (mid-shell). Also in ref. [9] shell effects are large and attractive for closed-shell nuclei, whereas in the present approach they range between 0 (closed-shell) to 11 MeV (mid-shell). Although these differences might appear large, they mainly concern the definition of the *offset* of the liquid-drop mass formula, which can be adjusted to the average of all nuclei, or only to closed-shell nuclei, or only to mid-shell nuclei. These differences should be taken into account when making the extrapolation $A \to \infty$ to infinite nuclear matter.

We wish to point out that there is a freedom in the choice of the offset of shell corrections in mass calculations. However, in this work we apply the shell corrections also to radii in the LDM; in describing radii it is common practice to describe spherical closed-shell nuclei in terms of a mean field and add deformation and other shell effects as corrections. Therefore for consistency reasons we choose as an offset for masses also closed-shell nuclei.

2.5 Two-nucleon separation energies

As an application of the LDM mass formula (9) plus shell correction (12), we show results for two-nucleon separation energies. Good insight in shell gaps and shell corrections is obtained by plotting the two-neutron separation energies $S_{2\mathrm{n}}$ *versus* the proton number Z and the two-proton separation energies $S_{2\mathrm{p}}$ *versus* the neutron number N (see figs. 1 and 2). Without shell corrections $S_{2\mathrm{p}}$ *versus* the N would give almost equidistant up-sloping curves (for fixed Z). The shell corrections lead to gaps at the proton magic numbers, with a width mainly determined by the strength of the term linear in S_2. However, closer inspection of the figures shows that, *e.g.*, the proton gap at $Z = 82$ is not constant but has a maximum width at the neutron magic number $N = 126$. Similar remarks apply for $S_{2\mathrm{n}}$.

Note that there are some remaining systematic deviations between experiment and theory, *e.g.*, at the $N = 126$ and $Z = 82$ shell closures. Also for very heavy nuclei a systematic discrepancy can be seen; however, that seems to be the case also in other studies based upon the LDM [9].

2.6 Symmetry energy revisited

Above we have obtained the volume and surface symmetry energies from a fit using the LDM mass formula plus shell corrections. Often more reliable results are achieved by isolating specific terms in a mass formula through the use of filters. To do this for the symmetry energy there are two possibilities: i) use experimental energies of isobaric analogue states (IAS) [19,20], or ii) use differences between neutron and proton separation energies (corrected for the Coulomb interaction). In the first approach there is no need to compute Coulomb corrections but in the second method a larger data base is available.

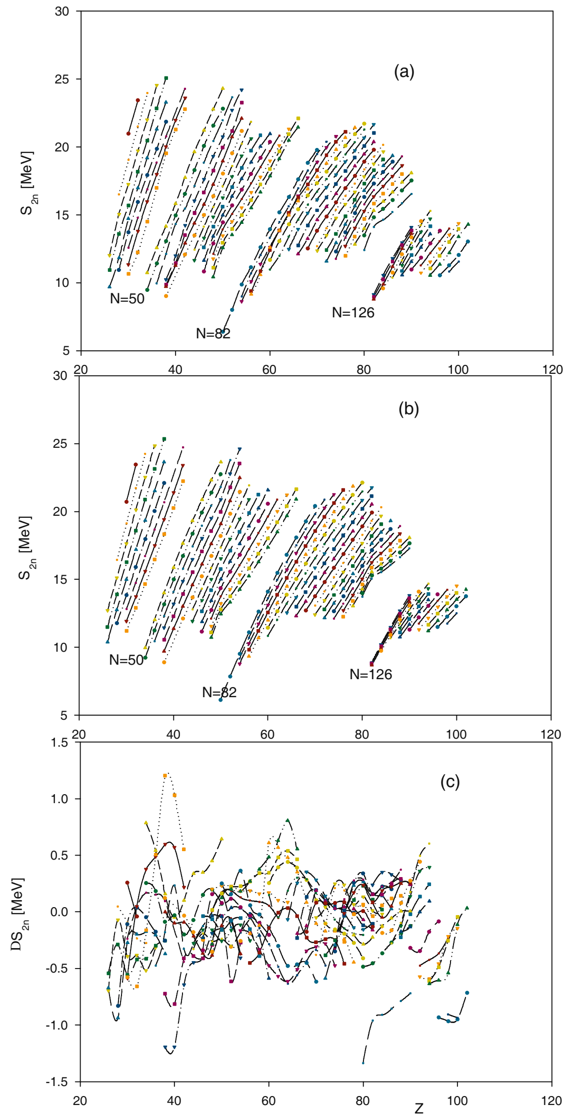

Fig. 1. (Color online) The two-neutron separation energies (in MeV) $S_{2\mathrm{n}}$ *versus* proton number Z: (a) experimental values, (b) calculated values from the LDM mass formula (9) plus the shell correction (12) and (c) differences. Nuclei with constant N (isotones) are connected.

We prefer here the approach ii) and define the isovector chemical potential $\mu_{\mathrm{a}} \equiv (\bar{S}_{\mathrm{n}} - \bar{S}_{\mathrm{p}})/2$ where the quantities $\bar{S}$ are nucleon separation energies, averaged to remove even-odd pairing effects,

$$\bar{S}_{\mathrm{n}} \equiv \frac{1}{2}(S_{\mathrm{n}}(N,Z) + S_{\mathrm{n}}(N-1,Z)),$$
$$\bar{S}_{\mathrm{p}} \equiv \frac{1}{2}(S_{\mathrm{p}}(N,Z) + S_{\mathrm{p}}(N,Z-1)), \qquad (14)$$

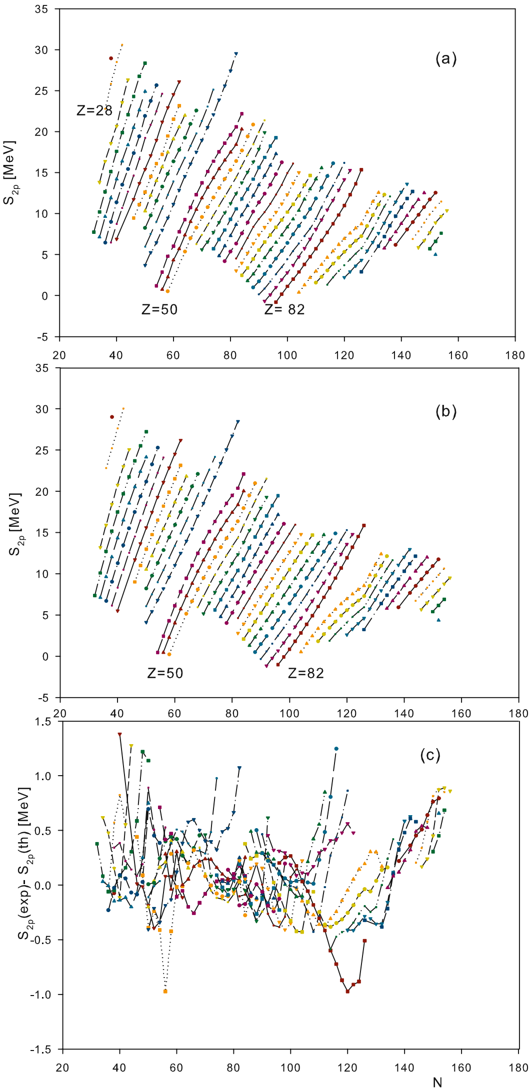

Fig. 2. (Color online) Same caption as fig. 1 but for two-proton separation energies S_{2p} plotted *versus* neutron number N. Nuclei with constant Z (isotopes) are connected.

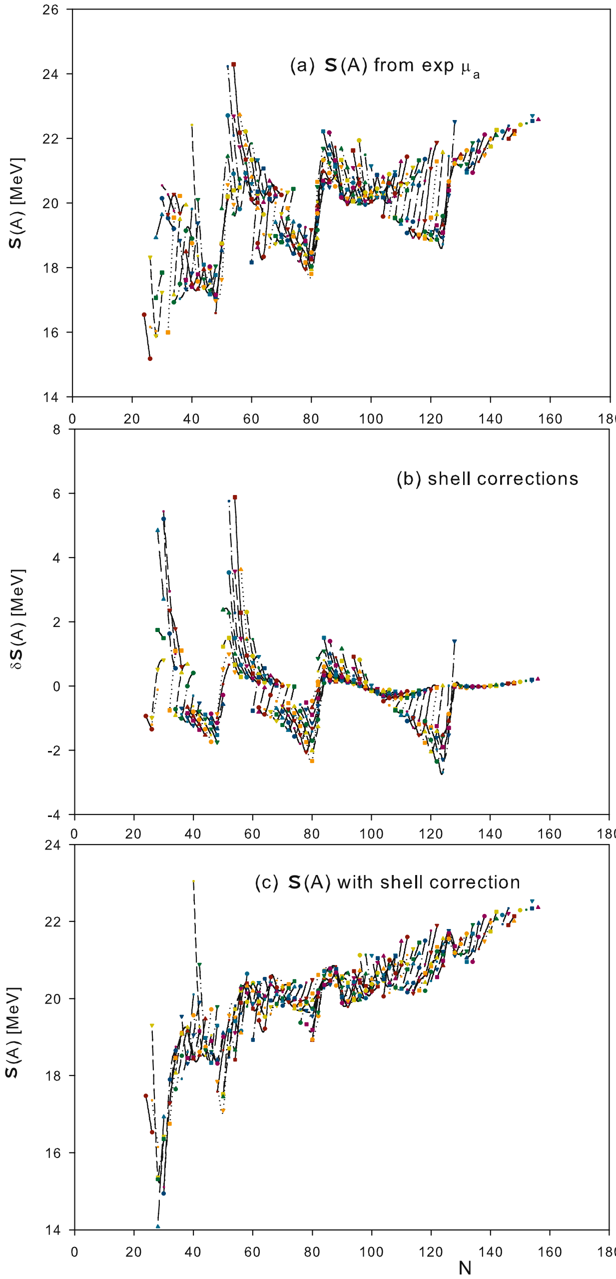

Fig. 3. (Color online) (a) The quantity $A(\mu_a + \delta E_C)/2(N - Z + 1)$ with μ_a taken from experiment. (b) The quantity $A\delta E_{\text{shell}}/2(N - Z + 1)$ with δE_{shell} calculated from the shell correction (12). (c) The difference between (a) and (b) corresponding to $\mathcal{S}(A)$ given in eq. (18). All plots are *versus* neutron number N. Nuclei with constant A (isobars) are connected.

with S_n and S_p the neutron and proton separation energies, *viz*

$$S_n \equiv B(N+1, Z) - B(N, Z),$$
$$S_p \equiv B(N, Z+1) - B(N, Z), \qquad (15)$$

in terms of the binding energies $B(N, Z) \equiv -E(N, Z)$. With the above definitions the isovector chemical potential can be written as a combination of four binding energies,

$$\mu_a = \frac{1}{4}(B(N+1, Z) - B(N-1, Z) - B(N, Z+1) + B(N, Z-1)), \qquad (16)$$

In terms of the parameters of the LDM mass formula this expression can be written as

$$\mu_a \approx \frac{2S_v}{1 + yA^{-1/3}} \frac{N - Z + 1}{A} - \delta E_C + \delta E_{\text{shell}}, \qquad (17)$$

where $\delta E_C \equiv a_c(Z - 1/2)/A^{1/3}$ and δE_{shell} is due to the shell corrections (12). A plot of the quantity $\mathcal{S}(A)^{-1}$ with

$$\mathcal{S}(A) \equiv (\mu_a + \delta E_C - \delta E_{\text{shell}}) \frac{A}{2(N - Z + 1)}, \qquad (18)$$

as a function of $A^{-1/3}$ should then yield a straight line with intercept $1/S_v$ and slope $1/S_s$.

To illustrate the importance of shell effects in this procedure, we plot in fig. 3 the quantity $\mathcal{S}(A)$ *without*

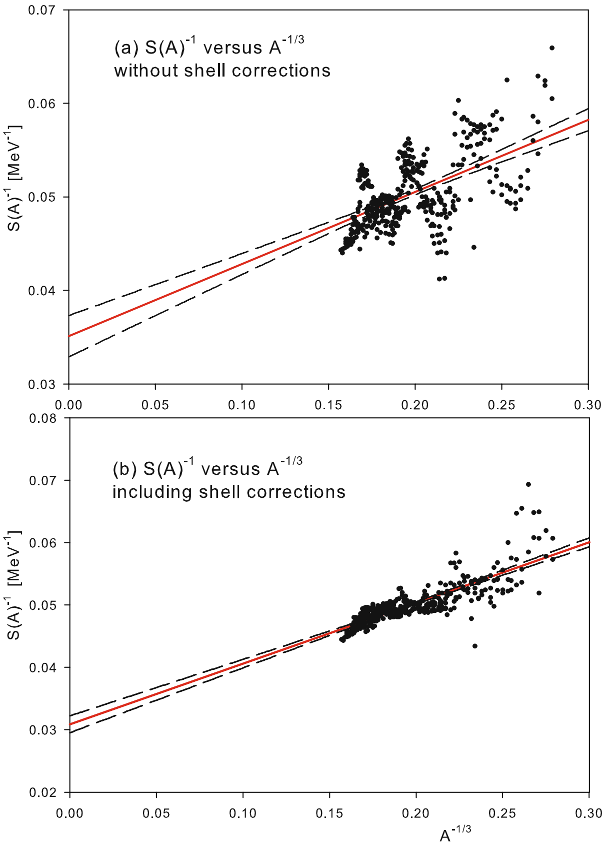

Fig. 4. (Color online) The inverse of $\mathcal{S}(A)$ given in eq. (18) as a function of $A^{-1/3}$ for all even-even nuclei. The red line represents the best fit and the dashed lines indicate the 95% confidence band.

the shell correction $\delta E_{\rm shell}$. Points that are connected represent isobaric nuclei and hence should be constant but for the correction $\delta E_{\rm shell}$. It is seen that shell corrections (mainly coming from the S_2 and $(S_2)^2$ terms) lead to up-sloping curves for neutron-hole/proton-particle situations (*e.g.*, N just below 126) or down-sloping for neutron-particle/proton-hole cases (*e.g.*, N just above 82), but have almost no effect in particle-particle (*e.g.*, $N > 126$, $Z > 82$) and hole-hole situations. They occur systematically and are qualitatively well reproduced by the terms (12). However, in magnitude shell effects seem somewhat underestimated. In particular, shell effects for particle-particle situations at $N > 126$ and $Z > 82$ appear to be too small. Also very heavy nuclei ($A > 240$) are not well reproduced, but that seems to be a common feature of mass formulas based on the LDM [9].

After correcting for shell effects one is able to deduce the symmetry energy in isolation from other LDM terms. The result is shown in fig. 4, where we compare for even-even nuclei with $N > Z$, the results of a linear fit to $\mathcal{S}(A)^{-1} = S_{\rm v}^{-1}(1+yA^{-1/3})$ without (a) and with (b) shell corrections. It is seen that inclusion of shell effects leads to an increase of the value of $S_{\rm v}$ and a reduction of the error band.

As best fit values we find $S_{\rm v} = 32.55\,\mathrm{MeV}$ and $y = 2.95$ to be compared with $S_{\rm v} = 31.51\,\mathrm{MeV}$ and $y = 2.75$ for the full LDM-mass fit (including shell corrections). Danielewicz and Lee [21] using experimental energies of isobaric analogue states and applying the shell corrections of Koura *et al.* [8] obtain a very similar result, $S_{\rm v} = 32.9\,\mathrm{MeV}$ and $y = 2.9$.

Note that the 1 in $N - Z + 1$ comes from the replacement of $(N-Z)^2$ by $4T(T+1)$. The Wigner term has the general form $T(T+r)$ with r a parameter. Without shell corrections this parameter is very poorly determined [14]; with shell corrections the minimum in r is less shallow and yields r close to 1. Values $r > 1$ were obtained by Jänecke and O'Donnell [22]. The present analysis shows the importance of shell effects in the extraction of the symmetry energy parameters and these were neglected in ref. [22].

3 Radii

In addition to binding energies, charge radii of nuclei provide valuable information on how ground-state properties of nuclei vary with N and Z. There also exists interest in precise predictions for charge and neutron distributions for specific applications, *e.g.*, they are needed as an input for the interpretation of experiments on atomic parity violation in heavy elements (large Z) [23]. Our aim here is to treat charge and mass radii in a similar fashion as masses, *i.e.*, in terms of a generalized LDM; in particular we use the parametrization of symmetry energy and of shell effects in sects. 2.1 and 2.4 to obtain results concerning neutron skins.

3.1 Charge radii

It has become clear that the simple parametrization $R = r_0 A^{1/3}$ provides only a very rough and qualitative description of charge radii. To obtain a quantitative description in a generalized LDM approach, one needs to take into account an isovector term $[\propto (N-Z)/A]$; furthermore it is necessary to include shell effects. In practice, the latter were mostly ascribed to deformation effects, and sometimes parametrized [5,24] in terms of the promiscuity term $P \equiv n_{\rm v} z_{\rm v}/(n_{\rm v}+z_{\rm v})$, where $n_{\rm v}$ ($z_{\rm v}$) represents the number of valence neutrons (protons).

Charge radii were considered in the context of microscopic mass formulas by Duflo and Zuker [5,25] and Royer [9]. In ref. [25] a good fit to charge radii of closed-shell nuclei was obtained with

$$R_{\rm p} = r_0 A^{1/3}\left(1 - v\frac{N-Z}{A^x} - w\frac{(N-Z)^2}{A^2}\right) e^{g/A}, \quad (19)$$

where v and w are parameters. The small correction $e^{g/A}$ (with $g \approx 1.04$) accounts for the larger radii of light nuclei, and x equals $4/3$ due to the "surface-skin" effect. For open-shell nuclei the inclusion of a shell correction was found to be necessary.

Assuming charge symmetry, we find it convenient to decompose the radius into an isoscalar part R_0 (representing the mass radius) and an isovector part R_1, which changes sign under the interchange of neutrons and protons. If one allows in addition for a small charge-symmetry–breaking Coulomb correction, the following parametrization results:

$$R_i(N,Z) = R_0(N,Z) \pm \frac{N-Z}{2A} R_1(N,Z) \pm \frac{1}{2}\delta R_{\mathrm{C}}(N,Z), \tag{20}$$

where $i = \mathrm{n}, \mathrm{p}$ and the upper (lower) sign applies to neutrons (protons). The explicit dependence of $R_i(N,Z)$ on N and Z will be suppressed in the following. The $R_{0,1}$ depend only weakly on the asymmetry $N-Z$. The structure corrections, *e.g.*, due to deformation, are known to be predominantly isoscalar in nature and are expected to affect strongly the first term on the right-hand side.

We parametrize the mass radius, $R_0 = (R_\mathrm{n} + R_\mathrm{p})/2$, in the following simple way:

$$R_0 = r_0 A^{1/3} + aA^{-2/3} + c\frac{(N-Z)^2}{A^2}. \tag{21}$$

Recently, Royer [9] has compared the fits to radii using various powers of A for the (small) second term; the fits show little preference for a particular power.

One may now argue that R_1 in eq. (20) is not an independent term but that it is related to the surface asymmetry discussed in sect. 2. Indeed, following Danielewicz [10] one has (in case of sharp radii)

$$\frac{R_\mathrm{n} - R_0}{R_0} \approx \frac{N_\mathrm{s}}{3N}, \qquad \frac{R_\mathrm{p} - R_0}{R_0} \approx \frac{Z_\mathrm{s}}{3Z}, \tag{22}$$

and hence for the skin (assuming $|\Delta R| \ll R_0$)

$$\frac{\Delta R}{R_0} \equiv \frac{R_\mathrm{n} - R_\mathrm{p}}{R_0} = \frac{A(N_\mathrm{s} - Z_\mathrm{s})}{6NZ}, \tag{23}$$

where the last equality follows from the leptodermic constraint $A_\mathrm{s} = 0$. Using eq. (7) and taking into account the Coulomb correction, one finds the following LDM estimates for the ratios of terms in eq. (20):

$$\left.\frac{R_1}{R_0}\right|_{\mathrm{LDM}} = \frac{A^2}{6NZ(1 + y^{-1}A^{1/3})}, \tag{24}$$

and

$$\left.\frac{\delta R_\mathrm{C}}{R_0}\right|_{\mathrm{LDM}} = -\frac{a_\mathrm{c}}{144 S_\mathrm{v}} \frac{A^{8/3}}{NZ(1 + y^{-1}A^{1/3})}. \tag{25}$$

The correction δR_C reflects the fact that, due to the Coulomb repulsion, the charge radius of an $N = Z$ nucleus is slightly larger than its neutron radius [10,26]. The expression (25) is somewhat different from the one given in ref. [10], eq. (33), because we have used here the exact conditions (7) without approximation.

As pointed out in ref. [10], additional small corrections are due to the conversion from sharp to rms radii, and to a possible difference in neutron and proton diffuseness.

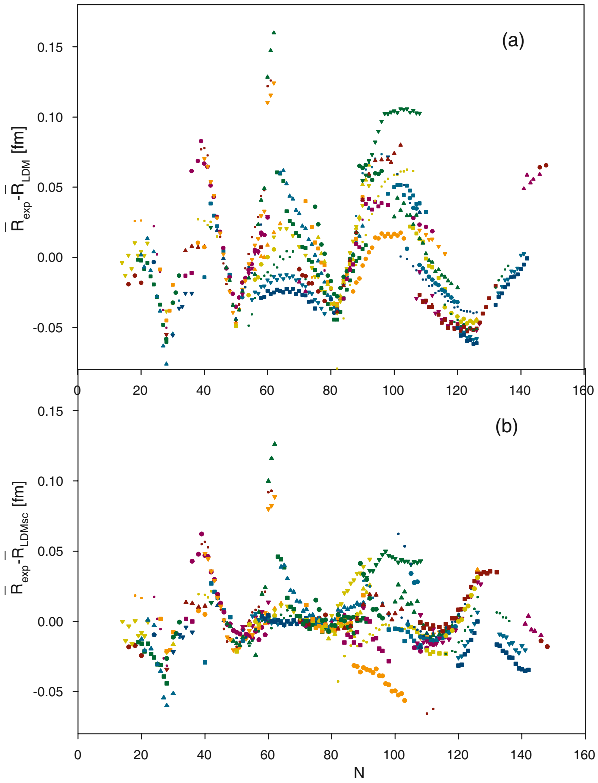

Fig. 5. (Color online) (a) Differences $\bar{R}_{\mathrm{exp}} - \bar{R}_{\mathrm{LDM}}$ between experimental rms charge radii and those obtained from LDM. Equation (20) is applied with parameters as given in the text. (b) Differences $\bar{R}_{\mathrm{exp}} - \bar{R}_{\mathrm{LDMsc}}$ between experimental rms charge radii and those obtained from a shell-corrected LDM. Equations (20) and (29) are applied with parameters as given in the text.

Due to the Coulomb force in the interior of the nucleus the proton distribution is slightly reduced with respect to that of the neutrons (also referred as a polarization effect). Using the notation $\bar{R} \equiv \langle r^2 \rangle^{1/2}$, one finds for the rms radius [10]

$$\frac{\Delta \bar{R}}{\bar{R}_0} \equiv \frac{\langle r^2\rangle_\mathrm{n}^{1/2} - \langle r^2\rangle_\mathrm{p}^{1/2}}{\langle r^2\rangle^{1/2}} = \frac{\Delta R_{\mathrm{LDM}}}{R_0} + \frac{\delta \bar{R}_{\mathrm{pol}}}{\bar{R}_0} \tag{26}$$

with

$$\frac{\delta \bar{R}_{\mathrm{pol}}}{\bar{R}_0} = -\frac{a_\mathrm{c}}{168 S_\mathrm{v}} \frac{A^{5/3}}{N}. \tag{27}$$

The diffuseness correction is small and is neglected here.

To fit the isovector term R_1 independently, we introduce a single parameter $b = R_1/R_1^{\mathrm{LDM}}$. We find an rms deviation $\sigma = 0.036\,\mathrm{fm}$ with the parameters $r_0 = 0.940 \pm 0.001\,\mathrm{fm}$, $a = 2.81 \pm 0.09\,\mathrm{fm}$, $c = -0.006 \pm 0.012\,\mathrm{fm}$ and $b = 1.1 \pm 0.1$. The latter value is consistent with 1 which is required from the surface asymmetry approach, suggesting that our procedure provides a good first-order estimate of the isovector term. This, however, might be fortuitous since we also find that there is a substantial correlation between the parameters of the $(N-Z)/A$ and $(N-Z)^2/A^2$ terms. In fact, there is a valley of values

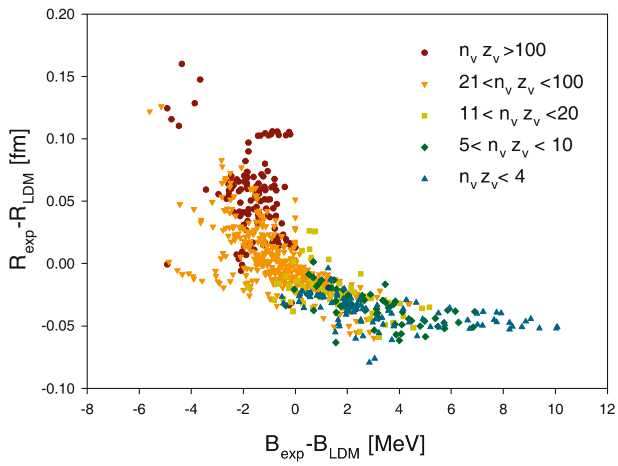

Fig. 6. (Color online) Correlation plot of the rms charge-radii differences $\bar{R}_{\mathrm{exp}} - \bar{R}_{\mathrm{LDM}}$ *versus* the binding-energy differences $B_{\mathrm{exp}} - B_{\mathrm{LDM}}$. The points are subdivided into 5 categories corresponding to the values of $d \equiv n_{\mathrm{v}} z_{\mathrm{v}}$: blue up-triangles $d \leq 4$; green diamonds $5 \leq d \leq 10$; light-green squares $11 \leq d \leq 20$; orange down-triangles $21 \leq d \leq 100$ and brown circles $d > 100$.

of these two parameters, yielding approximately the same rms deviation.

The differences between experimental rms charge radii [24] and those obtained from LDM are shown in fig. 5a; it is clear that the residuals are due to shell effects to which we now turn.

3.2 Shell corrections

It is well known [27] that, to obtain quantitative results, shell corrections must be added to eq. (20). In the literature one finds them of various forms. In several papers, *e.g.*, refs. [5,24], the promiscuity term P has been used, which does not contribute to singly closed-shell nuclei.

We now study to what extent shell corrections to masses and radii are similar in character. To this end we plot in fig. 6, for the ~ 600 nuclei listed in ref. [24], the differences $\bar{R}_{\mathrm{exp}} - \bar{R}_{\mathrm{LDM}}$ between experimental rms charge radii and those obtained from the LDM *versus* the similar differences for masses. (For clarity we have omitted a few nuclei with uncertainties in the radii larger than 0.10 fm.) To illustrate the close relation between the value of the differences and the number of valence nucleons we have divided the data points in 5 categories depending upon the number of valence nucleons for which (somewhat arbitrarily) we take the product $n_{\mathrm{v}} z_{\mathrm{v}}$. One observes a strong almost linear correlation whenever the LDM formula underbinds and predicted radii are too large (at and near closed-shell nuclei, right-hand side of the figure), and a much more diffuse correlation in case of overbinding and too small radii (for mid-shell nuclei, left-hand side of the figure). The explanation for the larger spreading for mid-shell nuclei is that a transition to deformation increases both the binding energy *and* the radius contrary to shell effects near closed shells that tend to increase the binding energy but decrease the radius. This clearly suggests the presence of appreciable and systematic shell effects and also that, in the neighborhood of closed shells, shell corrections to radii are similar to those for masses.

With this correlation in mind and neglecting for the moment the effect of deformation, we have tried two different forms of shell corrections to the LDM prediction (20) of charge radii.

1. We first used a shell correction proportional to the one fitted to masses, eq. (12), introducing just one new dimensionless scale parameter γ,

$$\frac{R_{\mathrm{shell}}(N,Z)}{R_0} = \gamma \frac{E_{\mathrm{shell}}(N,Z)}{a_{\mathrm{v}} A}. \tag{28}$$

We found that this prescription does not improve the fit substantially because of the difficulty in disentangling shell and deformation effects mentioned above.

2. We found that a better fit can be obtained with a simple sum of a one-body term (analogous to S_2 in eq. (13)) and a two-body neutron-proton term (similar to S_{np}):

$$R_{\mathrm{shell}}(N,Z) = \alpha_1 S_2(k) + \alpha_{\mathrm{np}} S_{\mathrm{np}}(k), \tag{29}$$

where

$$\begin{aligned} S_2(k) &= \frac{n_{\mathrm{v}} \bar{n}_{\mathrm{v}}}{(D_n)^k} + \frac{z_{\mathrm{v}} \bar{z}_{\mathrm{v}}}{(D_z)^k}, \\ S_{\mathrm{np}}(k) &= \frac{n_{\mathrm{v}} \bar{n}_{\mathrm{v}} z_{\mathrm{v}} \bar{z}_{\mathrm{v}}}{(D_n D_z)^k}. \end{aligned} \tag{30}$$

Whereas the two-body term with $k = 2$ (and an additional deformation term) is present in ref. [27], the one-body term is not. We have compared results with $k = 1$ to those with $k = 2$ in eq. (30), and obtained a slightly better fit with $k = 1$, which corresponds to the correction used in the masses.

After inclusion of the second shell correction the rms deviation reduces to $\sigma = 0.022$ fm. The LDM parameters change little: $r_0 = 0.927 \pm 0.001$ fm, $a = 2.77 \pm 0.09$ fm, $c = 0.02 \pm 0.03$ fm and $b = 1.18 \pm 0.09$. The parameters in the shell correction terms (30) are $\alpha_1 = 0.56 \pm 0.07$ fm and $\alpha_{\mathrm{np}} = 0.020 \pm 0.005$ fm. The differences between experimental charge radii [24] and those obtained from the shell-corrected LDM (denoted as LDMsc) are shown in fig. 5b. It seen that the shell corrections in general improve the fit near closed-shell nuclei; for mid-shell nuclei, where effects from deformation or contributions from high-spin intruder orbitals may play a role, the radii are generally underestimated.

3.3 Isotope shifts

In masses the effects of shell gaps are most clearly demonstrated by plotting nucleon separation energies; in radii the shell structure shows up most prominently by plotting isotope shifts as a function of neutron number N. Although we plan to address the calculation of isotope shifts

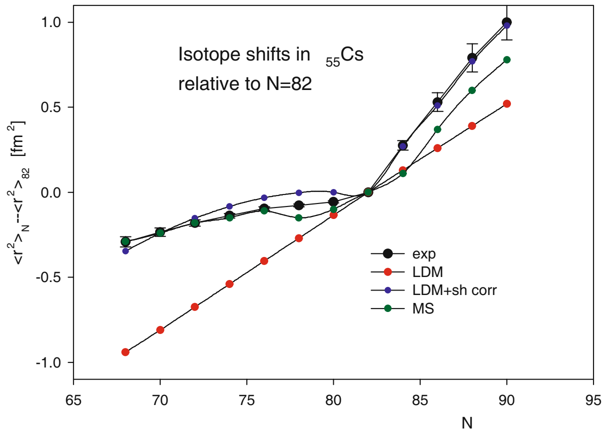

Fig. 7. (Color online) The isotope shifts $\langle r^2 \rangle_N - \langle r^2 \rangle_{N=82}$ in the Cs nuclei, compared with values calculated with the LDM, eq. (20), the shell-corrected LDM which includes the corrections (29) and the results of Myers and Schmidt [29] (labeled MS).

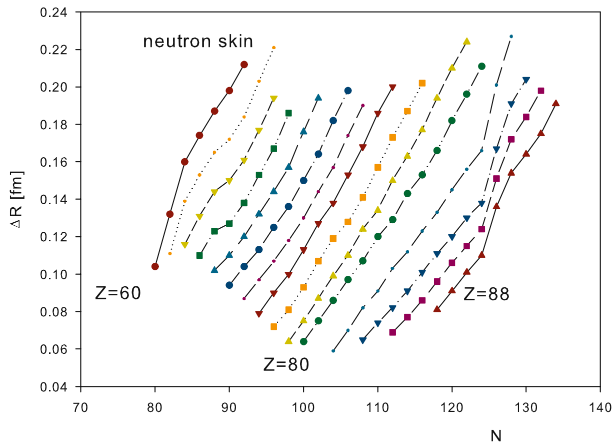

Fig. 8. (Color online) The neutron skin $\Delta\bar{R}$ (in fm) *versus* neutron number N for even-even nuclei with $Z > 60$. Equation (34) is used with the experimental isovector chemical potential μ_a (method 3). Nuclei with constant Z (isotopes) are connected.

in more detail in a following paper [28] in which deformation effects will be included, we show in fig. 7 results for the Cs ($Z = 55$) isotopes as a typical example for the behavior of isotope shifts near closed shells. The LDM provides a global trend only; for $N < 82$ the shell corrections lead to a reduced isotope shifts while for $N > 82$ they are increased. We note that in the older literature the deviation from the LDM was in general ascribed to the effect of deformation [29]; however, as can be seen from the figure, this leads to discrepancies just below and above the shell closure.

3.4 Neutron skin

The neutron skin in neutron-rich nuclei has become an important issue over the last few years. Up to now there does not exist a truely model-independent probe of the neutron distribution. Although in the past the results from antiprotonic atoms have been used for this purpose [30], the accuracy of this method has been questioned recently [31]. For a model-independent result one has to wait for the outcome of planned parity-violating electron scattering experiments. In the meantime experiments which use atomic parity violation in heavy nuclei to study possible extensions of the standard model require accurate information on neutron and proton radii.

Here we derive the neutron skin ΔR from the modified LDM. From the discussion above it is clear that we can use three different methods.

1. The most direct way is to use the isovector term in eq. (20) which has been fitted to experimental charge radii, corrected for Coulomb.
2. A second method uses the LDM expression for ΔR as given in eq. (23):

$$\frac{\Delta R}{R_0} = \frac{A(N-Z)}{6NZ(1+y^{-1}A^{1/3})} + \frac{\delta R_\mathrm{C}}{R_0}\,, \qquad (31)$$

where δR_C is the Coulomb correction (25). We note that Myers and Swiatecki [32] have derived a similar expression for the neutron skin in their droplet model.
3. A third way is by establishing a relation between the isovector chemical potential and the differences of neutron and proton radii. The latter is expressed in terms of the difference $N_\mathrm{s} - Z_\mathrm{s}$ through the expression (23). An alternative expression for this difference can be obtained [10] by noting that the isovector chemical potential μ_a is given by

$$\mu_\mathrm{a} \approx \frac{1}{2}\left(\frac{\partial B}{\partial N} - \frac{\partial B}{\partial Z}\right) = -\frac{\partial E}{\partial \delta}\,. \qquad (32)$$

We now express the symmetry energy E_S of eq. (1) and the Coulomb energy E_C of eq. (5) in terms of three independent variables A, δ and δ_v. With the use of the constraint $N_\mathrm{s} + Z_\mathrm{s} = 0$, we find

$$\mu_\mathrm{a} = 2S_\mathrm{s}\frac{N_\mathrm{s} - Z_\mathrm{s}}{A^{2/3}} - \frac{5a_\mathrm{c}}{6}\frac{Z}{A^{1/3}}\,. \qquad (33)$$

Turning to the difference of rms radii and adding the polarization correction of eq. (27), we find

$$\frac{\Delta\bar{R}}{\bar{R}_0} = \frac{\mu_\mathrm{a}}{12S_\mathrm{s}}\frac{A^{5/3}}{NZ} + \frac{5a_\mathrm{c}}{72S_\mathrm{s}}\frac{A^{4/3}}{N} - \frac{a_\mathrm{c}}{168S_\mathrm{v}}\frac{A^{5/3}}{N}\,. \qquad (34)$$

Since experimental separation energies are used in this approach, one may assume that shell effects are implicitly included. In this case the uncertainty in ΔR is almost completely due to the uncertainty in the surface symmetry energy S_s.

Comparison of methods 1 or 2 (which yield a smooth N-dependence) with method 3 should provide an idea about shell effects (assuming that S_s is constant). It is seen from fig. 8 that in methods 3 small kinks occur at neutron shell closures. The latter are absent in the results of methods 1 and 2, and also in the result of Brown *et al.* [23]. On the other hand unlike charge radii the neutron skin size appears to be quite insensitive to the deformation [33].

In the past mostly the experimental results on neutron skins from anti-protonic atoms were used [30]. However, recently it was pointed out [31] that there are large uncertainties in the analysis coming from the model dependence of the extrapolation of densities to large radii. Of particular interest is the neutron skin of ^{208}Pb in view of the planned parity-violating electron scattering experiment at Jlab [34] to measure the neutron distribution model independently. The result of a recent re-analysis [31] of anti-protonic atom data for the neutron skin for this nucleus is $\Delta R = 0.20 \pm 0.04 \pm 0.05\,\mathrm{fm}$, where 0.04 represents the experimental error and 0.05 the estimated theoretical error. Since in the case of ^{208}Pb the shell corrections vanish, methods 1, 2, or 3 are expected to yield very similar results. We obtain $\Delta R = 0.182$, 0.197, and 0.201 fm, for methods 1, 2, and 3, respectively. A recent calculation [23] using Skyrme interactions yields $\Delta R = 0.20\,\mathrm{fm}$ and so at this point good agreement is found. However, we note that the shell model calculation of ref. [23] does not seem to reproduce the experimental proton radii away from closed shells very well.

4 Summary and conclusions

In this paper we have used an extended liquid-drop model which includes a surface asymmetry and shell corrections to binding energies as well as radii. The shell corrections to masses are described by four terms leading to an rms deviation for 2149 nuclei of approximately 800 keV. As particular applications we have addressed the symmetry energy and the neutron skin.

Concerning the symmetry energy, we determined the volume S_v and surface S_s symmetry energy by applying a Coulomb correction to the experimental difference of neutron and proton separation energies. From these values one may infer two values of the density dependence of the symmetry energy in nuclear matter [10,14], namely $S(\rho_0) = S_\mathrm{v}$ and $S(\rho \approx \frac{2}{3}\rho_0)$, with ρ_0 the nuclear saturation density. These serve as convenient constraints for the equation of state of neutron stars.

To describe the charge of nuclei with a neutron excess within the framework of the LDM, the inclusion of an isovector term [$\propto (N - Z)$], strongly suggested by charge symmetry, yields a good description of closed-shell nuclei. For open-shell nuclei the inclusion of two terms suggested by the shell corrections to masses leads to a reduction of the rms deviation of the charge radii to about 0.020 fm. The fit may improve if the effects of deformation are treated explicitly.

While for the description of the neutron skin several options exist, its close relation to the surface symmetry energy suggests a rather direct computational approach, namely the use of the experimental differences between neutron and proton separation energies.

As to radii, information on the latter is required for quantitative tests of the standard model using atomic nuclei. For example, the necessary accuracy in nuclear inputs such as R_p and ΔR, required to reach a certain precision in atomic parity-violating experiments, has been addressed in ref. [35]. Specializing to Ra and aiming at an overall 10^{-3} precision, one needs an accuracy of 0.4% in R_p^2 and a 20% accuracy in $\delta_\mathrm{np} \equiv \bar{R}_\mathrm{n}^2/\bar{R}_\mathrm{p}^2 - 1$. Since for the Ra isotopes no absolute experimental radii are available (only isotope shifts), one has to rely on theoretical estimates. We feel that our predictions for both charge and neutron radii have an uncertainty similar to the quoted required values.

A related issue that been discussed recently [23] is whether the uncertainty in an atomic parity-violating experiment associated with the neutron radius can be reduced by considering ratios of more than one isotope. This would be the case if the neutron skin sizes for the different isotopes are correlated. The present study suggests that this is the case indeed: the smooth $(N-Z)/A$-dependence of the neutron skin is only slightly affected by shell effects.

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