Valence correlation scheme for single nucleon separation energies

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A simple valence correlation scheme is presented in which empirical neutron and proton separation energies, S_n and S_p , follow extremely compact, linear trajectories in terms of the variables $\alpha N_p - N_n$. This scheme often allows predictions for unknown nuclei by *interpolation* rather than extrapolation. A Taylor expansion shows that the Weizsäcker mass formula in fact behaves in first order as $\alpha N_p - N_n$ though such a functional dependence is not explicit and has not been noted before. [S0556-2813(96)50112-3]

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Nucleon separation energies, S_n and S_p , have a wellknown behavior across each major shell region. This is illustrated for the pair of half-major shells, Z=50-66 and N=82-104, in Figs. 1(a) and 1(b). In these figures, $S_n(S_p)$ are defined as functions of binding energies,

$$S_{n}(Z,N) = B(Z,N) - B(Z,N-1),$$
(1)

$$S_{n}(Z,N) = B(Z,N) - B(Z-1,N).$$

(a)

160

(b)

160

170

170

15

10

5

0

15

10

5

0

0

 S_p (MeV)

10

20

 $2.6N_p - N_n$

 $S_n (MeV)$

In Fig. 1(a), S_n increases (the last neutron becomes more bound) with increasing proton number, reflecting the attractive *p*-*n* interaction, but decreases with increasing neutron number, since the like-nucleon interaction is repulsive on

average [2]. This behavior is reproduced by mass formulas such as the Weizsäcker semiempirical relation [3], as given in Ref. [4]:

$$M(A) = ZM_{p} + NM_{n} - a_{1}A + a_{2}A^{2/3} + a_{3}\frac{Z^{2}}{A^{1/3}} + a_{4}\frac{(Z-N)^{2}}{A} + \delta(A), \qquad (2)$$

where the coefficients a_i are fit to the data, and the successive terms represent the nucleon masses, volume, surface, Coulomb, symmetry, and pairing energies. Other mass formulas (e.g., [1,5-8]) embody numerous refinements, and of-

(c)

30

(d)

30

20

 $2.0N_p - N_n$

40

FIG. 1. Experimental S_n and S_p values for even-even nuclei in the Z=50-66, N=82-104 region. Data are taken from [1]. S_n and S_p plotted against A on the left and against $\alpha N_p - N_n$ on the right.

140

15

10

5

0 L 130

15

10

5

O

130

 S_{p} (MeV)

140

150

А

150

A

 S_n (MeV)



10



FIG. 2. (a)–(c) The dependence of the correlation of S_p with $\alpha N_p - N_n$ for different α_p values. (d) The correlation coefficient of the fit, r^2 , as a function of α_p .

ten more parameters. Although numerical calculations with such formulas are quite successful, their overall dependence on N, Z, and A is hardly transparent due to the competing roles of several terms.

In the last decade, the concept of valence correlation schemes (VCS's) has been developed, in which the phenomenology of nuclear structure observables for ground state and low-lying levels is simple and compact when expressed in terms of valence nucleon numbers (e.g., N_pN_n) [9]. These VCS's are motivated by simple ideas concerning the essential microscopic ingredients in nuclear structural evolution.

It is the purpose of this Rapid Communication to ask whether single nucleon separation energies also can be correlated in the framework of a VCS. We will show that a remarkably simple parameterization works extremely well, that it has an intuitive underlying rationale, that it reveals a functional dependence hidden in the Weizsäcker formulation, that it is universal, and that it often provides predictions for unknown nuclei by *interpolation*.

The contrasting behavior of S_n [see Fig. 1(a)] against proton and neutron numbers (increasing against Z and decreasing against N) suggests immediately a scheme of the form:

$$S_n \sim \alpha_n N_p - N_n, \qquad (3)$$

where N_p and N_n are valence proton and neutron numbers relative to the nearest magic numbers, 20, 28, 50, 82, 126 and where α_n is a parameter that is constant for a given pair of proton and neutron half-major shells. From the slopes in Fig. 1(a), it is clear that α_n will be greater than unity and one can estimate visually values on the order of two or three.

Interestingly, the situation [Fig. 1(b)] for proton separation energies, S_p , is not merely the opposite of that for S_n because the Coulomb force plays an important role as well. Nevertheless, the behavior in Fig. 1(b) suggests that S_p still can be written

$$S_p \sim N_n - \alpha_p N_p = -(\alpha_p N_p - N_n), \qquad (4)$$

where we use the second form to emphasize the analogy to Eq. (3), because, for both S_n and S_p , α_n and α_p will turn out to be greater than unity. This second form also highlights the overall decrease of S_p across a major shell.

Of course, to obtain absolute values for S_n and S_p we need to write:

$$S = K(\alpha N_p - N_n) + C, \qquad (5)$$

where the slope K is positive (negative) for $S_n(S_p)$, and where α , K, and C are constants for the nuclei in a given pair of half-major proton and neutron shells, and in general can be different for S_n and S_p .

The use of the formulation in Eqs. (3)–(5) in terms of N_p and N_n , instead of Z and N, has several adavantages. First, as we shall see, this linearization of separation energies facilitates predictions for new nuclei and the investigation of shell structure in such regions (e.g., nuclei far from stability or the heaviest actinides): that is, separation energies calculated from Eqs. (3)–(5) depend on the choice of magic numbers in new regions. Also, Eqs. (3)–(5) properly focus attention on the effects and interactions of the valence nucleons and separate off the effect of the core (contained in the parameter *C*). In contrast, a functional dependence on $\alpha Z-N$ leads to *C* parameters that vary enormously from region to region with no obvious sensitivity to the underlying shell structure.



FIG. 3. S_n (left) and S_p (right) correlations with $\alpha N_p - N_n$ for several other mass regions spanning several major shells and including particle as well as hole structure. The shells used for the actinides [panels (e) and (f)] are Z=82-126 and N=126-184.

We have carried out least square fits of Eq. (5) to empirical S_n and S_p data for the Z=50-66 and N=82-104 halfmajor shells. The best-fit values are $\alpha_n = 2.6$ and $\alpha_p = 2.0$. The results are shown in Figs. 1(c) and 1(d). The correlations are remarkably simple and compact: all values lie along extremely well-defined, essentially linear trajectories. We illustrate the sensitivity of the correlations to the α values in Figs. 2(a)–(c). Figure 2(d) shows the explicit dependence of the correlation coefficient [10] r^2 on α_p .

Analysis of the data in other mass regions shows that the simple correlation of S_n and S_p with $(\alpha N_p - N_n)$ is quite general. For regions in which either (or both) neutrons and protons are holelike (past midshell), obvious modifications are necessary. The monotonic trends of S_n and S_p continue past midshell [in contrast to the mirrorlike behavior about midshell of observables such as $E(2_1^+)$ or $B(E2:0_1^+ \rightarrow 2_1^+)$ values]. Therefore if one or both kinds of nucleon is holelike, we change the sign preceding it: This gives a general expression

$$S = K(\pm \alpha N_p \mp N_n) + C, \qquad (6)$$

where the upper signs are for particles and the lower signs are for holes. Clearly, in order that expressions of the form of Eq. (6) link up at midshell, rather different coefficients K and C are necessary in adjacent half-shell regions. Using these definitions, we show the S_n and S_p correlations for several mass regions in Fig. 3. In each case, the correlations are linear and extraordinarily compact.

The universality of these results strongly suggests that they reflect a real, and simple, underlying physical effect. It is easy to understand the behavior qualitatively. The like nucleon interaction is, on average, repulsive [negative coefficient in the relevant term (e.g., N_n term for S_n). The unlike nucleon interaction is attractive and stronger than the like nucleon interaction. Hence α_n in Eq. (3) is positive and greater than unity. The slope (α_p) of S_p against N_p would be smaller in magnitude than the slope of S_p against N_n were it not for the Coulomb force. However, this force rapidly lowers S_p for increasing Z so that the dependence of S_p on N_p is large and α_p is also greater than unity, as indeed found in the fits. It is curious, but probably accidental, that the Coulomb p-p force is just the right magnitude that the Eqs. (3) and (4) for S_n and S_p are almost identical (apart from overall sign), that is, that α_n for S_n is approximately equal to α_p for S_p even though the physical mechanisms are so different (competition of short range nuclear and long-range electromagnetic forces).

The behavior in Figs. 1(c) and (d) and Fig. 3 is so smooth and the dependence of S_n and S_p on N_p and N_n so simple that it is interesting to see how such behavior is reflected in standard mass equations (which fit empirical masses). Separation energies calculated from the Weizsäcker mass formula of Eq. (2) do not contain an obvious $\alpha N_p - N_n$ behavior. Nevertheless, as Fig. 4 shows, separation energies obtained from the Weizsäcker formula behave almost exactly as $\alpha_n N_p - N_n$ for S_n and $-(\alpha_p N_p - N_n)$ for S_p with α values similar in magnitude to those found in our fits. It is interest-



FIG. 4. S_n and S_p values for the same region as in Fig. 1, but calculated with the Weizsäcker formula, as a function of $\alpha N_p - N_n$.

ing to study the origins of this dependence. To do so, we first note that, for a given pair of half-major proton and neutron shells in medium and heavy nuclei, A, N, and Z vary only slightly. Therefore we rewrite Eq. (2) (for a particle-particle region) in terms of the variables

$$Z = Z_0 + N_p \quad \text{and} \quad N = N_0 + N_n, \tag{7}$$

where Z_0 and N_0 are the nearest proton and neutron magic numbers. Since $N_p \ll Z_0$ and $N_n \ll N_0$ for the nuclei we consider, we can expand the Weiszäcker formula in terms of $(N_p + N_n)/(Z_0 + N_0)$. Keeping terms up to quadratic in N_p and N_n , we have

$$M(A = Z + N) = k_0 + k_1 N_p + k_2 N_n + k_3 N_p N_n + k_4 N_n^2 + k_5 N_p^2.$$
(8)

Estimates of the higher-order terms in N_p and N_n are at most 10% as large as those kept in Eq. (8). Separation energies calculated from differences of M(A) values, hence, will be clearly linear in N_p and N_n . In fact, it is easy to deduce that

$$\alpha_n = -\frac{k_3}{2k_4}, \quad \alpha_p = -\frac{2k_5}{k_3}.$$
 (9)

The full expressions obtained for α_n and α_p from Eq. (9) are naturally rather lengthy. However neglecting terms less than ~10% of the *k* coefficients, gives the relatively simple results:

TABLE I. Predicted S_n values (MeV) for nuclei in the A = 150

region using Eq. (5) with α =2.6, K=0.135 MeV, and C=4.62 MeV. Entries in boldface are made by interpolation, the others by extrapolation.

$Z \setminus N$	92	94	96	98	100	102	104
52	4.0	3.7	3.4	3.2	2.9	2.6	2.4
54	4.7	4.4	4.1	3.9	3.6	3.3	3.1
56	5.4	5.1	4.8	4.6	4.3	4.0	3.8
58	-	5.8	5.5	5.3	5.0	4.7	4.5
60	-	6.5	6.2	6.0	5.7	5.4	5.2
62	-	-	6.9	6.7	6.4	6.1	5.9

$$\alpha_n = \frac{Z_0 + N_0}{3Z_0 - N_0},\tag{10}$$

$$\alpha_p = \frac{Z_0 + 3N_0}{(Z_0 + N_0)^{1/3}} \left(\frac{a_3}{3a_4}\right) - \frac{Z_0 - 3N_0}{Z_0 + N_0},\tag{11}$$

where a_3 and a_4 are coefficients in the Weizsäcker relation in Eq. (2). These α_n and α_p values are thus very close to those obtained by fitting Eq. (5) to the separation energies obtained from the Weizsäcker formula.

We note that these, as well as the constants K and C in Eq. (6), depend only on Z_0 and N_0 and not on N_p and N_n . At the level of approximation represented by Eqs. (10) and (11), k_3 and k_4 depend only on a_4 . Hence, α_n , which involves their ratio [Eq. (9)], does not depend on the Weiszäcker coefficients. k_5 though, depends on both a_3 and a_4 and, hence, α_p does also. This reflects the fact that neutron separation energies are only very weakly dependent on the Coulomb term while, as noted above, S_p values result from the competition of nuclear and Coulomb forces.

Thus, exploitation of the VCS notion that separation energies should depend on a function of the form $\alpha N_p - N_n$, leads not only to the discovery of an extraordinarily simple behavior of empirical S_n and S_p values, but reveals that there is an unrecognized dependence of this kind lurking in the apparently complex form of semiempirical mass equations.

The compactness of the correlations in Figs. 1(c), (d), and 3 and a particular property of the quantity $\alpha N_p - N_n$ leads to an interesting facet of this VCS that is useful in the new nuclei that will become accessible with radioactive beams. Since α_n and α_p are typically in the range 1–3, values of the quantity $\alpha N_p - N_n$ for unknown nuclei far from stability are often within the range of values for known nuclei nearer stability. For such cases, separation energies can be predicted by *interpolation* along *existing* trajectories. As an illustration, Table I gives some S_n predictions for unknown nuclei in the rare earth region.

Finally, since N=Z nuclei are characterized by singularities in the $T=0 \ p-n$ interaction, one expects this VCS may break down for such nuclei. Preliminary inspection of S_n values for light N=Z nuclei (Z < 28) gives some evidence for this speculation. Indeed, the difference of measured values from the predictions of the $\alpha N_p - N_n$ scheme might give information on the strength of the $T=0 \ p-n$ interaction in such nuclei. Such information may soon be accessible in the N=Z nuclei of the $A \sim 100$ region with new radioactive beam facilities.

To summarize, a very simple valence correlation scheme tracks empirical values of single nucleon separation energies extremely well. Empirical values of S_n scale linearly with $\alpha_n N_p - N_n$ and S_p scales equally well with $-(\alpha_p N_p - N_n)$, where N_p and N_n are the valence proton and neutron numbers and α_n or α_p is a constant within a half-major shell and varies in a range from 1–3 for different mass regions. The remarkable universal behavior revealed reflects, in a extraordinarily simple way, the competing roles of the attractive valence p-n interaction, the net repulsive valence likenucleon interaction and, for S_p , the repulsive Coulomb interaction. It reveals a simplicity not readily apparent in standard mass equations, and it has predictive power, via interpolation, for many nuclei far from stability.

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