Nucleon separation energies in the valence correlation scheme

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In this paper we study the one- and two-nucleon separation energies $(S_n, S_p, S_{2n}, \text{and } S_{2p})$ by using the Atomic-Mass-Evaluation-2011 Preview. We show the linear dependence of separation energies, previously investigated for S_n and S_p of even-even nuclei, in terms of $\alpha N_p + \beta N_n$ (N_p and N_n is the valence proton number and valence neutron number, respectively, with respect to the nearest magic closure), hold in a broader sense. It is applicable equally well to odd-mass and odd-odd nuclei. New odd-even staggerings are found for S_n and S_p , and are discussed by using the pairing interaction and the symmetry energy. Predictive power of these simple relations is discussed.

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Nucleon separation energies and mass (or binding energy) are fundamental quantities of a nucleus. They provide us with useful information on structural evolutions of atomic nuclei as well as the key input for theoretical studies on the origin of the heavy elements, especially those on the rapid proton (rp) and rapid neutron (r) capture processes. Therefore, describing and predicting nuclear masses and separation energies have been one of the focuses of the nuclear structure physics in recent years. For comprehensive reviews, see Refs. [1,2].

In 1996 Streletz and collaborators discovered a very interesting fact [3]: S_n (one-neutron separation energy) and S_p (one-proton separation energy) of even-even nuclei follow compact and linear trajectories in terms of the variable $\alpha N_p + \beta N_n$. Here N_p and N_n are, respectively, the valence proton number and valence neutron number with respect to the nearest magic closure. α is a constant (positive for particles and negative for holes) optimized by using experimental data. β is set to be either -1 for particles or +1 for holes in each halfmajor shells. This valence correlation scheme of separation energies was studied by using the seniority mass equation [4]. There are a number of valence correlation schemes which are very useful in studies of evolution of various observables in different regions in the nuclear chart. See Refs. [5,6] for reviews.

The purpose of this paper is to revisit the linear relations of separation energies in terms of $\alpha N_p + \beta N_n$, discussed in Ref. [3], by using the latest version of experimental masses, the Atomic-Mass-Evaluation-2011 Preview (AME2011-preview) [7]. Here our discussion is not restricted to S_n and S_p of eveneven nuclei. We investigate S_n , S_p , and two-proton and twoneutron separation energies (S_{2n} and S_{2p}) of even-even, odd-A, and odd-odd nuclei, on the same footing. New features of odd-even staggering are discerned and discussed in terms of pairing interaction and symmetry energy. PACS number(s): 21.10.Dr, 21.60.Cs, 21.10.Re

Let us first define S_p , S_n , S_{2p} , and S_{2n} , by differences of the binding energies as follows:

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

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

$$S_{2p}(Z, N) = B(Z, N) - B(Z - 2, N),$$

$$S_{2n}(Z, N) = B(Z, N) - B(Z, N - 2).$$
(1)

We take the convention that binding energy B(Z, N) is positive. Under this convention, S_p , S_n , S_{2p} , and S_{2n} are all positive.

We begin our discussion by the linear relation between the separation energies S_n and $\alpha N_p + \beta N_n$ [3]:

$$S_n = K(\alpha N_p + \beta N_n) + C, \qquad (2)$$

where *K* and *C* are constants optimized by using experimental data. Here all single- and double-magic nuclei, and N = Z nuclei are excluded. S_p follow the same relation except that the constants are different.

The correlation of S_n and S_p with optimal $\alpha N_p \pm N_n$ are shown in Figs. 1 and 2. Here we take experimental data compiled in the AME2011-preview [7], and consider not only even-even but also odd-mass and odd-odd nuclei, with proton numbers $Z \ge 29$. The results in each panel correspond to different shells. The results of even-even, even-Z-odd-N, odd-Z-even-N, and odd-odd nuclei are denoted by squares, diamonds, stars, and circles, respectively. One sees from Figs. 1 and 2 that S_n and S_p in each of these four groups (eveneven, even-Z-odd-N, odd-Z-even-N, and odd-odd) follow compact linear trajectories versus $\alpha N_p \pm N_n$.

On the other hand, there are two types of odd-even staggerings as follows. First, S_n (see Fig. 1) of nuclei with even neutron numbers N are systematically larger than those of their odd-N neighbors, and S_p (see Fig. 2) of nuclei with even proton numbers Z are larger than those of their odd-Z neighbors. Such odd-even staggering in separation energies has been well known and understood in terms of the pairing interaction. Second, there is an interesting and subtle odd-even staggering in both S_n and S_p : If one scrutinizes the results of

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FIG. 1. (Color online) Experimental S_n (in MeV, taken from the AME2011-preview [7]) versus $\alpha N_p + \beta N_n$ for different mass regions. The numbers in each panel correspond to Z, N, α , and β , respectively; for instance (29 ~ 39, 39 ~ 49, +1.99, +1) in (a) means that Z = 29 ~ 39, N = 39 ~ 49, $\alpha = +1.99$, and $\beta = +1$. Strong linear correlation between S_n and $\alpha N_p + \beta N_n$ is easily noticed.

 S_n , one sees that the trajectory of S_n for even-even nuclei is very slightly higher than that of its neighboring nuclei with odd Z and even N, and the trajectory of S_n for odd-odd nuclei is very slightly larger than that of its neighboring nuclei with even Z and odd N. Similarly, the trajectory of S_p for even-even nuclei is slightly higher than that with even Z and odd N, and that for odd-odd nuclei is slightly higher than that with odd Z and even N. Such subtle odd-even staggerings are new, and are pointed out here for the first time.

We furthermore suggest that these odd-even staggerings can be essentially traced back to the pairing interaction [denoted by $V_{\text{pairing}}(Z, N)$] and the symmetry energy [denoted by $V_{\text{sym}}(Z, N)$] in the modified Bethe-Weizsäcker formula [8]. According to Ref. [8],

$$V_{\text{pairing}}(Z, N) = a_{\text{pairing}} A^{-1/3} \begin{cases} 2 - I & \text{for even } Z & \text{and even } N, \\ I & \text{for odd } Z & \text{and odd } N, \\ 1 - I & \text{for odd } Z & \text{and even } N & \text{with } Z < N, \\ 1 & \text{for odd } Z & \text{and even } N & \text{with } Z > N, \\ 1 - I & \text{for even } Z & \text{and odd } N & \text{with } Z > N, \\ 1 & \text{for even } Z & \text{and odd } N & \text{with } Z < N, \end{cases}$$
(3)

and

$$V_{\rm sym}(Z,N) = c_{\rm sym} I^2 A \left(1 - \frac{\kappa}{A^{1/3}} + \frac{2 - I}{2 + IA} \right),\tag{4}$$

where $a_{\text{pairing}} = 5.4423$ MeV, $c_{\text{sym}} = -29.1563$ MeV, $\kappa = 1.3484$, and I = |N - Z|/A.



FIG. 2. (Color online) Same as Fig. 1 except for S_p (in MeV) versus $\alpha N_p + \beta N_n$.

From Eq. (1) we obtain the energies in $[S_n(Z, N) - S_n(Z, N - 1)]$ contributed by the pairing interaction and the symmetry energy as follows:

$$[S_n(Z, N) - S_n(Z, N-1)]_{\text{pairing}} = V_{\text{pairing}}(Z, N) + V_{\text{pairing}}(Z, N-2) - 2V_{\text{pairing}}(Z, N-1)$$

$$\simeq 2a_{\text{pairing}}A^{-1/3} + a_{\text{pairing}}A^{-4/3} \begin{cases} 8/3 - 2IA & \text{even } Z, \text{ even } N\\ 14/3 - 4IA & \text{odd } Z, \text{ even } N \end{cases}$$
(5)

and

$$\begin{split} &[S_n(Z, N) - S_n(Z, N-1)]_{\text{sym}} \\ &= V_{\text{sym}}(Z, N) + V_{\text{sym}}(Z, N-2) - 2V_{\text{sym}}(Z, N-1) \\ &\simeq 2c_{\text{sym}}(A^{-1} - \kappa A^{-4/3}) + 2c_{\text{sym}}A^{-2}(3 - 2IA) \\ &+ 8c_{\text{sym}}\kappa A^{-7/3}(2IA/3 - 1), \end{split}$$
(6)

where N > Z is assumed. There are two terms on the right hand side of Eq. (5). The first term is very large which is ~1.90 MeV for A = 188. The second term is much smaller, and different for odd and even Z (~ -0.35 MeV for even Z and ~ -0.68 MeV for odd Z, taking ${}^{188}_{76}$ Os and ${}^{189}_{77}$ Ir as examples). Thus the average value of $[S_n(Z, N) - S_n(Z, N - 1)]_{\text{pairing}}$ is 1.40 MeV. The contribution from the symmetry energy of Eq. (6) is ~ -0.16 MeV for A = 188. Summing over these two terms, one obtains that the value of $S_n(Z, N)$ of even-N nuclei is larger than its odd-N neighboring nuclei by 1.24 MeV, on average. Because the contribution in $[S_n(Z, N) - S_n(Z, N - 1)]$ from other terms in the mass formulas are negligibly small (≤ 25 keV for $A \geq 100$), we conclude that the odd-even difference of S_n (for even-N and odd-N) is dominantly given by the pairing interaction and the symmetry energy.

According to Eq. (2),

$$S_n(Z, N) - S_n(Z, N-1) \simeq [C(Z, N) - C(Z, N-1)] - K,$$
(7)

where we assume the value of K is identical for even-even and even-odd nuclei. The magnitude of the staggering for C(Z, N) - C(Z, N - 1) of Fig. 1(j) is ~2.00 MeV for even Z and ~1.20 MeV for odd Z, K is ~0.14 MeV. Thus on average the values of $S_n(Z, N)$ with even N are larger than those with odd N by ~1.46 MeV. This difference is close to our evaluation (~1.24 MeV) contributed by pairing interaction and symmetry energy in Eqs. (5) and (6), by using A = 188 - 189 nuclei. Similarly, we obtain for N > Z + 1 and A > 100,

 $[S_n(Z, N) - S_n(Z-1, N)]_{\text{pairing}} = V_{\text{pairing}}(Z, N) + V_{\text{pairing}}(Z-1, N-1) - V_{\text{pairing}}(Z, N-1) - V_{\text{pairing}}(Z-1, N)$

$$\simeq a_{\text{pairing}} A^{-4/3} \begin{cases} (IA + II + I/6) & \text{for order } Z & \text{and order } I \\ (IA - 4I/3 - 1/3) & \text{for odd } Z & \text{and odd } N \end{cases}$$

$$\simeq a_{\text{pairing}} A^{-4/3} |N - Z|, \tag{8}$$

and

$$[S_n(Z, N) - S_n(Z - 1, N)]_{\text{sym}} = V_{\text{sym}}(Z, N) + V_{\text{sym}}(Z - 1, N - 1) - V_{\text{sym}}(Z, N - 1) - V_{\text{sym}}(Z - 1, N)$$

$$\simeq -2c_{\text{sym}}(A^{-1} - \kappa A^{-4/3}).$$
(9)

The value of $[S_n(Z, N) - S_n(Z - 1, N)]_{\text{pairing}}$ on the right hand side of Eq. (8) ~0.18 MeV for ${}^{188}_{76}$ Os and ${}^{188}_{77}$ Ir, and $[S_n(Z, N) - S_n(Z - 1, N)]_{\text{sym}}$ for A = 188 is ~0.24 MeV. Summing over these two terms, we obtain that the total contribution of pairing interaction and symmetry energy in $[S_n(Z, N) - S_n(Z - 1, N)]$ is ~0.42 MeV. According to Eq. (2),

$$S_n(Z, N) - S_n(Z - 1, N) \simeq [C(Z, N) - C(Z - 1, N)] + K|\alpha|.$$
(10)

The magnitude of staggering for C(Z, N) - C(Z - 1, N)in Fig. 1(j) is ~0.30 MeV for even Z and ~0.45 MeV for odd Z, $|K\alpha|$ is ~0.27 MeV. Therefore the value of $S_n(Z, N) - S_n(Z - 1, N)$ for A = 188 in Fig. 1(j) is 0.64 MeV (close to 0.42 MeV, evaluated in terms of pairing and symmetry energy). We note that the value of $[S_n(Z, N) - S_n(Z - 1, N)]$ is ~0.44 MeV by using Eqs. (8) and (9) and $[S_n(Z, N) - S_n(Z - 1, N)] \sim 0.53$ MeV in Fig. 1, on average for $A \ge 100$.

The results for S_p are very similar. We have very similar formulas and explanations of odd-even staggerings as above for S_n .

We also note that the above discussions are consistent with the previous interpretation [9] of the odd-even staggering in proton-neutron interaction [10–16] between the last one proton and one neutron, denoted by $\delta V_{1p-1n}(Z, N)$,

$$\delta V_{1p-1n}(Z, N) = S_n(Z, N) - S_n(Z-1, N) = S_p(Z, N) - S_p(Z, N-1).$$

In Ref. [9] it was noted that the values of $\delta V_{1p-1n}(Z, N)$ for even-A nuclei are systematically larger in magnitude than those of their odd-A neighboring nuclei.

Now we come to the two-proton and two-neutron separation energies S_{2n} and S_{2p} , the results of which are summarized in Figs. 3 and 4, respectively. It is easy to obtain

$$S_{2n}(Z, N) = S_n(Z, N) + S_n(Z, N - 1),$$

$$S_{2p}(Z, N) = S_p(Z, N) + S_p(Z - 1, N).$$
(11)

Thus nuclei with $Z = Z_{\text{magic}}$, $N = N_{\text{magic}}$, $N = N_{\text{magic}} + 1$, Z = N, and Z = N - 1 for S_{2n} , the nuclei with $Z = Z_{\text{magic}}$, $N = N_{\text{magic}}$, $Z = Z_{\text{magic}} + 1$, Z = N, and Z = N + 1 for S_{2p} (Z_{magic} and N_{magic} denote magic numbers for protons and neutrons, respectively) are excluded and should be treated as exceptions, as shown in Eq. (11).

Figures 3 and 4 show that both S_{2n} and S_{2p} are linear in terms of $\alpha N_p \pm N_n$, without noticeable differences between the results those of even-even, odd-mass, and odd-odd nuclei. Here also we note a few "exceptions" which show slight deviations to our linear correlations. These exceptions include S_{2n} with Z = 39 of panels (b) and (d), Z = 66 and N = 93of panel (h), Z = 83, 84 and N = 153, 154 of panel (l) of Fig. 3; and S_{2p} with Z = 30, 39 and N = 39 of panel (a), Z = 39 of panel (d) and Z = 84-86 of panel (l) of Fig. 4. These exceptional cases are either very close to closed shells or midshell. The reason for these deviations should be studied in the future.

From Eqs. (3)–(4) we obtain

$$[S_{2n}(Z, N) - S_{2n}(Z, N-1)]_{\text{pairing}} = V_{\text{pairing}}(Z, N) - V_{\text{pairing}}(Z, N-2) - V_{\text{pairing}}(Z, N-1) + V_{\text{pairing}}(Z, N-3)$$

$$\simeq -a_{\text{pairing}} A^{-4/3} \begin{cases} 8/3(1-I) & \text{for even } Z & \text{and even } N \\ 14/3 - 16I/3 & \text{for odd } Z & \text{and even } N \end{cases}$$

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$$[S_{2n}(Z, N) - S_{2n}(Z, N-1)]_{\text{sym}} = V_{\text{sym}}(Z, N) - V_{\text{sym}}(Z, N-2) - V_{\text{sym}}(Z, N-1) + V_{\text{sym}}(Z, N-3)$$

$$\simeq 4c_{\text{sym}}(A^{-1} - \kappa A^{-4/3}) + 2c_{\text{sym}}A^{-2}(9 - 4IA) + 8c_{\text{sym}}\kappa A^{-7/3}(4IA/3 - 3).$$
(12)

In Eq. (12) $[S_{2n}(Z, N) - S_{2n}(Z, N-1)]_{\text{pairing}} \sim -0.01$ and -0.02 MeV for $^{188}_{76}$ Os and $^{179}_{77}$ Ir, and $[S_{2n}(Z, N) - S_{2n}(Z, N-1)]_{\text{sym}} \sim -0.33$ MeV for $^{188}_{76}$ Os and $^{179}_{77}$ Ir. Eq. (12) shows that $S_{2n}(Z, N)$ is always smaller than $S_{2n}(Z, N-1)$ by ~ 0.3 MeV on average for $A \ge 100$. This is essentially originated from the symmetry energy. Without details we note a subtle odd-even effect as follows. Suppose that both Z and N are even. According to the experimental data, $S_{2n}(Z, N) - S_{2n}(Z, N-1) \simeq -0.41$ MeV, and $S_{2n}(Z, N-1) - S_{2n}(Z, N-2) \simeq -0.28$ MeV, on average. In Fig. 1(j), K is 0.14 MeV, and by using Eqs. (7) and (11) one obtains that $S_{2n}(Z, N) - S_{2n}(Z, N-1) \simeq -2K \simeq -0.28$ MeV. This is close to $[S_{2n}(Z, N) - S_{2n}(Z, N) -$

In Table I, we list the root-mean-squared deviations (RMSD) (in keV) of predicted values by using Eq. (2) with respect to experimental values for S_n , S_p , S_{2n} , and S_{2p} compiled in the AME2011-preview [7] in different shells. One sees large RMSD values for S_{2n} of Figs. 3(b), 3(d), 3(h), and 3(l) and for S_{2p} of Figs. 4(a), 4(d), and 4(l). The RMSD values of these cases would be reduced if our above exceptions were excluded: the RMSD values would be 368, 291, 368, and 380 keV for S_{2n} in Figs. 3(b), 3(d), 3(h), and 3(l); is 342, 336, 383 keV for S_{2p} in Figs. 4(a), 4(d), and 4(l), respectively.

The small RMSD of Eq. (2) from experimental data encourages us to go further. One might apply these linear relations in terms of $\alpha N_p \pm N_n$ in predicting unknown separation energies. Towards that goal, one should first investigate their predictive power. Here we take the experimental database



FIG. 3. (Color online) Same as Fig. 1 except for S_{2n} (in MeV) versus $\alpha N_p + \beta N_n$.



FIG. 4. (Color online) Same as Fig. 1 except for the S_{2p} (in MeV) versus $\alpha N_p + \beta N_n$.

of the AME2003 [17] and predict separation energies. We compare our predicted separation energies which were not

TABLE I. The root-mean-square deviations (RMSD) (in keV) of linear relations in terms of $\alpha N_p \pm N_n$ for S_n , S_p , S_{2n} , and S_{2p} with respect to the AME2011-preview [7], for different mass regions.

Ζ	S_n	S_p	S_{2n}	S_{2p}
(a)	254	305	335	455
(b)	267	197	422	158
(c)	170	287	190	185
(d)	258	230	328	452
(e)	166	283	190	235
(f)	201	211	108	185
(g)	195	138	225	184
(h)	259	241	432	303
(i)	191	215	245	304
(j)	174	213	248	299
(k)	92	120	88	96
(1)	291	277	473	479

accessible experimentally in the AME2003 [17] but were measured in the last decade and compiled in the AME2011preview [7]. These new experimental data include 131 S_n , 131 S_p , 104 S_{2n} , and 118 S_{2p} . In Table II the RMSD values of our predicted separation energies with respect to these new experimental data are listed and compared with those of predicted results in Refs. [9,17]. One sees that the predictions in this paper works very well except cases (a)-(c) and (l) (i.e., small-A and the largest A cases). Among them, for (d), (e), (g), and (k) the predicted results are competitive with those in Refs. [9,17]. Therefore, we present our predicted separation energies based on the AME2011 experimental database [7] for these four cases. Our predicted results include 480 unknown S_n , 296 S_p , 354 S_{2n} , and 221 S_{2p} by either interpolation or extrapolation according to Eq. (2). These predicted results are tabulated in [18].

To summarize, in this paper we study separation energies, S_n , S_p , S_{2n} , and S_{2p} , in the valence correlation scheme. These separation energies are linear in terms of $\alpha N_p \pm N_n$. This work is an extension of Ref. [3], in which S_n and S_p of even-even nuclei were investigated. Here we consider all types of nuclei,

TABLE II. The RMSD's (in keV) of our predicted separation energies based on the experimental database compiled in the AME2003 [17], with respect to new experimental data which are not experimentally accessible in the AME2003 but compiled in the AME2011-preview [7], including 131 S_n , 131 S_p , 104 S_{2n} , and 118 S_{2p} . (I, II, III) correspond to the RMSD of our predicted results assuming the experimental database of AME2003, and the RMSD of predicted results in the AME2003 [17] and in Ref. [9], respectively. We also present the numbers of these new experimental data of the AME2011-preview [7] in each mass region (denoted as N). One sees that the accuracy of our predictions are competitive in a few regions in comparison with Refs. [9,17].

Ζ	$\frac{S_n}{(I)/(II)/(III)/\mathcal{N}}$	$\frac{S_p}{(\mathrm{I})/(\mathrm{II})/(\mathrm{III})/\mathcal{N}}$	$\frac{S_{2n}}{(\mathrm{I})/(\mathrm{II})/\mathcal{N}}$	$\frac{S_{2p}}{(I)/(II)/(III)/\mathcal{N}}$
(b)	260/207/309/15	393/227/231/15	442/278/438/12	432/271/372/15
(c)	568/430/355/12	327/374/459/14	766/557/574/8	327/378/385/15
(d)	180/179/206/7	308/343/341/8	229/410/471/7	248/631/576/7
(e)	256/194/182/15	258/432/376/13	356/310/264/13	468/648/516/13
(f)	210/77/177/16	240/106/202/16	467/117/192/12	305/123/142/10
(g)	186/410/197/3	275/430/241/6	200/413/204/3	201/369/176/2
(h)	326/193/192/16	277/339/260/17	607/233/223/15	580/326/270/17
(i)	208/101/104/16	322/99/91/13	141/113/119/7	457/95/101/9
(j)	_/_/_/_	_/_/_/_	_/_/_/_	_/_/_/_
(k)	173/-/232/6	81/-/302/5	73/-/213/7	99/-/160/5
(1)	369/84/111/22	330/82/214/20	614/89/172/17	547/98/261/21

not only even-even but also odd-mass and odd-odd. In addition we also discuss S_{2n} and S_{2p} .

Two types of odd-even staggerings are discussed. First, S_n for nuclei with even neutron numbers N are systematically larger than those of their odd-N neighbors, and similarly, S_p for nuclei with even proton numbers Z are systematically larger than those of their odd-Z neighbors. This odd-even staggering has been known and understood well in the literature. Second, S_n for an even-even nucleus is very slightly larger than that of its neighboring nuclei with odd Z and even N, and S_n of an odd-odd nucleus is slightly larger than that of its neighboring nuclei si slightly larger than that of its neighboring nuclei with even Z and odd N. Similarly, S_p for an even-even nucleus is slightly larger than that of a even even even nucleus is slightly larger than that of its neighboring nuclei with even Z and odd N. Similarly, S_p for an even-even nucleus is slightly larger than that of its neighboring nuclei with even Z and odd N, and S_p of an odd-odd nucleus is slightly larger than that of its neighboring nuclei with odd Z and even N. This is a very subtle effect, and is discerned in this paper.

We discuss the above odd-even staggerings of these separation energies in terms of pairing correlation and symmetry energy of the mass formula in Ref. [8]. The pairing and symmetry energy terms present the staggerings reported here with desired behaviors, yet there are sizable differences (20–30%) in magnitude between staggerings exhibited by experimental data (i.e., Figs. 1–4) and those given by pairing and symmetry energy. Further studies in future are thus warranted to understand these staggerings.

We also discuss the accuracy of the linear relations between these separation energies in terms of $\alpha N_p \pm N_n$. For many cases these relations works remarkably well. We make use of these relations and predict S_n , S_p , S_{2n} , and S_{2p} for a few regions.

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