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Neutron-proton pairing reexamined

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We reexamine neutron-proton pairing as a phenomenon that should be explainable in a microscopic theory of nuclear binding energies. Empirically, there is an increased separation energy when both neutron and proton numbers are even or if they are both odd. The enhancement is present at some level in nearly all nuclei: the separation energy difference has the opposite sign in less than 1% of the cases in which sufficient data exist. We discuss the possible origin of the effect in the context of density functional theory (DFT) and its extensions. Neutron-proton pairing from mean-field theory does not seem promising to explain the effect. Gao and Chen have argued that a significant part of the increased binding in odd-odd deformed nuclei might arise as a recoupling energy, and we find a similar result for spherical nuclei. This suggests that the DFT should be extended by angular momentum projection to reach an accuracy capable of treating this effect.

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It has long been known that nuclear binding has a mild dependence on the combined even-odd parities of proton and neutron numbers [1–3]. Except for the study of Gao and Chen [4], there has been very little quantitative theoretical work to describe the phenomenon. In this Brief Report we re-examine the systematics and make some suggestions concerning the necessary theory to treat it.

The neutron-proton pairing effect is ubiquitous in the nuclear mass table. To see it visually, we show in Fig. 1 the neutron separation energies of an isotone chain, neutron number $N = 28$, as a function of proton number Z. Plotted is the separation energy, related to the binding energy by $S_n(N, Z) = B(N, Z) - B(N - 1, Z)$. One sees that the neutron separation energies for even Z are systematically larger than the average of the separation energies for the neighboring odd-Z nuclei. Similar behavior is found for proton separation energies S_p in chains of isotopes. In that case S_p is greater if the number of neutrons is even than when the number of neutrons is odd.

To study this behavior in more detail, we examine the separation energy differences S_{n2p}, S_{p2n}, defined as the difference between the separation energy and the average for the two neighboring nuclei. This is

$$\begin{aligned} S_{n2p} &= S_n(N, Z) - [S_n(N, Z + 1) + S_n(N, Z - 1)]/2 \\ S_{p2n} &= S_p(N, Z) - [S_p(N + 1, Z) + S_p(N - 1, Z)]/2 \end{aligned} \quad (1)$$

for neutrons and protons, respectively. These measures were first introduced by Jensen *et al.* [5]. Using this notation, the usual measure for ordinary pairing is given by Ref. ([1] Eqs. 2–92, 2–93)

$$\begin{aligned} 2\Delta_n \equiv S_{n2n} = S_n(N, Z) - [(S_n(N + 1, Z) \\ + S_n(N - 1, Z)]/2 \end{aligned} \quad (2)$$

for the neutron gap, Δ_n, and similarly S_{p2p} gives the proton gap. Most earlier studies of neutron-proton pairing used different measures for the effect. In early fits of the measured binding energies [3,6], the effect was parametrized as $\delta \sim \text{mod}(N, 2)\ \text{mod}(Z, 2)/A$ and attributed to an enhancement in the neutron-proton interaction. In Ref. [7], the parameterization was changed to one have an approximate $A^{-2/3}$ dependence on nuclear mass number,

$$\delta = K\ \text{mod}(N, 2)\ \text{mod}(Z, 2)/A^{2/3}. \quad (3)$$

In Ref. [8] a nine-point difference formula was proposed to describe a neutron-proton pairing energy. This is to be compared the six-point difference formula we use in Eq. (1). We also mention the shell-based mass fits of Zeldes [2], which invoke a shell-dependent term similar to δ.

The signs of S_{n2p} and S_{p2n} are remarkably consistent across the nuclear mass table. Taking experimental data from the 2003 Audi-Wapstra mass tables [9], there are 1412 nuclei that have values of S_{n2p} that are significant, i.e., have magnitudes larger than the accumulated error in the experimental binding energies needed to construct the difference. Of these only 10 nuclei had a sign for S_{p2n} opposite to that seen in Fig. 1. Of the 1448 measured proton separations S_{n2p}, only nine had the opposite sign. The nuclei with significant values of S_{p2n} for proton separations are shown in Fig. 2, with the few opposite-sign cases shown as the black squares. The plot for neutron separations is very similar. There is concentration in the light nuclei near the $N = Z$ line but no obvious pattern elsewhere.

We next display the magnitude of the separation energy differences as a function of the mass numbers, A, of the nucleus. This is plotted in Fig. 3. There is a great deal of scatter, but the trend is consistent with an $A^{-2/3}$ dependence as in Eq. (3). The heavy line shows a least-squares fit to the data, $|S_{p2n}| = 7.3/A^{2/3}$ MeV. The values for $|S_{n2p}|$ have a similar distribution. An obvious question is whether the size of the effect correlates with proximity to shell closures. To see if there any obvious trends, we plot in Fig. 4 the measured nuclei whose $|S_{p2n}|$ is larger than the average. There is no visible dependence on shell closures. The behavior of $|S_{n2p}|$ is very similar in that there is no obvious pattern in the location of the larger values.

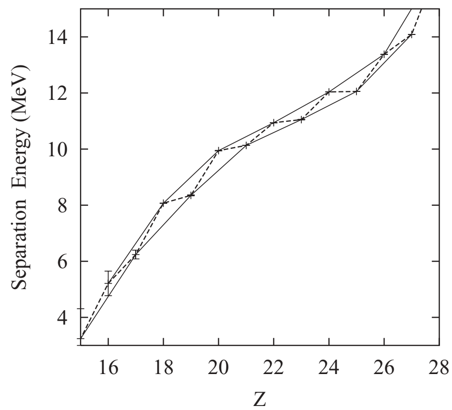

FIG. 1. Neutron-proton pairing effect as seen in the neutron separation energy for $N = 28$ as a function of proton number Z. There is a consistent offset of the separation energies of odd-Z nuclei as compared with the average of the neighboring even-Z nuclei.

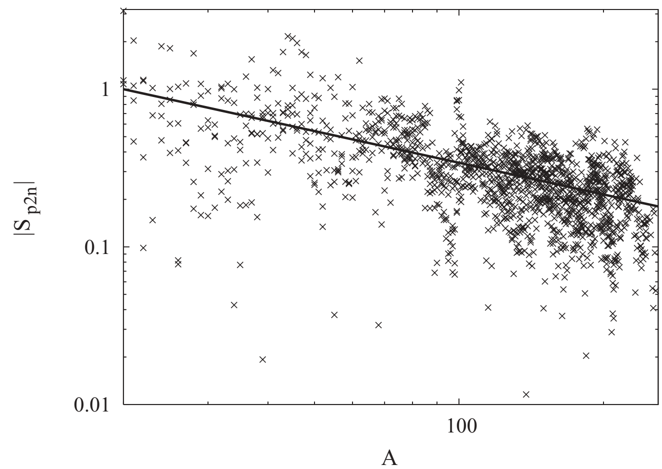

FIG. 3. $|S_{p2n}|$ as a function of A. The line shows the $A^{-2/3}$ fit Eq. (3) with $K' = 7.3$ MeV.

There is another strong neutron-proton pairing effect that does not appear in nuclei away from the $N = Z$, the Wigner energy. It is often expressed [10]

$$W(A)|N - Z| + d(A)\delta_{NZ}[1 - \mathrm{mod}(N, 2)][1 - \mathrm{mod}(Z, 2)]. \quad (4)$$

The second term has the obvious form of a neutron-proton pairing. The Wigner energy has been much discussed in the the literature (see, e.g., Refs. [10,11]) and we have nothing to add here. Note however that the most of the cases where S_{n2p} or S_{p2n} has the opposite sign are for nuclei near $N = Z$.

We now turn to the question of how to understand the global neutron-proton pairing effect. The enhanced binding could arise by an increased attraction between an odd neutron and an odd proton. It could also arise by a mechanism that produced an increased binding in a nucleus with even numbers for both protons and neutrons. There is no way to distinguish these pictures by the observed systematics of the separation energy differences, because even-even and odd-odd binding energies contribute to the separation energy difference with the same weights. Both pictures are consistent with the strong similarity between the proton and neutron separation energy differences. Still, it is important to understand the origin of the effect if one is to construct accurate theories of nuclear binding based on microscopic theories such as the self-consistent mean-field theory, also called density functional theory (DFT) [12,13].

We first examine whether the usually DFT treatment produces a significant neutron-proton pairing. We calculated values of S_{n2p} for a small sample of cases for which the measured values are large. Also, we have picked cases where $N - Z > 6$ to avoid the influence of the Wigner energy. To carry out these calculations we used the code ev8 [14] with the SLy4 density functional that is widely used for global studies [15]. Ordinary nn and pp pairing are treated in the BCS approximation. The code was modified to calculate the binding energies for odd-even, even-odd, and odd-odd isotopes by blocking the odd orbitals. The modification allowed the odd nucleon to occupy a quasiparticle orbital near the Fermi level of the even neighbor. With this modification, ev8 treats the

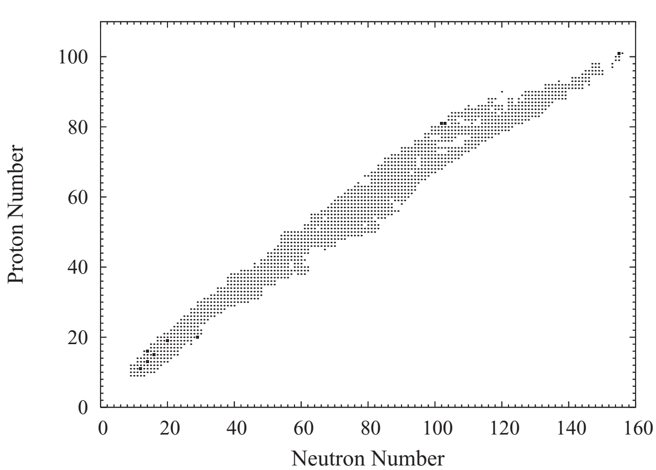

FIG. 2. Nuclei with measured proton separation energy differences S_{p2n} showing the cases (black squares) with opposite sign from the normal.

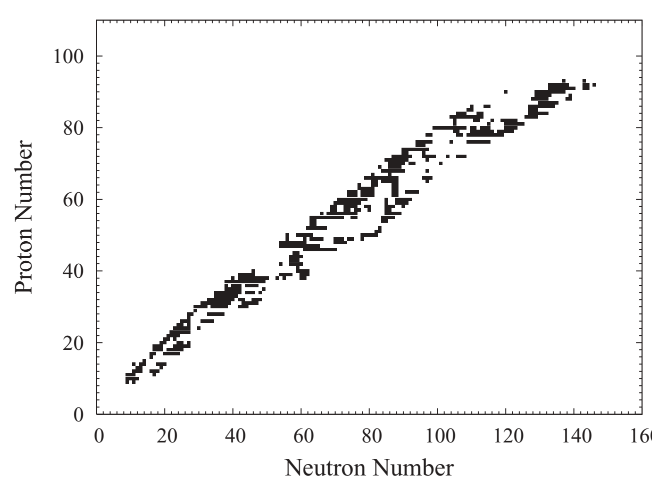

FIG. 4. Chart of nuclides showing those that have $|S_{p2n}|$ values higher than the average trend $|S_{p2n}| = 7.3/A^{2/3}$ MeV.

TABLE I. Comparison of DFT+BCS calculations of S_{n2p} with measured values. Energies are in MeV.

N	Z	Calculated	Measured
27	21	−0.023	0.526
37	27	−0.047	0.616
40	32	−0.049	0.699

interaction of the odd particles due to the time-even fields generated by the energy functional. The calculated values for S_{n2p} are compared to the measured values in Table I. It can be seen that these are all more than an order of magnitude smaller than the measured values. It is clear that some extension is needed to the usual DFT+BCS with time-even fields.

Next we discuss an explicit treatment of neutron-proton pairing in the framework of a generalized HFB theory. The extension of DFT in this way is formally quite straightforward [16]. Certainly, at the $N = Z$ line neutron-proton pairing is on the same footing as like-particle pairing and could contribute to the Wigner energy. It is usually parametrized in a way that does not exhibit a neutron-proton pairing effect away from the $N = Z$ line and we shall consider it irrelevant to explain the effect. There have also been limited studies of neutron-proton pairing in the HFB theory [11,17,18]. Typically, away from the $N = Z$ line, condensates form in the like-particle sectors and prevent any pairing between neutrons and protons. We therefore doubt whether the effect can be explained without make some extension of the usual DFT+HFB theory.

There is a possible mechanism that only requires a mild extension of the DFT. That is to exploit the higher degeneracy of states in the odd-odd nucleus to recouple the neutron and proton more favorably. This is easiest to understand in the situations where the mean-field theory approaches either the spherical shell model or the strongly deformed limit. Indeed, Zeldes and Liran [2] may have had this mechanism in mind in their shell-based mass parametrization. For the shell-model limit, consider even-even nucleus (N, Z) that has a spherical mean field. An added neutron goes into a spherical shell j_n with an energy ϵ_{j_n}. Similarly, an added proton goes into a shell j_p. When there are both added neutrons and protons, there is an additional neutron-proton interaction energy $\langle j_n j_p|V_{np}|j_n j_p\rangle_J$ depending on the angular momentum of the pair J. The neutron separation energies for the nuclei with proton numbers Z, $Z + 1$, $Z + 2$ are, respectively,

$$S_n(N+1, Z) = -\epsilon_{j_n} \tag{5}$$

$$S_n(N+1, Z+1) = -\epsilon_{j_n} - \langle j_n j_p|V_{np}|j_n j_p\rangle_{J_g} \tag{6}$$

$$S_n(N+1, Z+2) = -\epsilon_{j_n} - \left\langle j_n \left(j_p^2\right)^{J=0} \middle| V_{np} \middle| j_n \left(j_p^2\right)^{J=0}\right\rangle_{j_n}. \tag{7}$$

In the second equation, J_g denotes the angular momentum of the odd-odd nucleus ground state. The last equation gives the neutron separation energy for the nucleus with two additional protons. Here the angular momentum coupling is determined by the three-particle wave function. In the spherical shell model, the two protons are coupled to angular momentum zero in the three-particle wave function $|j_n(j_n^2)^{J=0}\rangle$. Standard angular momentum recoupling gives the neutron-proton interaction as

$$\begin{aligned}\left\langle j_n \left(j_p^2\right)^{J=0} \middle| V_{np} \middle| j_n \left(j_p^2\right)^{J=0}\right\rangle_{j_n} &= 2 \sum_{J=|j_n-j_p|}^{j_n+j_p} (2J+1)\langle j_n j_p| \\ &\quad \times |V_{np}|j_n j_p\rangle_J/(2j_n+1)(2j_p+1).\end{aligned} \tag{8}$$

Thus, in the shell model, the additional energy of the odd neutron when the proton pair is added is twice the $(2J + 1)$-weighted average over the possible neutron-proton couplings.

This value can be estimated empirically from the spectrum of the odd-odd nuclei as the quantity

$$\delta_s = \sum_{J=|j_n-j_p|}^{j_n+j_p} (2J+1)E_J/(2j_n+1)(2j_p+1). \tag{9}$$

Here E_J are measured excitation energies of the levels of the multiplet in the odd-odd nucleus. The quantity δ_s is thus a measure of the enhancement of the neutron separation energy for an odd neutron in a nucleus with an odd number of protons.

For most odd-odd nuclei, the recoupling spectrum is difficult to determine due to the presence of other levels. However, near doubly magic nuclei it is often possible to make a spectroscopic identification [19]. Some cases where we could plausibly assign the members of the multiplet are shown in Table II. These results are also shown in Fig. 5. The recoupling energy δ_s has the same order of magnitude as the separation energy differences and also varies from case to case in a similar way. However, there is considerable scatter leaving room for other mechanisms is to have a role.

The recoupling effect has also be estimated in strongly deformed nuclei [4]. Odd-odd deformed nuclei have a two-fold degeneracy of the ground state depending on whether the K quantum numbers of the odd particles are parallel or antiparallel. The quantity analogous to δ_s in Eq. (3) is half the energy difference of the two intrinsic states. The K-dependent interaction energies have been tabulated [21] and compared with the separation energy differences in Ref. [4]. The recoupling energies are significant but about a factor of two smaller than the separation energy differences.

TABLE II. Comparison of neutron-proton pair interaction energies with the recoupling model [Eq. (9)]. Energies are in MeV. The quantity δ_s is defined in Eq. (9).

N	Z	S_{p2n}	S_{n2p}	δ_s
21	19	0.49	0.32	0.44
27	21	0.39	0.53	0.70
29	21	0.25	0.30	0.32
29	27	0.30	0.31	0.38
29	29	0.81	0.78	0.65
33	27	0.20	0.29	0.15
81	51	0.24	0.22	0.14
125	83	0.03	0.03	0.06
127	81		0.15	0.04
127	83	0.36	0.36	0.42

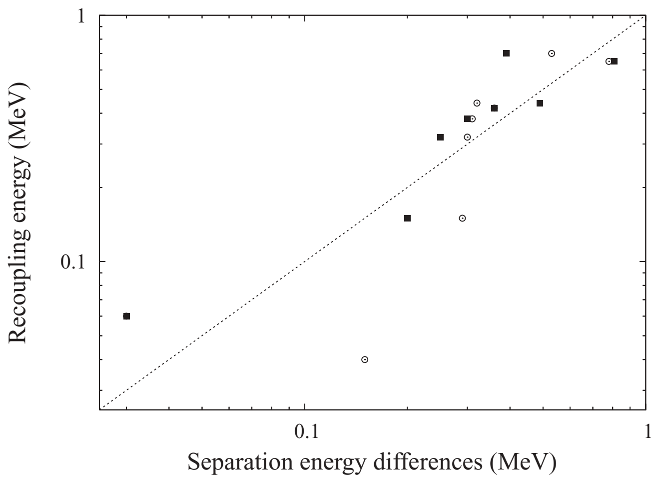

FIG. 5. Scatter plot of δ_s, Eq. (3), compared with S_{p2n} (solid squares) and S_{n2p} (circles). The nuclei plotted are ^{40}K, ^{48}Sc, ^{50}Sc, ^{56}Co, ^{60}Co, ^{58}Cu, ^{208}Tl, ^{208}Bi, and ^{210}Bi.

Independently, we have examined whether the separation energy differences are altered in deformed nuclei. One might expect the recoupling effect to be smaller in deformed nuclei because of the greater restriction on orientations. We took the classification of deformed nuclei from Ref. [20], which used the theoretical criterion that the static deformation of the nucleus be larger than the fluctuations about the minimum. There are 92 nuclei with measured S_{n2p} that meet the criterion. Fitting Eq. (3) to these nuclei, we find a slightly lower value for K, 5.7 MeV compared to 7.3 MeV. Also a larger fraction of the deformed nuclei have very small values of the separation energy differences: 23% of the deformed nuclei have S_{n2p} less than $3.7/A^{2/3}$ MeV versus 9% for the other nuclei. The difference is not very large, suggesting that other mechanism beyond the recoupling effect may be needed.

In conclusion, neutron-proton pairing is pervasive in the nuclear mass table, but there is no apparent systematic theory that can account for it. The effect is clearly beyond the mean-field theory calculated with the usual BCS pairing. We regard HFB with static neutron-proton pairing as unlikely to explain the effect. We showed that recoupling effects in the odd-odd nucleus can account for much of the effect in some nuclei. Other correlation effects may have a role as well and should be investigated.

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