Pairing and shell gaps in nuclei

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Abstract. The pairing contribution to the odd-even oscillations in the nuclear binding energies is considered in the framework of the nuclear shell model. Schematic and realistic Hamiltonians are used to understand the trends related to pairing and shell gaps. Detailed results are shown and discussed for the calcium isotopes. Results are also shown for carbon, oxygen and neon as well as the overall trends for all nuclei.

1. Introduction
One of the most robust signatures of pairing in nuclei is the odd-even oscillation in binding energies (BE) as a function of neutron or proton number. This is illustrated in Fig. 1 which shows the energies, $E$, and one-neutron separation energies, $S_n$, for the calcium isotopes. The figure shows the results of a shell-model calculation in the $(0f_{7/2}, 0f_{5/2}, 1p_{3/2}, 1p_{1/2})(fp)$ model space with the GX1A Hamiltonian (also referred to as GXPF1A in the literature [1]) compared with experiment. We will discuss the oscillation in the one-neutron separation energies as a function of neutron number in terms of the energy differences

$$D_n(N) = (-1)^{N+1}[S_n(Z, N+1) - S_n(Z, N)] = (-1)^N[2BE(Z, N) - BE(Z, N-1) - BE(Z, N+1)]$$

(1)

where $S_n(N) = BE(Z, N) - BE(Z, N - 1)$ is the one-neutron separation energy (BE = -$E$). $N$ is the number of neutrons and $Z$ is the number of protons. This quantity turns out to be always positive and reflects the fact that the even nuclei are always more bound on the average than the neighboring odd nuclei. We will distinguish the results for even and odd $N$ value by, $D_{ne}$ and $D_{no}$, respectively. In the literature one commonly finds the related quantity $\Delta_n(N) = \frac{D_n(N)}{2}$. We use $D$ rather than $\Delta$ because its values are more directly connected to simple underlying quantities associated with pairing and shell gaps. Equivalent equations as a function of proton number are obtained by fixing $N$ and varying $Z$.

Fig. 2 shows values of $D_n$ for the calcium isotopes ($N > 20$) obtained from experiment and from two commonly used Hamiltonians in the $fp$ model space, KB3G [2] and GX1A [1]. We also show the excitation energies for the lowest $2^+$ states of the even nuclei. The trends observed in Fig. 2 will be understood on the basis of both simple and realistic models. This will lead to an understanding of the results for all nuclei.

One observes in Fig. 2 a rather complicated experimental trend that is rather well reproduced by the calculations. The results for the two Hamiltonians are similar up to $N = 33$ where the experimental data are known. Beyond $N = 33$ there are differences, in particular for $N = 34$.
Figure 1. The bottom panel shows the ground-state energies for the calcium isotopes obtained from the $pf$ shell-model calculation with the GX1A Hamiltonian relative to $^{40}$Ca with filled circles even $N$ and open circles for odd $N$, all connected by a line. The crosses are the experimental data. The top panel shows the one-neutron separation energies for GX1A and experiment.

($^{54}$Ca), where the GX1A result for the $D$ and $E_x(2^+)$ values are nearly two times larger than for those for KB3G.

Fig. 2 also shows the results obtained for GX1A when all of the single-particle energies are set equal to each other. The result does not depend on the value of the single-particle energy since in this degenerate case the one-body part of the Hamiltonian does not contribute differences of Eq. (1). The result is a very regular oscillating pattern. What we learn from this is that the larger irregularities observed in the upper panels of Fig. 2 are due to the finite spacing of the single-particle energies related to the shell gaps.

In this contribution we show how the results for $D$ in Fig. 2 and other nuclei arise from schematic and realistic interactions between nucleons. An essential ingredient will be the pairing part of the interaction, but the consequences of pairing will be influenced by shell gaps and other components of the interactions. We start with the schematic surface-delta interaction in the next few sections, and then come to more realistic interactions. In the last sections we examine the results for $D$ in light nuclei out to the neutron-drip line, and also show the experimental results.
for all nuclei. The experimental masses were taken from the intermediate evaluation of Audi and Wang [3] supplemented by more recent data on $^{51,52}$Ca [4] and $^{26}$O [5].

2. The surface-delta interaction model

To get some insight into the reasons for the patterns observed in Fig. 2, we start with the simple “surface-delta-function” (SDI) model for $V$ [6]. The two-body matrix elements for a delta function $V(| \vec{r}_1 - \vec{r}_2 |) = \delta A | \vec{r}_1 - \vec{r}_2 |$ can be obtained analytically as a product of angular and radial matrix elements, $< V > = < V >_{\text{ang}} < V >_{\text{rad}}$ where

$$< V >_{\text{rad}} = \int R_a(r)R_b(r)R_c(r)R_d(r)r^2dr. \quad (2)$$

where $a, b, c$ and $d$ label the single-particle states with quantum numbers $(n, \ell, j)$, and $R(r)$ are the radial wavefunctions. For the SDI one evaluates this integral at the surface, $r = r_o$, and assumes that

$$| R_a(r_o) | = | R_b(r_o) | = | R_c(r_o) | = | R_d(r_o) | = R. \quad \text{Then} \quad < V >_{\text{rad}} = (-1)^{n_a+n_b+n_c+n_d}R^2_{r_o} = (-1)^{n_a+n_b+n_c+n_d}C,$

where the phase factor is used for the radial wavefunction convention of being positive near the origin. The SDI two-body matrix elements for $J = 0$ are

$$< aaJ = 0 | \text{SDI} | bbJ = 0 > = (A'/2)\sqrt{(2j_a + 1)(2j_b + 1)}. \quad (3)$$

The results obtained with SDI for the $fp$ model space with degenerate single-particle energies is shown in Fig. 3. We have chosen the constant $A' = 4\pi A(-1)^{n_a+n_b+n_c+n_d}C = 0.4$ MeV in order to make the value $D = 4$ MeV similar to that obtained for the GX1A Hamiltonian when the single-particle energies are degenerate.

For the SDI the $D$ and $E_x(2^+)$ are constant. The SDI with degenerate single-particle energies has some very simple and interesting properties [7]. The $J = 0$ pairing properties are determined only by strength of the interaction and by the total number of possible pairs, $m/2 = 10$ in our example, where $m = 20$ is the maximum number of valence neutrons. Exactly the same results for $D$ are obtained if there were a single orbital with $j = 19/2$, but the value of $E_x(2^+)$ depends upon the $j$ values. Use of a delta function with the radial integral evaluated with oscillator or Woods-Saxon radial wavefunctions gives results that are close to SDI (within about 5%), but the properties are more complicated but analytic (oscillator) or non analytic (Woods-Saxon).

In addition to $D$ and $E_x(2^+)$ we show in Fig. 3 the energies obtained when the degenerate single-particle energies are zero (if the energies were not zero there would be an additional linear dependence to the total energies). The total energy for SDI [line (a) in Fig. 3] as a function of the number of valence neutrons, $n$, is very simple

$$E(n) = \frac{nV_o}{2} \quad \text{even} \ n, \quad \text{and} \quad E(n) = \frac{(n-1)V_o}{2} \quad \text{odd} \ n, \quad (4)$$

where $V_o$ is the interaction energy for two-nucleons in the $J = 0$ paired state. We also have $D = -V_o$. All of the odd $N$ nuclei have four degenerate states with $J^\pi = 1/2^-, 3/2^-, 5/2^-$ and $7/2^-$.  

One can also make a “mean-field” approximation for the total energy [line (b) in Fig. 3] with $\bar{E}(n) = n(n-1)V/2$, where the average (monopole) energy, $\bar{V}$ is the total closed-shell energy divided by the total number of $m$ state two-particle combinations ($m = 20$ in this case). We can define the pairing correlation energy as the difference $E^{\text{corr}}(n) = E(n) - \bar{E}(n)$. This is shown by curve (c) in Fig. 3.
3. The modified surface-delta interaction model

One observes two differences between the results in the two lower panels of Fig. 2. One is that the GX1A result tends to fall off as a function of the number of neutrons whereas the SDI result is flat. A part of this is due to the fact that GX1A contains an assumed smooth mass dependence of the form $(A/42)^{-0.3}$ that is meant to take into account a smooth increase in the harmonic oscillator parameters $\bar{h}\omega$ as a function of $A$. This was not included in the SDI. The main reason for the fall off is that the average interactions, $\bar{V}_{ab}$, differ from SDI and lead to a splitting in the single-hole energies for $^{60}$Ca that reduces the effective pairing for larger $N$ values.

The other feature is that the GX1A result for $D$ oscillates whereas the SDI result does not. In the 1960’s this was recognized as a basic failure of the delta and SDI Hamiltonians. It was empirically fixed by adding a constant to the interaction to make the so-called modified-delta interaction [8] of the form $V(| \vec{r}_1 - \vec{r}_2 |) = A\delta(| \vec{r}_1 - \vec{r}_2 |) + B$ where $B$ is the added constant. In terms of two-body interaction it is infinitely long range. With the SDI form of the radial integral this becomes the so-called modified-surface-delta interaction (MSDI). The modern interpretation of this constant is that it comes from core-polarization corrections and three-body interactions. The energy and $D$ values obtained with $B = 0.2$ MeV are shown in Fig. 4. This constant simply adds a term $n(n-1)B/2$ to the all energies, and does not change the correlation energy. It gives an oscillation in $D$: $D_o = -V_o - B$ for odd $n$ and $D_e = -V_o + B$ for even $n$. Half the sum of neighboring even and odd $D$ gives the pairing contribution: $D_a = \frac{1}{2}[D_e(N) + D_o(N-1)] = -V_o$, and half of the difference gives quadratic dependence: $D_b = \frac{1}{2}[D_e(N) - D_o(N-1)] = B$. Fig. 2-5 in Bohr and Mottelson [9] is based upon the $D_a$ combination ($\Delta = D_a/2$).

The Coulomb interaction between protons behaves like the addition of a long-range monopole term ($B \approx 0.31$ MeV for $Z$=20). There is also a small anti-pairing addition to $D_a$ of (about +0.17 MeV for $Z = 20$). This is important for understanding the trends in $D_p(Z)$ compared to
those for $D_n(N)$.

A microscopic calculation of these quadratic monopole corrections requires an explicit consideration of core-polarization the real and induced three-body interactions (those between two-valence nucleons and one in the core). It has been proposed that the density-dependent interactions empirically included in the Skyrme interaction can be used to obtain $B$ values for the valence shell-model interactions [10]. This method improves the relative binding energies obtained for shell-model calculations in heavy nuclei.

![Figure 5](image1)

**Figure 5.** Results obtained with the SDI interaction as a function of the shell gap between the $0f_{7/2}$ and $(0f_{5/2}, 1p_{3/2}, 1p_{1/2})$ set of orbitals. The top panel also show the results for $D$ (thin lines) obtained when the shell gap is infinite.

![Figure 6](image2)

**Figure 6.** Values for $D$ and $E_x(2^+)$ obtained from the one-pion exchange (top two panels), the N$^3$LO interaction (middle panels), and by including three-nucleon interactions [11] (bottom panel).

4. The surface-delta interaction model with a shell gap

Next we show how $D$ changes when the single-particle energies are not degenerate. This requires a computational experiment with the SDI applied to the fp orbits divided into two groups, $f = (0f_{7/2})$, and $r = (0f_{5/2}, 1p_{3/2}, 1p_{1/2})$ with a variable gap in between them, so that the second group is raised in energy relative to the the $0f_{7/2}$. The result is shown in Fig. 5 where
the gap starts at zero and is increased up to four MeV. Four MeV is approximately equal to the experimental shell gap found for \(^{48}\text{Ca}\) \((N = 28)\). When the gap is small (one MeV), the energies of the \(2^+\) states remain flat, and the pairing correlation starts to fall off away from the break at \(N = 28\). When the gap is two MeV there is a small rise in the \(2^+\) energy and a small increase in \(D\) at \(N = 28\). When the gap is above two MeV there is an obvious increase in the \(2^+\) energy and \(D\) and \(D \approx E_x(2^+)\) at the gap. Thus, the relative values of \(D\) and \(E_x(2^+)\) provide a confirming measure of shell gaps. For the calcium isotopes the calculations are carried out with only neutrons in the \(fp\) model space and the \(2^+\) energies are those for neutrons. The experimental states used for comparison are also dominated by the neutron configuration. In other cases when the gap is between orbitals with difference parity, the excitation energy of the relevant negative parity state (like \(3^-\)) should be used. When experimental values of \(E_x(2^+)\) are used one should confirm that the \(2^+\) state in question has the appropriate neutron or proton configuration. Away from semi-magic nuclei the \(2^+\) states usually have strongly mixed proton and neutron configurations.

One can truncate the full \(fp\) calculation by considering only the \(J = 0\) part of the Hamiltonian \([12]\). This method provides a good approximation to ground-state energies for identical-particle systems with realistic Hamiltonians that includes the affects of both pairing and shell gaps.

In the limit of an infinite gap, the results are those shown by the thin line in the top panel of Fig. 5. In this case the total pairing energy that starts out at \(V_\pi = -4\) MeV in the degenerate cases gets divided into two parts, \(V_\pi^f = -1.6\) for the \(0f_{7/2}\) below \(N = 28\) and \(V_\pi^r = -2.4\) for the other three orbitals above \(N = 28\). Unlike the \(D\) which shows a large increase at the shell gap at some even \(N\), the \(D\) for odd \(N\) does not show any direct evidence of the shell gap. As in this example, the \(D\) values often change across a gap because the number of \(m\) states that are involved in the pairing change.

5. Features for the calcium isotopes

We can now understand the features of the calcium isotopes shown in Fig. 2. With the GX1A Hamiltonian there are two large shell gaps at \(N = 28\) and \(N = 34\), and a smaller shell gap at \(N = 32\), related to preferential filling of the orbitals in the order \(0f_{7/2}, 1p_{3/2}, 1p_{1/2}\) and \(0f_{5/2}\). The results for KB3G are similar except that above \(N = 32\) the \(1p_{1/2}\) and \(f_{5/2}\) orbitals are closer together and there is no shell gap at \(N = 34\). The smallest \(D_{no}\) value occurs for \(^{53}\text{Ca}\) \((N = 33)\) (0.43 MeV for GX1A). If confirmed experimentally this would be smallest \(D_{no}\) value in all nuclei. It is related to the fact that there is some shell gap on both sides of the \(1p_{1/2}\) orbital which has the smallest possible pairing matrix element (see Eq. (3)). Experimental confirmation of this is important.

The results for \(D\) and \(E_x(2^+)\) obtained with the bare one-pion exchange potential are shown at the top of Fig. 6. One-pion exchange provides almost no pairing. The middle of Fig. 6 shows the results obtained with the N²³LO potential \([13]\) in first order and in second order. Almost half of the pairing comes from the second-order corrections, and most of this comes from the bubble diagrams mediated by the tensor interaction. This is also seen in calculations for the heavy nuclei \([10]\). Also the second-order correction changes the sign of the quadratic term (the sign of the odd-even oscillations) to bring the result into close agreement with experiment. The bottom panel of Fig. 6 shows the results obtained with the inclusion of three-nucleon interactions from \([11]\). The three-nucleon interactions improve the agreement with experiment for the shell gap at \(N = 28\), but at the expense of giving an upward trend in the \(D\) values as one approaches \(N = 28\) that does not agree very well with experiment. The empirical interactions KB3G and GX1A reproduce the shell gap at \(N = 28\) due to monopole adjustments of the two-body matrix elements. We can conclude that these type of monopole adjustments take into account the (missing) three-nucleon interactions.
6. Light nuclei toward the neutron drip line

How do the $D$ values change as we approach the neutron drip line? The heaviest isotope for which the neutron drip line has been reached is oxygen where it is located at $N = 16$ ($^{24}$O). Recent experiments on neutron decay have established the energies of the lowest neutron-unbound state in $^{25}$O [14] and $^{26}$O [5]. These results together with other mass data have been used for Fig. 7 that shows the $D_n$ values for carbon, oxygen and neon. For oxygen large shell gaps are observed for $N = 6$ (a) and 8 (b) with two smaller ones at 14 (c) and 16 (d). $^{20}$Ne with $N = 10$ shows the Wigner-cusp at (e) due to proton-neutron pairing ($T = 0$ and $T = 1$) [15]. $^{12}$C at $N = 6$ (a) should also have a Wigner-cusp, but it is on top of the shell gap at $Z = 6$. The $2^+$ states for neutron-rich carbon and oxygen are dominated by the the neutron configuration and can be compared to the $D$ values. The $2^+$ states for carbon and neon have mixed proton-neutron configurations.

![Figure 7](image1.png)

**Figure 7.** Experimental values for $D$ and $E_x(J^\pi)$ for the carbon, oxygen and neon isotopes. $J^\pi$ is $2^+$ except for $^{14}$C, $^{16}$O and $^{18}$Ne where it is the lowest observed negative parity state.

![Figure 8](image2.png)

**Figure 8.** $D_n$ for all nuclei. Values for for even $Z$ are given as a function of the number of neutrons ($N > Z$) connected by lines. $D_{ne}$ are for even $N$, $D_{no}$ are for odd $N$ values, $D_{na}$ are the averages and $D_{nb}$ are the differences given in Sec. 3. The vertical lines show the location of the magic numbers 20, 28, 50, 82 126.
The small $D_{no}$ values at $N = 15$ (f) is related to the filling of the $1s_{1/2}$ orbital at this point; $^{25}$O and $^{27}$Ne have $1/2^+$ ground states. Shell-model calculations such as those in the $p-sd$ model space with the WBP Hamiltonian [16], and in the $sd$ model space with the USDA/B Hamiltonians [17] are in general good agreement with these data. The main exception is that WBP strength needs to be reduced by about 25% in order to reproduce the experimental energies for the neutron-rich carbon [18]. For WBP one assumed that the interaction (including pairing) is the same for oxygen and carbon. A similar situation exists for a reduction of the interaction strength in the silicon isotopes ($Z = 14$) compared to calcium [19]. Two possible reasons for this reduction are: (1) The radial matrix for the bare interaction elements become smaller for more loosely bound neutrons. This can be qualitatively modeled by evaluating Eq. (2) with Woods-Saxon or Hartree-Fock radial wavefunctions. (2) The core-polarization corrections to the matrix elements are reduced.

Both of these effects have been considered in Ref [20], where it was found that (1) is most important for silicon. Thus we may expect pairing to be reduced as one approaches the drip line simply due to the fact that the neutrons are on the average further apart. This is confirmed by the small value of $D_{no}$ for $^{25}$O ($N = 17$) (g) where the $0d_{3/2}$ and the $1p_{3/2}$ orbitals start to fill. Understanding the situation near and beyond the neutron drip line will require an explicit consideration of the continuum part of the wavefunctions.

The examples we have discussed are part of the complete set of data shown in Fig. 8. It is interesting to compare the experimental systematics with those obtained from various mean-field (e.g. [21]) and configuration-mixing models. In the next decade we expect a tremendous growth in the data for masses of neutron-rich nuclei from radioactive beam facilities. These are essential for understanding how the pairing and shell gap properties evolve as one approaches the neutron drip line.

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References
[1] Honma M, Otsuka T, Brown B A and Mizusaki T 2002 Phys. Rev. C 65 061301(R); 2004 Phys. Rev. C 69 034335; 2005 Euro. Phys. Jour. A 25 Suppl. 1 499
[2] Poves A, Sanchez-Solano J, Caurier E and Nowacki F 2001 Nucl. Phys. A 694 157
[3] Audi G and Wang M 2011 private communication
[4] Gallant A T, et al. 2012 Phys. Rev. Lett. 109 032506
[5] Lunderberg E, et al. 2012 Phys. Rev. Lett. 108 142503
[6] Plastino A, Arvieu R and Moszkowski S A 1966 Phys. Rev. 145 837
[7] Talmi I 1993 Simple Models of Complex Nuclei, Contemporary Concepts in Physics vol 7 (Harwood Academic Publishers)
[8] Glaudemans P W M, Brussaard P J and Wildenthal B H 1967 Nucl. Phys. A 102 593
[9] Bohr A and Mottelson B R 1998 Nuclear Structure vol I (World Scientific Publishing Company)
[10] Brown B A, Signoracci A and Hjorth-Jensen M 2011 Phys. Lett. B 695 507
[11] Holt J D, Otsuka T, Schwenk A and Suzuki T 2012 J. Phys. G 39 085111
[12] Volya A, Brown B A and Zelevinsky V 2001 Phys. Lett. B 509 37
[13] Entem D R and Machleidt R 2003 Phys. Rev. C 68 041100
[14] Hoffman C R, et al. 2008 Phys. Rev. Lett. 100 152502
[15] Senkov R, Bertsch G F, Brown B A, Luo Y L and Zelevinsky V 2008 Phys. Rev. C 78 044304
[16] Warburton E K and Brown B A 1992 Phys. Rev. C 46 923
[17] Brown B A and Richter W A 2006 Phys. Rev. C 74 034315
[18] Stanoiu M et al. 2008 Phys. Rev. C 78 034315
[19] Nowacki F and Poves A 2009 Phys. Rev. C 79 014310
[20] Signoracci A, Brown B A and Hjorth-Jensen M 2011 Phys. Rev. C 83 024315
[21] Bertsch G F, Bertulani C A, Nazarewicz W, Schunck N and Stoitssov M V 2009 Phys. Rev. C 79 034306