Mass differences and neutron pairing in Ca, Sn and Pb isotopes

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Abstract: Various estimates of the even-odd effect of the mass shell of atomic nuclei are considered. Based on the experimental mass values of the Ca, Sn, and Pb isotopes, the dependence of the energy gap on the neutron number is traced and the relationship of this characteristic to the properties of external neutron subshells is shown. In nuclei with closed proton shells, effects directly related to neutron pairing and effects of nucleon shells are discussed.

Keywords: nucleon interaction, models of atomic nuclei, nucleon pairing in atomic nuclei

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1 Introduction

The creation of the shell model of the atomic nucleus [1, 2] is one of the most significant achievements of theoretical nuclear physics. The first attempts at its development were based on the model of atomic electron shells. The prospects for this approach were not that obvious, since there is a significant difference between the electrons in the atom and the nucleons in the atomic nucleus. In the case of an atom, the electrons are in the strong Coulomb field of the atomic nucleus, and the interactions of electrons with one another are a correction to the total potential (the “screening” of the nuclear field by the electrons is very important). In the case of an atomic nucleus, the total self-consistent field is the result of nucleon-nucleon interactions and effectively takes its properties into account. Accordingly, the total atomic nucleus potential changes with transitions from isotope to isotope.

For a correct description of the properties of atomic nuclei, in addition to changing the mean-field potential it is also necessary to take into account the residual interaction. This, in spite of its small value, is crucial in determining the specific properties of the system of nucleons. In the first approximation, the so-called pairing forces are considered as the residual interaction — an effective short-range interaction, which leads to an increase of the binding energy of a pair of nucleons when summation of their spins gives the total moment \( J = 0 \). The pairing of identical nucleons makes it possible to explain many experimental facts, including the spin \( J^P = 0^+ \) of all even-even nuclei and the enhanced stability of even-even isotopes [3–5].

2 Even-odd staggering and nucleon pairing

The increasing of stability of even-even nuclei leads to the stratification of the mass surface on three components: one for even-even nuclei, one for odd-odd nuclei and one intermediate for nuclei with odd mass number \( A \). A systematic study of the binding energies of a nucleus \( B(A) \) shows that for even-even nuclei the following rule is fulfilled:

\[
B(A) > \frac{1}{2} [B(A+1)+B(A−1)].
\]

The observed even-odd mass staggering (EOS) has been extensively explored in the literature [6–10]. The EOS effect is generally associated with the pairing gap \( \Delta \), as suggested by BCS theory. To estimate its value various more or less averaged equations are used: three-, four- or five-point [4, 11–14] formulas (so-called indicators):

\[
\Delta_n^{(3)}(N) = \frac{(-1)^N}{2} [S_n(N)−S_n(N+1)],
\]

\[
\Delta_n^{(4)}(N) = \frac{(-1)^N}{4} [−S_n(N+1)+2S_n(N)−S_n(N−1)],
\]

\[
\Delta_n^{(5)}(N) = \frac{1}{2} [\Delta_n^{(4)}(N)+\Delta_n^{(4)}(N+1)]
\]

\[
= \frac{(-1)^N}{8} [3S_n(N+1)−3S_n(N) + S_n(N−1)−S_n(N+2)],
\]

where \( S_n(N) = B(N)−B(N−1) \) is the neutron separation energy of a nucleus \((N,Z)\). In the formulas (2–4) for neutron EOS, the proton number \( Z \) is fixed. Similar
formulas (here and below) for protons can be obtained by fixing the neutron number \(N\) and replacing \(N\) by \(Z\).

It is seen from the formulas above that the expression (3) is also an averaging between \(\Delta_n^{(3)}(N)\) and \(\Delta_{n}^{(3)}(N-1)\).

The relations (2) and (3) were originally obtained in order to get an analytic dependence of EOS on \(A\) to introduce it as an additional pairing term to the semi-empirical Bethe-Weizsäcker mass surface formula. From this point of view, the values of \(\Delta_n^{(3)}\) fluctuate much more strongly depending on \(A\), but the result of their approximation differs slightly from the results for \(\Delta_n^{(4)}\) [4]. So, the four-point formula (3) became the basis for describing the EOS effect, and consequently for describing the pairing effect, for a long time. In some modern calculations even more smoothing formulas are used, taking into account five [12, 13, 15] or six experimental binding energies of isotopes [11]. An increase in the number of isotopes does not significantly affect the EOS calculation result, but the expansion of the range of experimental data in the region far from stability can lead to the usage of experimental data with significant errors. Modern mass formulae use more complicated pair approximations depending not only on power of \(A\) but also on isospin relations [17, 18]. The relationship between different variants of the EOS estimation, as well as various variants of the \(\Delta(n)(A)\) approximation for protons and neutrons, are considered in Refs. [10, 19–21].

Many studies are devoted to the evaluation of both the direct nucleon pairing contribution to the EOS and the contributions of other microscopic effects [6, 8, 22–25]. It is shown [8, 23] that the best estimation for identical nucleons pairing in the even \(N\) nucleus is the three-point indicator (2) for neighbor odd neutron number \(\Delta_n^{(3)}(N+1)\). This conclusion corresponds to the direct determination of the two-neutron pairing \(\Delta_{nn}(N)\) as the difference between the two-neutron separation energy \(S_{2n}(Z,N)\) from the even-even nucleus and the doubled neutron separation energy \(S_n(Z,N-1)\) from the neighboring odd nucleus \((N-1,Z)\) [26]:

\[
\Delta_{nn}(N) = S_{2n}(N) - 2S_n(N-1) = S_n(N) - S_n(N-1) = 2\Delta_n^{(3)}(N-1),
\]

where \(S_{2n}(N) = B(N) - B(N-2)\). This definition considers the nucleus as a core with a pair of external “valence” nucleons, and does not take into account how the mean-field potential changes when “valence” nucleons are added or removed.

It is known that the \(\Delta_{nn}(N)\) dependence for even-even nuclei is much smoother, and it produces an EOS estimate lower than that given by other formulas. Also, unlike the others, this characteristic is diminished for closed-shell nuclei, which corresponds to the common expectation that the pairing at shell closure should decrease in connection with the level density reduction. It can be expected that \(\Delta_{nn}(N)\) includes the mean field contributions to the least extent, but it is apparently impossible to completely exclude their influence [8, 10]. In Ref. [20] it was noted that, as \(\Delta_{nn}(N)\) includes the second differences of the binding energies, its value may be non-zero even without EOS.

3 Seniority model

With the pairing phenomena taken into account, the \(A\)-nucleon system Hamiltonian is:

\[
\hat{H} = \hat{H}_0 + \hat{H}_{\text{pair}},
\]

where \(\hat{H}_0\) is the intrinsic singe-particle Hamiltonian, determined by the nucleus mean-field, and the residual interaction corresponds to the monopole pairing:

\[
\hat{H}_{\text{pair}} = -G \hat{P}^\dagger \hat{P}.
\]

Here \(G\) is the pairing strength parameter, and \(\hat{P}^\dagger\) and \(\hat{P}\) denote the pair creation and annihilation operators. A rough experimental estimate gives \(G_n = 25/A\) MeV for neutrons and \(G_p = 17/A\) MeV for protons [3].

The seniority model [27, 28] is one of the simplest models. It describes the filling of a shell with the total angular momentum \(j\) over a closed core. Following Ref. [8], let us consider \(n\) nucleons moving in a \(2\Omega\)-fold degenerated shell \((2\Omega = 2j+1)\), described by the Hamiltonian in Eq. (7). The energy eigenvalues in the seniority model can be expressed in terms of nucleon number \(n\) and seniority \(\nu\) (the number of unpaired nucleons (quasiparticles) in the configuration considered):

\[
E(n,\nu) = \frac{1}{4} G(n-\nu)(2\Omega-\nu-n+2).
\]

The nuclear ground state has seniority \(\nu = 0\) for even nucleon number \(n\) (all nucleons are paired), and \(\nu = 1\) for odd number \(n\). The value of EOS according to the formula for the three-point indicator (2) is:

\[
\Delta^{(3)}(n) = \begin{cases} 
\frac{1}{2}G\Omega + \frac{1}{2}G & \text{for even } n, \\
\frac{1}{2}G\Omega & \text{for odd } n.
\end{cases}
\]

The index \(\tau = n,p\) denotes the nucleon type. Since this result depends only on whether the number of particles \(n\) is even or odd and does not depend on the absolute value of \(n\), the average four- and five-point indicators (3) and (4) in the seniority model are the same:

\[
\Delta^{(5)}_\tau(n) = \Delta^{(4)}_\tau(n) = \frac{1}{2}G\Omega + \frac{1}{4}G, \quad \text{for all } n.
\]

The pairing energy direct estimation \(\Delta^{(5)}(n)\) for an even neutron number will be smaller than the doubled...
In this case the pairing value is equal to the doubled EOS effect $\Delta_{\tau\tau}(n)=2\Delta^{(3)}(n-1)$ and does not depend on the absolute value of $n$.

4 Nucleon separation energy

In the simplest case of two neutrons pairing over the closed core, the pairing energy $\Delta_{nn}(N)$ (5) corresponds to the doubled EOS effect $\Delta^{(3)}_n(N-1)$. Hereafter we consider the corresponding doubled indicators:

\[
\Delta_{nn}^{(3)}(N)=2\Delta_n^{(3)}(N),
\]
\[
\Delta_{nn}^{(4)}(N)=2\Delta_n^{(4)}(N),
\]
\[
\Delta_{nn}^{(5)}(N)=2\Delta_n^{(5)}(N).
\]

Since relations (12 - 14) depend on the nucleon separation energies, let us consider the neutron separation energy $\Delta_{nn}(N)$ in Ca isotopes ($Z=20$). The dependence $S_n$ in Ca isotopes ($Z=20$) is plotted. The separation energy $S_n$ shows a saw-tooth form, as a consequence of the pairing effect.

The values $S_n(N)$ for even and odd $N$ are divided into two groups lying well on two straight parallel lines. Sharp leaps between groups of $S_n$ values for $N=20, 28, 32$ correspond to subshell transitions. Since the distance between single-particle levels is large in light nuclei, a consistent filling of the subshells $1d_{3/2}-1f_{7/2}-2p_{3/2}$ in Ca isotopes is traced well.

Figure 1(a) shows the neutron separation energy $S_n(N)$. In Fig. 1(a), the measured neutron separation energy $S_n$ in Ca isotopes ($Z=20$) is plotted. The dependence $S_n$ shows a saw-tooth form, as a consequence of the pairing effect.

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Figure 1(a) also gives the proton separation energy $S_p(N)$. Despite the fact that the number of protons remains constant at $Z=20$, this dependence has a saw-tooth shape as well. Although it is not so pronounced as that for $S_n(N)$, it nevertheless reflects the influence of the neutron pairing on the total mean-field potential changes.

The measured two-neutron separation energy $S_{2n}(N)$ (see Fig. 1(b)) does not show the effect of neutron pairing, because only even $N$ or odd $N$ isotopes are used for its calculation.

In Refs. [28, 29] it was shown that in seniority model the energy of $n$ valence nucleons in the field of the closed core $B(j^n)$ can be expressed as

\[
B(j^n) = B_{\text{core}}(n=0)+n\varepsilon_j+n(n-1)\alpha
+\frac{1}{2} \left[ n-\frac{1-(-1)^n}{2} \right] \beta. \tag{15}
\]

So the single nucleon separation energy

\[
S_n(N) = B(j^n)-B(j^{n-1})
= \varepsilon_j+(n-1)\alpha+\frac{1+(-1)^n}{2} \beta \tag{16}
\]

includes the energy $\varepsilon_j$, and depends on the kinetic energy of the nucleon on the $j$ shell and on the energy of interaction of an external nucleon with the core. The third term, proportional to $\beta$, corresponds to the pairing effect, and the second one, proportional to $\alpha$, provides a common gradient of the curve $S_n(N)$. The values of the coefficients $\alpha$ and $\beta$ can be determined from the two-body matrix elements of “valence” nucleon interactions, so the pairing interaction not only determines the saw-tooth shape of $S_n(N)$, but makes a contribution to the self-consistent mean-field changes too. Sharp leaps between groups of $S_n$ values for $N=20, 28, 32$ are determined by the difference $\varepsilon_{j1}-\varepsilon_{j2}$ in the transition between subshells $j_1$ and $j_2$.

Fig. 1. Neutron $S_n(N)$, proton $S_p(N)$ (a) and two-neutron $S_{2n}(N)$ (b) separation energies in Ca isotopes. Data from Ref. [30].

5 Identical nucleon pairing

Due to the total gradient of the $S_n(N)$ dependence in one subshell, the pairing energy $\Delta_{nn}$, obtained from (5),
is always less than the result obtained from the three-point formula (2) for even \( N \):

\[
\Delta_{nn} < \Delta_{nn}^{(3)},
\]

which is consistent with the seniority model (9, 11).

In Fig. 2, values of pairing energy indicators \( \Delta_{nn} \) from (5), \( \Delta_{nn}^{(2)} \) and \( \Delta_{nn}^{(4)} \) in the Ca isotopes are plotted. All calculations were made on the base of measured nuclear masses from Ref. [30]. If even and odd \( N \) are considered together one can clearly see that \( \Delta_{nn} \) and \( \Delta_{nn}^{(3)} \) values coincide accurately on the \( N=1 \) shift (Fig. 2(a)), and the \( \Delta_{nn}^{(4)} \) values are their average. The leap in \( S_{n}(N) \) dependence due to the closure of the \( 1d2s \) subshell and the start of the \( f_{7/2} \) subshell filling occurs at \( N=20 \) and \( N+1=21 \). As a result the three-point pairing energy indicator \( \Delta_{nn}^{(3)} \) (2) has a sharp leap even at \( N=20 \), but for \( \Delta_{nn}^{(5)} \) (5) the corresponding change is at odd \( N+1=21 \).

That is why for even-even nuclei the three-point indicator \( \Delta_{nn}^{(3)} \) has significant fluctuations near the magic numbers, while the dependence of \( \Delta_{nn}^{(5)} \) has a smoother behavior (see Fig. 2(b)). The values of the averaged indicators \( \Delta_{nn}^{(4)} \) and \( \Delta_{nn}^{(3)} \) are almost the same, but it should be noted that an increase in the number of points used to calculate the averaged characteristics narrows the range of isotopes under consideration.

It of interest is to consider the behavior of the difference between \( \Delta_{nn} \) and \( \Delta_{nn}^{(3)} \), formally coinciding with the pairing strength parameter \( G \) in the simplest seniority model (9):

\[
\delta\epsilon(N) = (-1)^N \left( \Delta_{nn}^{(3)} - \Delta_{nn}(N) \right).
\]

At the same time, the definitions (2, 5) imply

\[
\delta\epsilon(N) = S_{n}(N-1) - S_{n}(N+1).
\]

As the behavior of the \( S_{n}(N) \) dependence (Fig. 1(a)) shows, the value \( \delta\epsilon(N) \) excludes the pairing effect and can be regarded as a correction associated with the core polarization and/or the contribution of the three-body interaction [31].

6 Results for semimagic nuclei

In Fig. 3 the dependencies \( \Delta_{nn}^{(3)}, \Delta_{nn} \) and \( \delta\epsilon \) in even-even Ca isotopes are plotted. In Fig. 3(a), in addition to \( \Delta^{(3)} \), the experimental values of the first excited states \( J^p=2^+ \) are also given. In the \( ^{40}\text{Ca} \) case, which is typical for doubly magic nuclei, the \( 2^+ \) state is not always the first excited state, which is associated with increasing of the rigidity and spherical symmetry of nuclei with filled shells [4].

The spectroscopy of Ca isotopes was considered in detail in Ref. [32]. The low-energy spectra of odd Ca isotopes and the single-particle structure demonstrate the isolation of the subshell \( f_{7/2} \) with respect to the closed core \( ^{40}\text{Ca} \), leading to a pronounced sequential filling of neutron subshells. In Fig. 3 the vertical dashed lines denoting the subshells filling correspond strictly to the maxima in the \( \Delta_{nn}^{(3)} \), \( \delta\epsilon \) and \( E_{jj}(2^+) \) dependencies on the neutron number in the Ca isotopes. Thus, all three characteristics strongly correlate with each other.

As mentioned above, the \( \Delta_{nn}(N) \) value for even nuclei has a more smoothed character, but, nevertheless, it is rather complicated and undergoes significant changes at the shell boundaries. One should note the similarity of values of \( \Delta_{nn}^{(3)} \) and \( \Delta_{nn} \) (and, correspondingly, small \( \delta\epsilon \) value) for isotopes \( ^{42,44,46}\text{Ca} \). An approximation which considers the closed core \( ^{40}\text{Ca} \) with \( f_{7/2} \) shell filled consequently fits well for these isotopes [33–35] and one can assume that in this case the indicators \( \Delta_{nn}^{(3)} \) and \( \Delta_{nn} \) (and respectively their averaging four- and five-point indicators \( \Delta_{nn}^{(4)} \) and \( \Delta_{nn}^{(5)} \)) reflect the neutron pairing effect most accurately. The values \( \Delta_{nn}(N) \) more clearly demonstrate the dependence of the pairing energy on \( j \) quantum number. The ratio between the values for different subshells corresponds to the ratio of the number of projections for the corresponding \( j \) [36]:

\[
\frac{\Delta_{nn}}{2j+1} = \frac{\Delta_{nn}(22)}{8} \approx \frac{\Delta_{nn}(30)}{4} \approx \frac{\Delta_{nn}(36)}{6} \approx 0.35
\]

A value of 0.35 agrees well with the accepted ap-
proximation of the neutron pairing strength parameter $G_n \sim 25/A$ MeV (denoted in Fig. 3, 4 by a blue dashed line).

The behavior of indicators $\Delta^{(3)}_{nn}$ and $\delta e$ for semi-magic isotopes Sn and Pb with $Z = 50, 82$ have the same features. Figure 4 (a, b) shows the dependencies of $\Delta^{(3)}_{nn}$ and $E_g(2^+)$ on the neutron number $N$ in tin isotopes. For clarity, the dotted line also plots the value $\Delta^{(3)}_{nn} = \Delta^{(3)}_{nn}/2$, which corresponds with good accuracy to the excitation energy $E_g(2^+)$ for most isotopes in the chain.

From the single-particle structure point of view, the consequential filling of subshells does not exist in tin isotopes. Occupations of single-particle orbitals rise rather smoothly with neutron number from $N = 50$ to $N = 80$ [37]. Consequently, the $S_n(N)$ and $S_{nn}(N)$ dependencies have a smoothed variation without significant gaps associated with transitions between the subshells. In the $\Delta^{(3)}_{nn}(N)$ dependence, there is a small leap at $N = 66$, indicating the presence of a gap between the $(d_{5/2}, g_{7/2})$ and $(s_{1/2}, d_{3/2}, h_{11/2})$ subshell groups. One should also
note the proximity of the values and the explicit correspondence of the form of $\Delta_{nn}(3)$ and $\Delta_{nn}$ dependencies throughout the shell. Nevertheless, $\delta e$ values have pronounced changes, but they are minimal for $N > 70$. In this region, the subshells with large values of $j$, $1h_{11/2}$ and $2f_{7/2}$, are filled, which leads to the characteristic spectra of the low-energy excited states in these isotopes [38]. A sharp leap in the three-point indicator $\Delta_{mn}(N)$ for $N=82$ values corresponds to the transition to a new shell, and the decrease in the pairing effect that occurs can be related to a decrease in the number of projections $j$ on the outer shells [39], 16 on the subshell $(d_{3/2}, h_{11/2})$ compared to 8 on the more isolated subshell $f_{7/2}$:

$$\frac{\Delta_{nn}(76)}{16} \approx \frac{\Delta_{nn}(84)}{8} \approx 0.15$$

The same regularities can be traced in the $\Delta_{nn}(3)$, $\Delta_{nn}$ and $\delta e$ dependencies for lead isotopes (Fig. 5 a, b). The behavior of $\Delta_{nn}(3)$ and $\Delta_{nn}$ is almost the same, which leads to $\delta e \approx \text{Const}$ for most Pb isotopes. A general decrease in the pairing effect $\Delta_{nn}$ can be associated with the transition from filling the high-momentum subshell group $(i_{11/2},h_{13/2})$ to states with a smaller value of $j$, up to $j = 1/2$ for $N = 124$. Of course the behavior of the characteristics under consideration for neutron-rich isotopes with $N > 132$ is very interesting. For example, in Ref. [31] it was shown that negative values of $\delta e$ may indicate a sharp change in the type of deformation of the nucleus during the transition from one isotope to another. However, the error in determining the neutron separation energies for these isotopes amounts to tens of percentages and it is somewhat premature to make unambiguous conclusions about the magnitude of the characteristics based on the difference of separation energies $S_n$.

7 Summary

The main features of various atomic nucleus characteristics based on the mass differences, the neutron separation energy and various options for calculating the mass-surface EOS effect have been considered in this paper. For semi-magic isotopes with $Z = 20, 50$ and $82$, for example, the complex nature of the even-odd effect, which includes both the nucleon pairing and other mean-field effects such as shell and subshell filling or symmetry effects, has been shown. The behavior of the characteristics involving the neutron separation energies from two neighboring isotopes, $\Delta_{nn}^{(3)}$ and $\Delta_{nn}$, strongly depends on the properties of the external nucleons and reflects not only the nucleon correlations in the middle of the shell filling, but also the closed shells and subshell formation as the nucleon number goes through the magic numbers.

The $\Delta_{nn}$ value for even-even nuclei has a smooth $N$ dependence, since it involves isotopes with the numbers $N$ and $N-1$ and in the case of even $N$ does not include the peak associated with a change in the neutron single-particle energy upon transition to the next subshell. The systematic underestimation of the EOS value calculated by the formula $\Delta_{nn}$, compared with other three-, four- and five point indicators ($\Delta_{mn}^{(3)}, \Delta_{mn}^{(4)}, \Delta_{mn}^{(5)}$) is in accordance with the conclusions of the simplest seniority model. The smallest discrepancy between the various variants of the calculation is observed in the middle of the subshell filling. In this case the EOS value corresponds most closely to the pairing energy $\Delta \approx G\Omega$, and the difference between the $\Delta_{nn}^{(3)} - \Delta_{nn}^{(3)}$ corresponds to the pairing strength parameter $G = 25/A$. In this area, far from magic numbers, pairing is most vividly manifested. A characteristic manifestation of the pairing effect is the low-lying $2^+$ states of collective nature, which form an energy gap 1–2 MeV between the ground and first exited state in even-even nucleus spectra.

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