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Partial-wave contributions to pairing in nuclei

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Abstract. We present a detailed study of partial-wave contributions of nuclear forces to pairing in nuclei. For $T = 1, J = 0$ pairing, partial waves beyond the standard $^1\mathrm{S}_0$ channel play an interesting role for the pair formation in nuclei. We explore the impact of including partial waves beyond the $^1\mathrm{S}_0$ channel on the odd-even mass staggering in semi-magic isotopic chains. The additional contributions are dominated by the repulsive $^3\mathrm{P}_1$ partial wave.

1. Introduction

Phenomenological Energy-Density Functional (EDF) theories are able to describe to a good accuracy properties of medium- and heavy-mass nuclei [1], but they lack a connection to microscopic nuclear forces. This brings to a poorly reliable theory at the outskirts of the mass table. Time has come to step forward and bring our knowledge of nuclear forces into the many-body problem [2, 3, 4, 5, 6]. A deeper understanding of the physics and a higher reliability of the method will be the final harvest of this work. Recently independent studies in this direction have been carried out to better describe pairing correlations, responsible for the superfluid properties of the nuclei.

These studies relied on two recent major theoretical advances. One the one hand, Effective Field Theory can provide us with a consistent and well-ordered picture of the nucleonic interaction [7, 8, 9, 10]. On the other hand, plugging these realistic potentials in the many-body theories is now a feasible yet challenging task, thanks to Renormalization Group techniques [11, 12, 13, 14, 15, 16].

A few exploratory studies have already been made at the first order in the pairing interaction. First, the importance of S-superfluidity has been assessed [17, 18, 19] and further contributions from P-, D-, ... waves have then been characterized [20]. Higher partial waves were also included in Ref. [21]. An approximate description of the effects coming from three-body forces is also available in the S-wave channel [22]. The coupling to collective density, spin and isospin modes (higher-order correlations) has been shown to play an important role [23, 24]. A quantitative and reliable description of these higher-order effects can only be achieved by means of a microscopic interaction and by strictly imposing the consistency with the description of all the other effects.

In this work we focus on partial-wave contributions to the first-order pairing interaction. Calculation details are given in Sect.2. In Sect. 3, we discuss which partial waves can contribute to the Cooper-pair formation. We then explore the impact on the odd-even mass staggering (OEMS) in semi-magic isotopic chains in Sect. 4. We conclude and give an outlook in Sect. 5.

2. Calculational details

The minimization of the energy-density functional in the presence of pairing leads to solving the self-consistent Hartree-Fock-Bogoliubov (HFB) equations [1, 25] that determine the quasiparticle (q) basis,

$$\begin{pmatrix} h-\mu & \Delta \\ -\Delta^* & -(h-\mu) \end{pmatrix} \begin{pmatrix} U^q \\ V^q \end{pmatrix} = E_q \begin{pmatrix} U^q \\ V^q \end{pmatrix} . \tag{1}$$

Here h denotes the single-particle Hamiltonian, μ the Fermi level, E_q is the quasiparticle energy and U^q, V^q the corresponding coefficients of the Bogoliubov transformation from single-particle to quasiparticle states. We use the Skyrme functional SLy4 [26] and first solve the Hartree-Fock (HF) equations, $h\phi_a = \varepsilon_a^{\mathrm{HF}}\phi_a$, on a spherical mesh with 0.1 fm spacing and 16.0 fm box radius. Our results are stable with respect to increasing the radius and decreasing the mesh spacing. This defines the single-particle basis $|a\rangle$, using the shorthand label $a \equiv n_a l_a j_a$ with radial quantum number n_a, orbital angular momentum l_a and total angular momentum $j_a = l_a \pm 1/2$.

Using the HF single-particle Hamiltonian, we then solve the HFB equations fully self consistently. The HFB state-dependent gap matrix Δ for $T = 1, J = 0$ pairing is given by

$$\Delta_{ab} = -\sum_{cd}\left(\sum_q U_c^q V_d^q\right)\sqrt{\frac{2j_c+1}{2j_a+1}}\,\frac{\sqrt{(1+\delta_{ab})(1+\delta_{cd})}}{2}\langle a\, b\,|\,(1-P_{12})\,V_{\mathrm{low}\,k}\,|\,c\, d\,\rangle_{J=0,T=1,T_z=-1} . \tag{2}$$

This defines the gap equation and we focus on neutron-neutron ($T_z = -1$) pairing properties. The matrix elements of the pairing interaction in the second line of Eq. (2) are antisymmetrized using the exchange operator P_{12} and normalized, and δ_{ab} is shorthand for $\delta_{n_a n_b}\,\delta_{l_a l_b}\,\delta_{j_a j_b}$. For completeness, the gap equation above is in the so-called phase convention II [27], for which the operation of the time-reversal operator $\mathcal{T}$ on a single-particle state is given by $\mathcal{T}\,|l_a j_a m_a\rangle = (-1)^{j_a - m_a}\,|l_a j_a - m_a\rangle$, with magnetic quantum number m_a.

For the neutron-neutron pairing interaction, we start from the chiral N^{3}LO two-nucleon (NN) potential ($\Lambda = 500\,\mathrm{MeV}$) of Ref. [10] and use the RG to evolve this NN potential to low-momentum interactions $V_{\mathrm{low}\,k}$ with a smooth $n_{\mathrm{exp}} = 4$ regulator with $\Lambda = 2.0\,\mathrm{fm}^{-1}$ [12]. This evolution renders the many-body calculation more controlled [14, 15, 16] and provides a good starting point for connecting energy-density functionals to nuclear forces [2, 28]. Based on the universality of $V_{\mathrm{low}\,k}$ [12, 15], we do not expect large differences starting from different N^{3}LO potentials.

We calculate the jj-coupled pairing matrix elements entering the gap equation, Eq. (2), by expanding the HF single-particle states on the harmonic oscillator (HO) basis:

$$|n_a l_a j_a\rangle_{\mathrm{HF}} = \sum_{n_b=0}^{9} {}_{\mathrm{HO}}\langle n_b l_b j_b | n_a l_a j_a\rangle_{\mathrm{HF}}\, |n_b l_b j_b\rangle_{\mathrm{HO}} , \tag{3}$$

with $l_a = l_b$ and $j_a = j_b$. The HFB predictions for the ground-state energies are stable against an increase of the HO shells. The jj-coupled two-particle matrix elements in the HO basis are calculated from the different partial-wave contributions using the standard recoupling formula [20].

For the ground-state binding energy of the isotopes presented in Sect. 4, we have found that the HFB single-particle space can be restricted to states below 120 MeV for $\Lambda = 2.0\,\mathrm{fm}^{-1}$. For hard potentials with large cutoffs, states up to $\sim 1\,\mathrm{GeV}$ are needed for convergence [24, 29]).

Calculations for odd-A nuclei are performed in the Equal Filling Aproximation [30].

3. Partial-wave contributions to pairing interactions in nuclei

We use the standard notation ${}^{2S+1}l_{J_{\rm rel}}$ to denote the different partial waves. This describes the relative motion of the two particles in the Cooper pair. S is the total spin of the pair, while l and $J_{\rm rel}$ are the relative orbital angular momentum and the total relative angular momentum, respectively. The relation $\boldsymbol{J}_{\rm rel} = \boldsymbol{l} + \boldsymbol{S}$ holds. In general, all partial waves fulfilling the fermionic symmetry relation $(-1)^{l+S+T} = -1$ can contribute to the vacuum nucleon-nucleon interaction. We list them for completeness:

$$\text{for } T=1: \quad {}^1\mathrm{S}_0 \quad {}^3\mathrm{P}_{0,1,2} \quad {}^1\mathrm{D}_2 \quad {}^3\mathrm{F}_{2,3,4} \quad {}^1\mathrm{G}_4 \quad \ldots$$

$$\text{for } T=0: \quad {}^3\mathrm{S}_1 \quad {}^1\mathrm{P}_1 \quad {}^3\mathrm{D}_{1,2,3} \quad {}^1\mathrm{F}_3 \quad {}^3\mathrm{G}_{3,4,5} \quad \ldots$$

Additional restrictions come into play in the pairing problem when the total angular momentum of the paired nucleons is $J = 0$. Both the center-of-mass angular momentum L and the relative total angular momentum $J_{\rm rel}$ of the pair can contribute to the total angular momentum $\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{J}_{\rm rel}$. One therefore has $L = J_{\rm rel}$ for $J = 0$. Moreover, because the parity of the pair is positive, it follows that the relative and center-of-mass orbital angular momentum l and L must have the same parity. As a result, the relative orbital and total angular momentum l and $J_{\rm rel}$ also have the same parity, and therefore only uncoupled channels ${}^{2S+1}l_{J_{\rm rel}=l}$ contribute to $T = 1, J = 0$ pairing matrix elements. On the other hand, $T = 0, J = 1$ matrix elements are not affected by these additional constraints and coupled channels also contribute to the pair formation in nuclei.

In summary, this shows that the ${}^1\mathrm{S}_0$ and ${}^3\mathrm{S}_1 - {}^3\mathrm{D}_1$ partial waves are not the only channels contributing to $T = 1$ and $T = 0$ pairing in nuclei. In addition, the following partial waves are part of the pairing interaction:

$$T=1, J=0: \quad {}^1\mathrm{S}_0 \quad {}^3\mathrm{P}_1 \quad {}^1\mathrm{D}_2 \quad {}^3\mathrm{F}_3 \quad {}^1\mathrm{G}_4 \quad \ldots$$

$$T=0, J=1: \quad {}^3\mathrm{S}_1 \quad {}^1\mathrm{P}_1 \quad {}^3\mathrm{D}_{1,2,3} \quad {}^1\mathrm{F}_3 \quad {}^3\mathrm{G}_{3,4,5} \quad \ldots$$

Interestingly, both ${}^3\mathrm{P}_1$ and ${}^1\mathrm{P}_1$ partial waves are repulsive at the relevant energies [31]. We therefore expect a reduction of the pairing gap compared to studies based on the standard S-wave interactions.

4. Odd-even mass staggering

We compute the ground-state binding energies $B(N, Z)$ of even-even and odd-A nuclei and then extract the odd-even mass staggering using the three-point mass formula [32, 33],

$$\begin{aligned} \Delta^3(N) &= \frac{(-1)^N}{2}\Big[B(N+1,Z) - 2B(N,Z) + B(N-1,Z)\Big] \\ &\approx (-1)^N \frac{\partial^2 B}{\partial N^2}\Big|_N \\ &\approx \frac{(-1)^N}{2}\frac{\partial S_n}{\partial N}\Big|_N \end{aligned} \tag{4}$$

The OEMS for lead, tin and calcium isotopes are shown in Figs. 1-3. The theoretical results are shown with increasing partial-wave contributions to the pairing interaction and in comparison to the experimental values based on experimental binding energies of Ref. [34]. The additional contributions beyond the standard ${}^1\mathrm{S}_0$ channel are dominated by the ${}^3\mathrm{P}_1$ partial wave. They lead to a decrease of the OEMS of up to 15% and can change the isotopic dependence at this level.

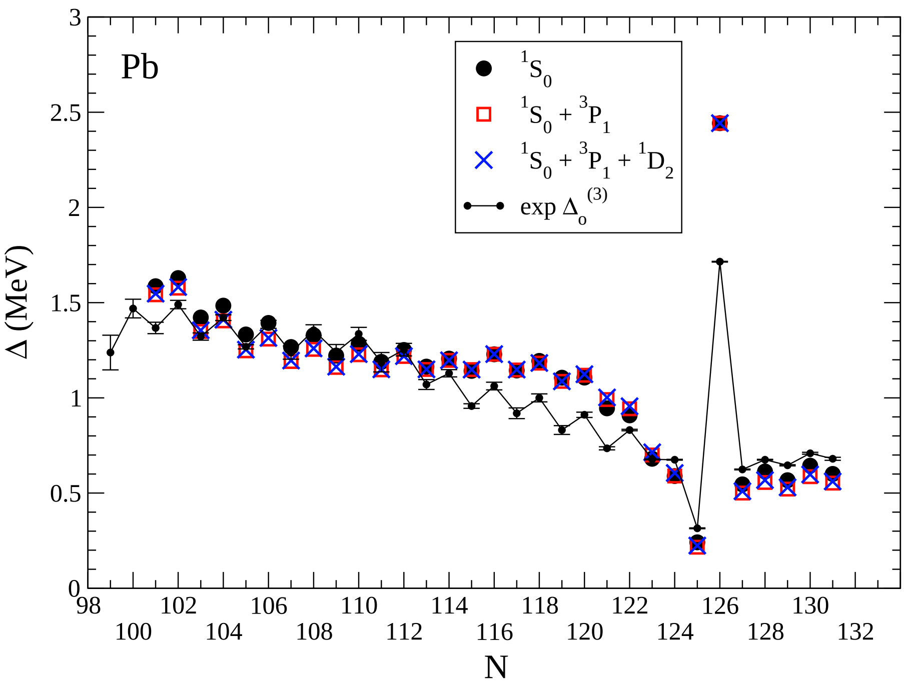

Figure 1. (Color online) Odd-even mass staggering for the lead isotopes with increasing partial-wave contributions to the pairing interaction. Experimental values are shown for comparison.

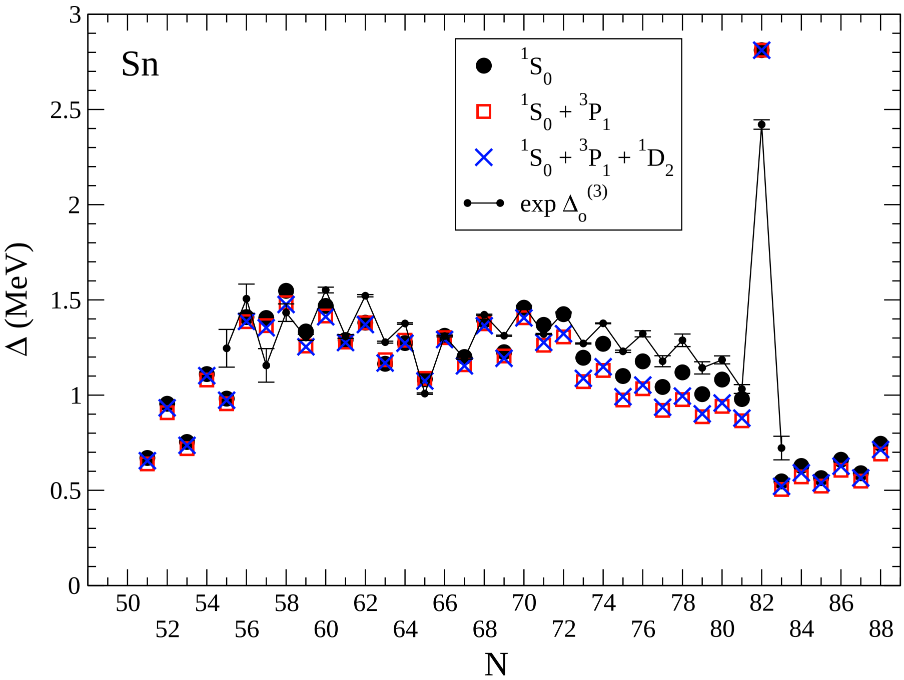

Figure 2. (Color online) Same as Fig. 1, but for tin isotopes.

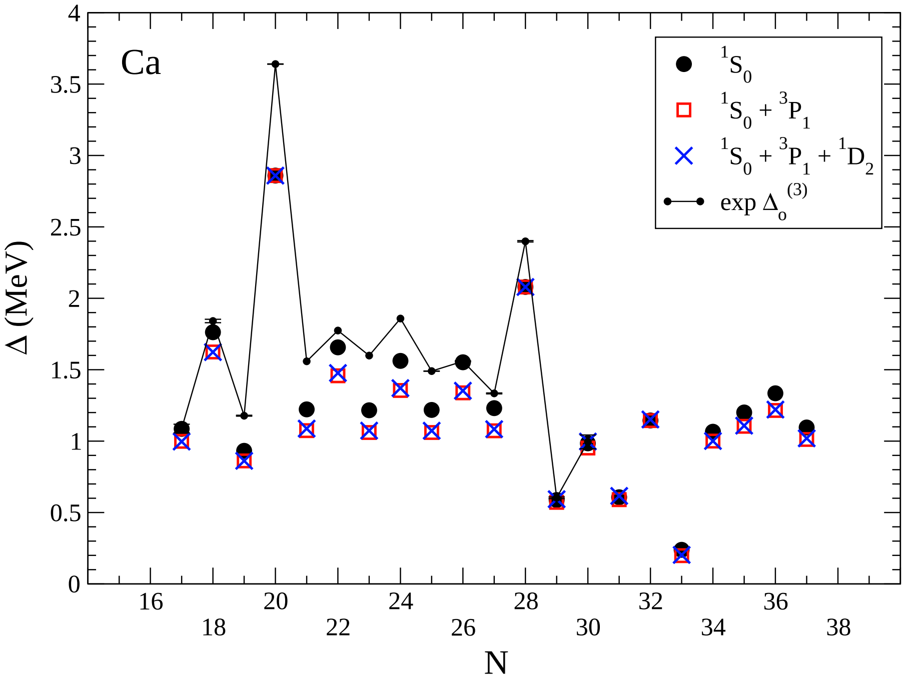

Figure 3. (Color online) Same as Fig. 1, but for calcium isotopes.

For magic numbers N, both the experimental and the theoretical OEMS have a peak. There are no contributions from pairing correlations at the magic numbers. The odd-even effect comes from the shell structure only. According to the third line of Eq. 4, it is about half of the single-particle shell gap.

5. Conclusions and outlook

We have studied partial-wave contributions of nuclear forces to pairing in nuclei for semi-magic isotopic chains. For $T = 1, J = 0$ pairing, the repulsive $^3\mathrm{P}_1$ channel decreases the OEMS by up to 15% compared to the effect obtained from the standard $^1\mathrm{S}_0$ contribution. While we have focused on neutron-neutron pairing, our conclusions equally apply to proton-proton pairing.

The effect of the different partial waves to the isocalar channel and a study of the effect of the spin-orbit field on both $T = 0$ and $T = 1$ channels can be found in [20].

For future work, an effort is required to include three-body forces in all partial waves to achieve consistent first-order calculations. A quantitative and reliable description of higher-order contributions can only be achieved starting, in a consistent fashion, from the same microscopic two- and three-body interactions that are also used to compute the first-order pairing correlations. More than that, the effect of higher-order pairing correlations on the single-particle energies (dressing of particles) is also essential for the consistency of the theoretical predictions. Studies in this direction are currently under development both in the HFB framework [35] and with the ab-initio Nambu-Gorkov Green's Function method [36].

In addition, deformation could affect the relative importance of the higher partial waves, especially at high-spins [37].

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