Pairing gaps in the Hartree-Fock-Bogoliubov theory with the Gogny D1S interaction

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As part of a program to study odd-A nuclei in the Hartree-Fock-Bogoliubov (HFB) theory, we have developed a new calculational tool to find the HFB minima of odd-A nuclei based on the gradient method and using interactions of Gogny's form. The HFB minimization includes both time-even and time-odd fields in the energy functional, avoiding the commonly used "filling approximation". Here we apply the method to calculate neutron pairing gaps in some representative isotope chains of spherical and deformed nuclei, namely the $Z = 8, 50$, and 82 spherical chains and the $Z = 62$ and 92 deformed chains. We find that the gradient method is quite robust, permitting us to carry out systematic surveys involving many nuclei. We find that the time-odd field does not have large effect on the pairing gaps calculated with the Gogny D1S interaction. Typically, adding the T-odd field as a perturbation increases the pairing gap by 100 keV, but the re-minimization brings the gap back down. This outcome is very similar to results reported for the Skyrme family of nuclear energy density functionals. Comparing the calculated gaps with the experimental ones, we find that the theoretical errors have both signs implying that the D1S interaction has a reasonable overall strength. However, we find some systematic deficiencies comparing spherical and deformed chains and comparing the lighter chains with the heavier ones. The gaps for heavy spherical nuclei are too high, while those for deformed nuclei tend to be too low. The calculated gaps of spherical nuclei show hardly any A dependence, contrary to the data. Inclusion of the T-odd component of the interaction does not change these qualitative findings.

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I. INTRODUCTION

The Hartree-Fock-Bogoliubov (HFB) theory is now very well developed for the Skyrme and Gogny families of interactions. However, up to now the calculational tools for odd-A nuclei and for other HFB wave functions that are not time-reversal invariant have not reached the point where systematic surveys can be easily carried out. The problems are less severe in the so-called filling approximation, and that approximation has become very commonplace in the literature. Two of us [1] have proposed a methodology based on the gradient method that avoids most of these computational issues. The first aim of this work is to demonstrate that the method is practical under "field conditions" of typical isotope chains across the chart of nuclides. The second aim is to assess the error in the filling approximation for an interaction in the Gogny family that has been widely used, namely the D1S interaction [2].

There is a very large literature on the application of HFB to odd-A systems and the filling approximation. References [3,4] first showed how to using blocking to calculate odd-A nuclei in the HFB theory. While exact blocking has been carried out with realistic interactions and with schematic forces [4], the HFB based on global energy density functionals has largely relied on the filling approximation. There are exceptions dealing with very specific examples like the high-spin study of Ref. [5] with the Gogny force. The filling approximation is defined as a full minimization of the HFB functional but neglecting spin-dependent and other time-odd densities. This is equivalent to neglecting the time-odd fields in the functional when expressed as products of fields and densities.

The filling approximation can also be portrayed as a statistical quantum system where the blocked orbital and its time reversed partner share the same probability [6]. This formulation may have advantages with respect to further generalizations. The approximation was used for example in setting the parameters of the Gogny functional in Ref. [7]. More recent applications with a Gogny functional are in Refs. [8,9]. There was an early study of time-odd fields with the Skyrme interaction [10], but most of the recent work has used the filling approximation. Notably, it was used for surveys of odd-A nuclei with Skyrme energy functionals in Refs. [11,12]. Very recently, the effect of time-odd fields in the Skyrme functional has been re-examined in two surveys [13,14]. The filling approximation has also been used with the relativistic mean field theory [15], and the role of the time-odd fields there have been examined in Refs. [16,17].

The physical quantity we calculate in this paper is the neutron pairing gap, defined for odd-N nuclei as

$$\Delta_o^{(3)}(Z,N) = \tfrac{1}{2}(B(Z,N-1) + B(Z,N+1) - 2B(Z,N)), \tag{1}$$

where $B(Z,N)$ is the (positive) binding energy of the nucleus. In the BCS theory it is calculated as the BCS gap parameter. In finite nuclei there can be considerable rearrangement in the wave functions from one nucleus to the next, and the gaps should be determined from Eq. (1) using the calculated binding energies. We use this definition in the present paper.

We consider a representative sample of isotope chains, spanning the nuclear size range from oxygen to uranium isotopes. We include both spherical and strongly deformed nuclei in the survey, permitting us to examine effects of the nuclear shape. As mentioned above, a particular focus in our survey is the validity of the filling approximation. We consider this to be important to examine because the filling approximation can give rise to an unphysical self-energy of

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the odd particle, as explained in the Appendix. Beyond that, our survey is extensive enough to uncover possible systematic problems with the Gogny functional we employ. Particular aspects are the overall mass-dependence of the pairing gaps, and the possible differences between pairing is spherical and deformed nuclei. Both these aspects can indicate nonpairing contributions to the gaps [18,19].

II. COMPUTATIONAL ASPECTS

The calculations reported below were carried out with a new code based on the program HFBAXIAL written by one of us [20] to carry out HFB calculations for Gogny-type interactions. The algorithm to find the HFB minima uses the analytic expression for the derivative of the HFB energy function with respect to a generalized Thouless transformation ([21], Eq. (7.32)) of the HFB wave function. Other aspects of the HFBAXIAL that are important for the algorithm are described in Ref. [1]. That reference also introduces the generalization of the gradient method to wave functions with odd particle numbers. We defer details of our new code to later publication [22]. For the present purposes, the main points on the computational side are the definition of the basis states and the assumed block structure of the Bogoliubov transformation matrices UV. We use an oscillator basis with equal oscillator length parameters in each direction. The basis states are cylindrically symmetric, with orbitals labeled by n_z, n_r, m, and s_z. We assume a block structure that preserves axial symmetry in the wave function and does not mix neutrons and protons. Thus the blocks may be labeled by t_z, the nucleon isospin, and j_z, the angular momentum about the z axis. In fact we also have to include $-j_z$ in the same block as j_z because these are coupled by the anomalous HFB field.

The original HFBAXIAL code assumes that the wave functions are time-reversal invariant, and thus the HFB fields are even under T, the time-reversal operator. The T-odd fields added to the new code arise from various terms in the Gogny interaction including the spin-orbit and density-dependent contact terms. In addition, there is a T-odd field associated with the exchange Coulomb interaction as well with the two-body correction to the center-of-mass kinetic energy. It should be mentioned that there is an intrinsic ambiguity in the T-odd field of the density-dependent interaction; we evaluate this term taking the density to be real. This term does not contribute to the pairing field in first order due to its assumed exchange character. However, it does contribute to the mean field potential giving an impact on $\Delta^{(3)}$.

Among the tests we made of the code, there are two that are worthy of mention because they are very powerful in finding inconsistencies in the coding. The first test is of the gradient method itself. As mentioned above, the gradient of the energy with respect to the degrees of freedom in the UV Bogoliubov transformation is computed analytically. One can also monitor the gradient numerically from the difference in energies when the UV matrices are changed by a small amount. If these two are not equal to the expected precision, there is a coding error that must be corrected. The second test is a very simple one. The interaction energy must vanish if the wave function is a one-particle state.[1] The vanishing is not trivial, as it comes about by an exact cancellation of the direct and exchange fields of the interaction. This provides a good test of exchange part of the Gogny interaction, which is computed in a highly optimized code.

There are two purely numerical parameters in the calculation. The first is the number of oscillator shell N_{sh} included in the basis. We follow the Madrid practice taking N_{sh} in the range 10 to 14 depending on mass region as given in the figure captions. The oscillator length parameter is taken at a fixed value $b = 2.1$ fm for all nuclei. Obviously one could do better by including more shells and allowing the oscillator parameter to vary. For our purposes here, the differences in total energies largely cancel out. The reported pairing gaps are converged to within several tens of keV, which is certainly acceptable for this survey of pairing trends and the validity of the filling approximation.

To find the HFB minima of odd-A nuclei, we start with the converged wave functions for the even-even nuclei on either side of the target nucleus, taking oblate, prolate and spherical minima. A set of trial odd-A wave functions is generated from them by the usual procedure of exchanging the U and V components in one of the columns of the UV matrix. Besides having odd particle number, these wave functions can be characterized by the angular momentum K about the symmetry axis, equal to $\pm j_z$ of the block in which the U-V interchange was carried out. Applying the gradient solver for each of the trial wave functions, a large set of local minima is obtained, many of which are identical. We select the lowest of these. There is no guarantee that one will always find the global minimum with this protocol. Still, for the spherical and strongly deformed nuclei that we calculate here, the possibility of other, deeper minima is slight.

III. RESULTS

We now compare the calculated neutron energy gaps for a variety of nuclei ranging from light to heavy and including both spherical and deformed isotope chains. We report three treatments of the theory. Besides the full minimizations with and without the time-odd fields, we report the results when the time-odd field is treated perturbatively. That is, we take the wave function from minimization without the field, and then take the expectation value of the field as a first-order perturbation to the energy of the state.

A. Spherical chains

We begin our survey with nominally spherical nuclei, presenting results for neutron pairing gaps in the three semimagic isotope chains, $Z = 8$, 50, and 82. The experimental data shown in the figures are based on the Audi *et al.* mass table Ref. [23] with some additions from Ref. [24]. We start with the lightest chain in our survey, the $Z = 8$ (oxygen) isotopes with

[1] A one-particle wave function is necessarily of Hartree-Fock form since the Bogoliubov transformation mixes particle numbers.

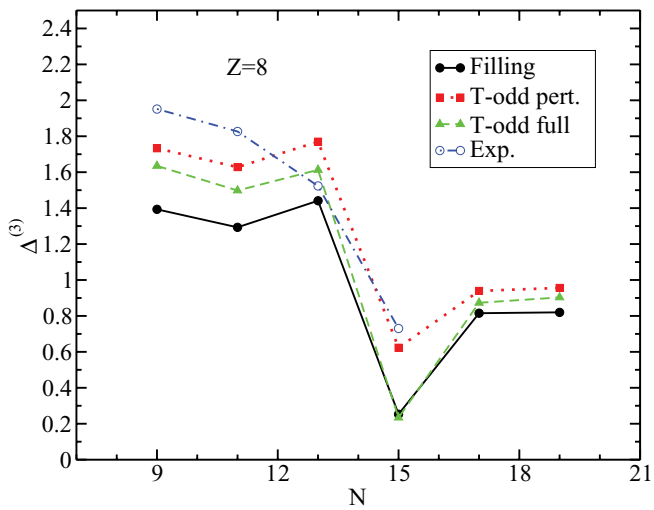

FIG. 1. (Color online) Neutron pairing gaps $\Delta^{(3)}$ in the oxygen isotope chain. Energies were computed in the $N_{sh} = 10$ harmonic oscillator space.

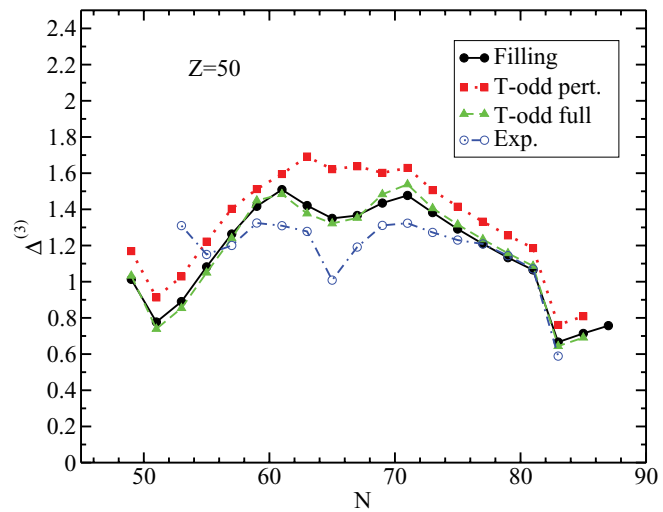

FIG. 2. (Color online) Neutron pairing gaps $\Delta^{(3)}$ in the Sn isotope chain. Energies were computed in the $N_{sh} = 12$ harmonic oscillator space.

$N > 8$. These are calculated to have very large pairing gaps when the $d_{5/2}$ subshell is being filled and smaller gaps in the upper sd shell. These qualitative features are the same in all three approximations in our study. The shell differences is of course expected because the shell degeneracy at the Fermi level should be a strong determinant of the gap. There is an especially strong decrease at $N = 15$, corresponding to an open $s_{1/2}$ shell. This "gap quenching" is a general feature of pairing gap systematics as noted in Ref. ([12], see Table III). From Fig. 1, we see experiment agrees with the theory at a qualitative level, showing large gaps in the $d_{5/2}$ shell and with a strong quenching at $N = 15$. On a more quantitatively level, the calculated pairing gaps are somewhat to low in the $d_{5/2}$ filling region.

The next chain, the $Z = 50$ Sn isotopes, has 16 measured pairing gaps and has been the subject of many theoretical studies of pairing, e.g. [16,25,26]. Our calculated gaps are shown in Fig. 2. As with the oxygen isotopes, the filling approximation gives very similar results to the full calculation with T-odd fields. The calculated gaps start out moderate at the beginning of the $N = 50$–82 major shell, smoothly increase through the shell with a mild dip around $N = 65$. The gaps then smoothly decrease toward the end of the shell, and drop sharply beyond the $N = 82$ shell closure. There is no gap quenching associated with the $s_{1/2}$ subshell, probably because of a degeneracy with other subshells in the single-particle spectrum. These features are also present in HFB calculations based on the Skyrme [12] and the Fayans energy functionals [26], so they seem to be generic for HFB with short-ranged functionals. Experimentally, the gaps are rather large, and one sees the sharp decrease at $N = 83$. However, other details differ from the calculated pattern of gaps. The predicted decrease at $N = 53$ is not seen experimentally. The mild decrease in the middle of the shell is smoother in the theoretical gaps than the experimental ones, which is very sharp at $N = 65$. Overall, the predicted gap is somewhat too high.

Concerning the effect of the T-odd field, at a perturbative level it makes the gap even larger, but the full calculation is hardly distinguishable from the filling approximation.

The heaviest spherical chain in our survey is the $Z = 82$ Pb isotope chain, which also has the greatest number of measured pairing gaps (18). The calculated gaps are shown in Fig. 3. The theoretical gaps start out very large, decrease to moderate at the upper end of the $N = 82$–126 major shell, and show the shell quenching effect at the $p_{1/2}$ shell. Again, all the theory curves are similar. Experimentally, the gaps have these qualitative features but the overall scale for the large gaps is markedly smaller.

In summary, the main qualitative features within an isotope chain are reproduced by the theory with or without inclusion of the T-odd field.

B. Deformed nuclei

The HFB energies of strongly deformed nuclei should be interpreted more cautiously. The minima now correspond to the bandheads of the rotational bands that characterize the

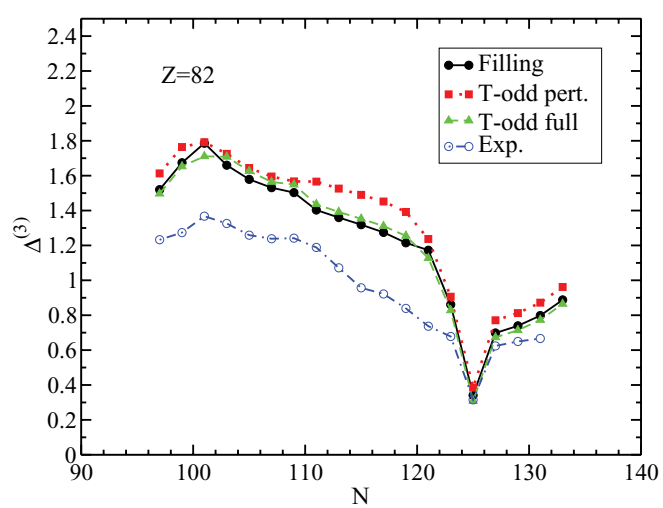

FIG. 3. (Color online) Neutron pairing gaps $\Delta^{(3)}$ in the Pb isotope chain. Energies were computed in the $N_{sh} = 12$ harmonic oscillator space.

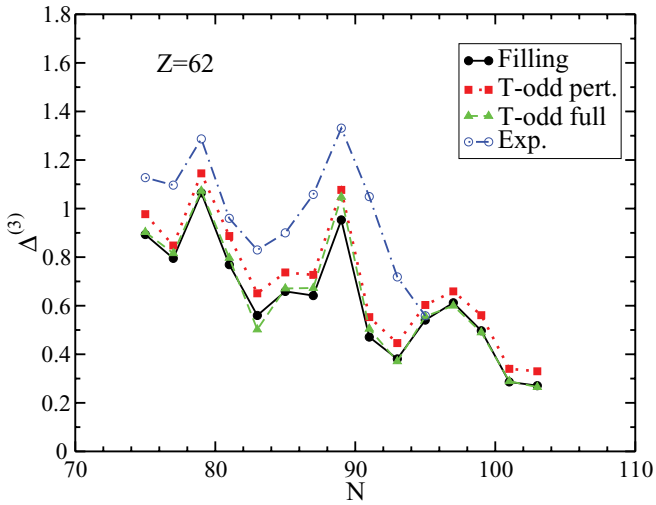

FIG. 4. (Color online) Neutron pairing gaps $\Delta^{(3)}$ in the Sm isotope chain. Energies were computed in the $N_{sh} = 12$ harmonic oscillator space.

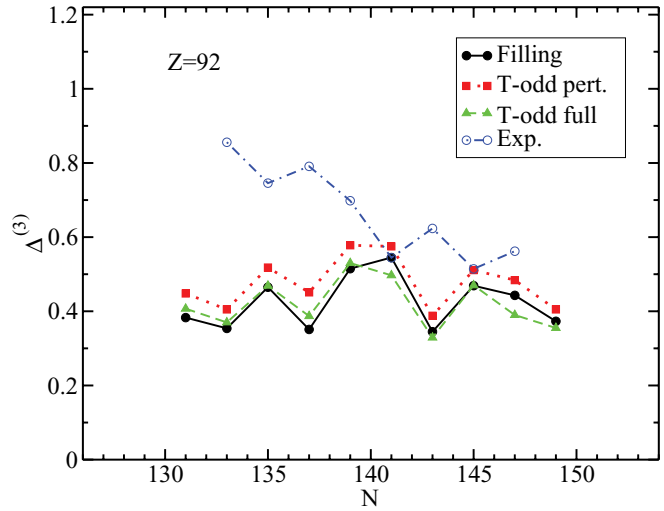

FIG. 5. (Color online) Neutron pairing gaps $\Delta^{(3)}$ in the U isotope chain. Energies were computed in the $N_{sh} = 14$ harmonic oscillator space.

spectra of these nuclei. In a systematic study of ground state spins of odd-A nuclei [27], it was found that only 40% of the spins of deformed nuclei agreed with their self-consistent mean field calculations. This raises an ambiguity in comparing the $\Delta^{(3)}$ to experiment, whether to take the ground state energies or energies of states of the same spin. We will come back to this point after reporting our comparison for ground state energies.

We first show the pairing gaps for the samarium isotope chain, well known for showing the transition from spherical to deformed nuclei. The calculated gaps are shown in Fig. 4. The theoretical gaps are smaller than would be expected from the systematics we found for the semimagic chains. As in the other cases, the T-odd field is significant at the perturbative level but hardly affects the gaps in the full treatment. The experimental data are somewhat higher than theory, but the variations along the chain follow the theory quite well.

The last isotope chain we consider is the uranium chain, shown in Fig. 5. The first isotope shown, $N = 131$, is weakly deformed but all the higher members have large (theoretical) quadrupole deformations. One sees in the graph that the calculated gaps are quite small throughout the chain. The experimental gaps are reduced with respect to the systematics for the semimagic nuclei, but not as much as the theory predicts. Also, one sees that the T-odd field has a very small effect in this very heavy chain, in fact negligible on the scale of the accuracy of the theory.

In the two chains we treated above, 11 of the gaps were for strongly deformed nuclei defined by the criterion that the calculated deformation β_2 satisfies $\beta_2 > 0.2$. Of these, the j_z and parity of the ground state agrees with experiment in five cases, including one where there is a near degeneracy of the lowest states. This is roughly the proportion as found in the very extensive survey of Ref. [27]. If we calculated the theoretical $\Delta^{(3)}$ demanding that the j_z agree with the observed ground state spin, the values would be some somewhat larger. We note that in some cases the theoretical ground state has mixed parity, so no spectroscopic identification is possible. For now, we take the present disagreement on the spectroscopy identity of the levels as an indicator of the accuracy of the mean-field theory. We anticipate extending the theory to restore angular momentum symmetry, and then a more complete comparison of the spectroscopy could be made.

IV. SYSTEMATICS

To better see the overall trends in the pairing gaps, we show in Table I average values of the pairing gaps for each isotope chain. The range of measured gaps in the isotope chain and the experimental average is shown in the second and third columns, respectively. One sees that the experimental gaps vary smoothly with the size of the nuclei, undergoing a mild decrease as a function of Z. If one takes the usual phenomenological parametrization of pairing gaps, varying as $A^{-1/2}$, one finds that the gaps for deformed nuclei are somewhat lower than one would expect from the spherical A-systematics. This in not surprising, given that the pairing depends on the single-particle level density at the Fermi surface and the levels of deformed nuclei are more spread out.

The last three columns of the table show theoretical results for the filling approximation and the two treatments of the

TABLE I. Average measured pairing gaps in selected isotope chains and the errors in the corresponding quantities for the various treatments of the time-odd fields.

Z	N range	Exp.	Filling	T-odd pert.	T-odd full
8	9–15	1.51	−0.41	−0.07	−0.36
50	53–83	1.18	+0.06	+0.22	+0.06
62	75–99	0.99	−0.29	−0.21	−0.30
82	97–131	0.98	+0.27	+0.37	+0.27
92	135–147	0.64	−0.19	−0.13	−0.21

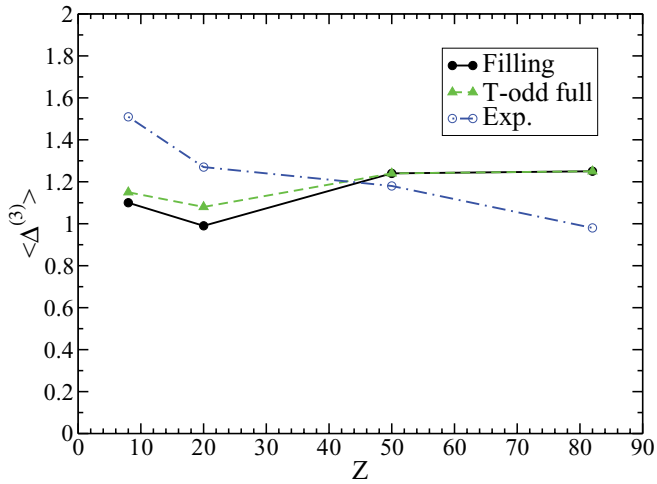

FIG. 6. (Color online) Average pairing gaps in the four spherical chains $Z = 8$, 20, 50, and 82, comparing theory and experiment.

T-odd fields. The entries in the table are the differences of the average theoretical and experimental gaps, taking the same nuclei to make the averages. For example, there are 4 measured gaps in the $Z = 8$ chain with an average of $\Delta^{(3)} = 1.51$ MeV. In the HFB theory with the filling approximation the average gap of those triplets is 1.10 MeV for an error of -0.41 MeV.

The errors for HFB + D1S theory in the filling approximation are shown in the fourth column. Both positive and negative errors are found, which we attribute to a dependance on deformation and on size of the nucleus. Namely, the theory predicts much smaller gaps in deformed nuclei than in the spherical ones. Also, in the medium and heavy nuclei the spherical nuclei are somewhat overpredicted while the deformed nuclei are substantially underpredicted. This highlights a deficiency of the HFB + D1S theory that cannot be cured by simply adjusting the overall strength of the interaction responsible for the pairing. Another deficiency of the theory can be seen by comparing the spherical chains, namely that there is very little Z dependence compared to experiment. This be seen more clearly in Fig. 6, which includes the $Z = 20$ chain along with the three other spherical chains in Table I. The lack of a significant Z dependence affects in particular the $Z = 8$ chain, which is seriously underpredicted.

The effect of including the T-odd field as a first-order perturbation is shown in the fifth column. The effect is to increase the pairing gaps, in qualitative agreement with the simple model described in the appendix. The increase is rather uniform over the isotope chains in the table, and the above-discussed deficiencies remain.

The full minimization of the HFB functional including the T-odd field gives gap errors shown in the last column of the table. One sees that the reminimization largely restores the calculate gaps to the filling approximation values. Thus, the filling approximation seems to be accurate enough to assess the HFB + D1S theory to the point of uncovering its systematic deficiencies.

The $\Delta^{(3)}$ values shown in the figures are available as a table (see Supplemental Material, Ref. [28]).

V. OUTLOOK

With our implementation of the new technique [1] for finding HFB minimum of odd-A nuclei we showed that it is a practical algorithm for the interactions in common use. Note that there is nothing in method that restricts the wave function to the one-quasiparticle space. We plan in the future to apply the method to two-quasiparticle wave functions, starting with the ground states of odd-odd nuclei. The energy splitting of the states with different K quantum numbers in strong deformed nuclei will provide a good test of the T-odd part of the interaction [29].

Concerning the validity of the filling approximation, we found that T-odd fields of the Gogny D1S interaction have a small effect and their inclusion does not noticeably improve the theoretical gaps. The same conclusion can be drawn for the T-odd field of a Skyrme interaction, from the HF-BCS study of gaps in Ref. [13] and HFB study of proton gaps in deformed nuclei in Ref. [14].

Concerning the performance of HFB on reproducing the experimental pairing, we found that the overall strength of the pairing in the D1S functional is close to optimal that it could reliably predict gap quenching. However, the mass dependence and the deformation dependence seems to deviate from the observed phenomenology.

This raises the question, what is missing in the theory that could be significant for pairing gaps? First of all, although the present T-odd effects are weak, the T-odd interaction should be re-examined with a view to making better energy functionals. In particular, the mean-field contribution to pairing gaps could affect the overall A dependence [18,19].

There are a number of correlation effects that could affect the pairing gaps. The most obviously ones are those that restore broken symmetries that may occur in the HFB wave functions. For example, projection of good particle number has been shown to have a non-negligible effect on the performance of Skyrme functionals [12,25,30]. However, improvement comes mostly from nuclei having weak pairing condensates. Restoration of angular momentum symmetry can be very important, giving rise to correlation energies of the order of several MeV in deformed nuclei. This is much larger than the 0.1 MeV accuracy scale of pairing gap energies we would like to achieve. Particularly critical to odd-even differences is the presence of so-called Coriolis coupling effects in odd-N systems with small j_z ([31], Chap. 4). Also, the energy gain by angular momentum projection is quite different in spherical and deformed nuclei, so it could affect the gaps in transitional nuclei. We consider the problem of restoration of angular momentum symmetry the most important computational issue to be address in future work. It is needed to make spectroscopic predictions, and it is needed to treat soft deformed nuclei on the same footing as the others. Unfortunately, the computational effort to carry out angular momentum restoration is heavy.

Another correlation is associated with the polarization of the nucleus by the valence nucleons. The resulting induced pairing interaction has been calculated to give as strong a contribution as the nucleon-nucleon interaction in the pairing channel [32], Such induced interactions are long-ranged and energy-dependent, and vary from nucleus to nucleus

depending on its structure. It would not be surprising that the effects were beyond the scope of the simple energy functionals in current use.

Lastly, there are correlation effects associated with the parts of the Hamiltonian that are neglected in the HFB theory. In the theory of the ground state, 4-quasiparticle excitations are neglected. In the usual formulation of the odd-N theory in terms of quasiparticle excitations of the even-N wave functions, there is coupling to 3qp excitations that give a significant contribution to the pairing gaps [33]. In our formulation, the odd-N wave function is an HFB local minimum and therefore a quasiparticle vacuum. The 2qp matrix elements of the Hamiltonian vanish because of the minimization in the odd-N space. Thus only 4qp excitations need to be considered. However, the quasiparticles energies can be negative in odd-N systems, because the qp creation operator can in effect unblock one of the orbitals. This would give smaller energy denominators in the second-order perturbative contribution for the H^{40} term in the Hamiltonian. Besides reducing the pairing gaps, its contribution might have a different dependence on A and on deformation.

ACKNOWLEDGMENTS

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APPENDIX

The HFB energy contains a spurious self-energy in the filling approximation for the unpaired particle in the wave function of an odd-A system. As a consequence, the filling approximation cannot be considered reliable for calculating quantities related to odd-even energy differences. This problem has been known for a long time in both condensed matter physics [34] and nuclear physics [35]; see Ref. [36] and its citations for recent discussions. Reference [36] considers the Skyrme family of energy functionals and points out that the problem disappears if the time-odd fields satisfy certain constraints. In this appendix, we estimate the possible error in the calculated pairing gaps when the time-odd fields are neglected.

To see how this comes about, let us consider a the t_0 term in the Skyrme interaction, i.e. the simple δ-function interaction $v(r_{12}) = t_0\delta^3(r_{12})$. The density entering the Skyrme functional will be a matrix in spin and isospin, see, e.g., [37]. In the absence of spin-orbit splitting, the density can be decomposed into time-even and time-odd parts by dividing the orbitals into two groups depending on the spin quantum number s_z. Labeling the groups by "+" and "−", the t_0 contribution to the identical-particle energy functional is

$$\langle v\rangle = t_0 \int d^3r\rho_+(r)\rho_-(r). \tag{A1}$$

Next the densities are decomposed into time-even and time-odd densities as $\rho_{e,o} = \rho_+ \pm \rho_-$. Then the interaction energy becomes

$$\langle v\rangle = \frac{t_0}{4}\int d^3r(\rho_e)^2 - \frac{t_0}{4}\int d^3r(\rho_o)^2. \tag{A2}$$

For the paired ground states, the second term is nonzero when there is an odd number of particles, but it is dropped in the filling approximation. To assess the magnitude of the error, we examine the simplest cases: (a) a state with one particle; (b) the two-particle state in which a particle is put into the time reversed orbital. Let us call the ρ_+ density associated with the one-particle state ρ_1. Then

$$\rho_e = \rho_o = \rho_1 \quad \text{(1 particle)}. \tag{A3}$$

Taking both T-even and T-odd terms in Eq. (A2), the terms cancel giving zero interaction of a particle with itself. In the filling approximation, the energy is

$$\langle v\rangle_{1,f} = \frac{t_0}{4}\int d^3r(\rho_1)^2. \tag{A4}$$

This may be compared with the two-particle interaction energy $\langle v\rangle_2$ given by Eq. (A2) with

$$\rho_e = 2\rho_1; \quad \rho_o = 0 \quad \text{(2 particles)}. \tag{A5}$$

From this it follows that the spurious self-energy is related to the two-particle matrix element by

$$\langle v\rangle_{1f} = \tfrac{1}{4}\langle v\rangle_2. \tag{A6}$$

This can only be small if the diagonal two-particle interaction matrix elements are small.

Of course in actual nuclei the spin-orbit field is very important, contrary to what was assumed here. Nevertheless, the model shows that T-odd fields can be significant, and are likely to be repulsive in the perturbative limit for interactions that are attractive in the filling approximation. We note further that the problem of spurious self-energies is particularly severe in theories that do not have an accurate treatment of the exchange (Fock) interaction. For example, in the relativistic mean field theory [17], the perturbative T-odd contribution is always negative, i.e., opposite in sign to HFB.

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