Microscopic Structure of Fundamental Excitations in $N = Z$ Nuclei

Wojciech Satuła[1,2] and Ramon Wyss[1]

[1]*Royal Institute of Technology, Frescativ. 24, S-104 05 Stockholm, Sweden*

[2]*Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, PL-00 681, Warsaw, Poland*

(Received 1 December 2000; published 17 July 2001)

An extended mean-field model is presented that describes states of different isospin in odd-odd and even-even nuclei. Excitation energies of the $T = 1$ states in even-even as well as $T = 0$ and $T = 1$ states in odd-odd $N = Z$ nuclei are calculated. It is shown that the structure of these states can be determined in a consistent manner when both isoscalar and isovector pairing collectivity as well as isospin projection (treated here within the isocranking approximation) are taken into account. In particular, in odd-odd $N = Z$ nuclei, the interplay between quasiparticle excitations (relevant for the case of $T = 0$ states) and isorotations (relevant for the case of $T = 1$ states) explains the near degeneracy of these states.

DOI: 10.1103/PhysRevLett.87.052504 PACS numbers: 21.10.Hw, 21.10.Re, 21.60.Ev, 74.20.–z

It is well known that pairing properties of finite Fermi systems are number-parity dependent. This is particularly well documented in atomic nuclei which exhibit phenomena such as odd-even mass staggering or odd-even staggering of the moments of inertia. These phenomena originate from simple phase-space quenching due to the odd (quasi)particle known as the blocking effect. Within the standard BCS theory of superconductivity the blocking effect can naturally be accounted for by assuming the ground state of the odd system to be a one-quasiparticle (QP) [or two-quasiparticle (2QP) in odd-odd (o-o) nuclei] excitation on top of the even-even (e-e) vacuum, $\alpha^\dagger|\text{vac}\rangle$. In fact, the simplicity and consistency of the BCS treatment of even and odd nuclei were of paramount importance to establish the theory of superconductivity in atomic nuclei [1,2].

The classical BCS theory requires to be extended only in the closest vicinity of the $N = Z$ line. In these nuclei, apart from the isovector pairing mode, isoscalar neutron-proton Cooper pairs coupled to non-zero angular momentum can also be formed. However, the empirical fingerprints of this pairing phase are not very clear. The problem is rather complex, because it requires a detailed understanding of both pairing phenomena and the nuclear symmetry energy. An invaluable source of information allowing one to disentangle these effects, is the isobaric excitations in $N = Z$ nuclei, as already discussed in [3–6]. Unfortunately, most of these studies were either purely phenomenological or based on, in our opinion, inconsistent models. In this Letter, we argue that the proper understanding of the isobaric excitations can be obtained only on a microscopic level. It requires that both isoscalar and isovector pairing as well as isospin projection (at least approximate) be taken into account. Moreover, within such a model, the standard BCS scheme of elementary excitations does not apply any longer. We provide the necessary extensions of the BCS theory which allow for a simultaneous description of (i) the mass excess in $N = Z$ nuclei, (ii) isospin $T = 1$ excitations in even-even $N = Z$ nuclei (theory of $T = 2$ states in e-e nuclei was given in our previous Letter [7]), and (iii) $T = 0$ and $T = 1$ states in o-o nuclei.

We begin with the description of $T = 1$ states in e-e nuclei. Similar to our Letter [7] we start with a single-particle (SP) model, $\hat{H}^\omega = \hat{H}_{\text{SP}} - \hbar\omega\hat{t}_x$, where $\hat{H}_{\text{SP}}$ generates (for the sake of simplicity) an equidistant and isosymmetric, i.e., four fold degenerate spectrum, $e_i = i\delta e$. For nonzero frequency each level splits into a pair of upsloping ($|-\rangle$) and downsloping ($|+\rangle$) Routhians, carrying alignment $t_x = \mp 1/2$. The SP Routhians cross at the frequencies: $\hbar\omega_c^{(n)} = (2n-1)\delta e$, where $n = 1, 2, 3, \ldots$. As shown in [7] the reoccupation process which takes place at each level crossing [$\omega_c^{(n)}$] conserves the isosignature symmetry. In other words, cranking the lowest SP configuration (vacuum) gives only the states of *even* isospin. Hence, states of odd isospin are obtained by promoting one particle from the $|-\rangle$ state to the lowest $|+\rangle$ state, as depicted in Fig. 1. The lowest odd-T branch of the isorotational band is obtained by cranking this particle-hole (p-h) excited state. The excitation energy and initial alignment of this p-h state are δe and $T_x = 1$, respectively.

The p-h excitation modifies the isorotational spectrum in the following manner: It blocks the level crossing at $\hbar\omega = \delta e$. The allowed crossings appear at frequencies $\hbar\omega_c^{(n)} = 2n\delta e$ $(n = 1, 2, 3, \ldots)$. At each level crossing the isospin changes by $\Delta T_x = 2$, giving rise to an odd-T isorotational band. The total excitation energy of the band is

$$\Delta E = \frac{1}{2}\,\delta e + \frac{1}{2}\,\delta e T_x^2\,. \qquad (1)$$

The formula (1) is similar to the one obtained previously [7] for the states of even isospin. Indeed, the moments of inertia come out identical. However, the odd-T band is shifted in energy by $\delta e/2$ due to the p-h excitation.

One should note that the $|+\rangle|-\rangle$ $T = 0$ p-h excitation is odd with respect to time-reversal symmetry, whereas the remaining pair $|+\rangle\overline{|+\rangle}$ is time-even. Hence, the $T = 1$ pair creates the initial isoalignment, whereas the p-h

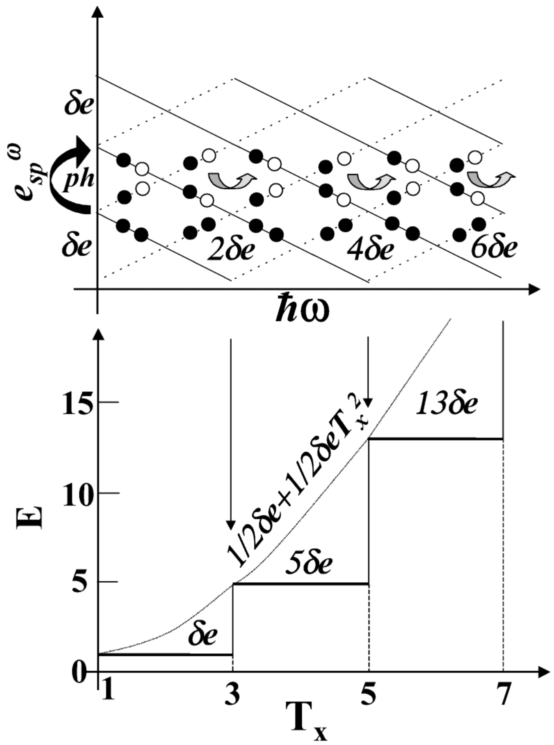

FIG. 1. The single-particle Routhians (upper panel) versus isocranking frequency for the equidistant level model. Solid and dashed lines depict downsloping, $|+\rangle$, and upsloping, $|-\rangle$, SP states carrying isoalignments of $\pm 1/2$, respectively. At each level crossing (indicated by arrows) the configuration changes, as well as the energy and isoalignment (lower panel).

excitation breaks *time-reversal* symmetry. This explicit mechanism of time-reversal symmetry breaking is *crucial* since all $T = 1$ states in e-e nuclei carry angular momentum. Although the SP model is oversimplified, it reveals the nature of odd- and even-T states in e-e nuclei: Both time-reversal and isosignature symmetries imply that odd-T states are based on an excited p-h configuration and cannot be reached by isocranking the vacuum configuration to an odd-T_x value. Obviously, since the ground state wave function in e-e nuclei is time-even, the $T = 1$ state can be realized in a realistic model with pairing correlations only by blocking the lowest 2QP state.

We now proceed to investigate how the excitation scheme is modified in the presence of pairing correlations. Our Hamiltonian is based on the deformed single-particle potential of Woods-Saxon– (WS-)type. The two-body correlations contain both isovector and isoscalar seniority-type pairing:

$$\hat{H}^{\omega} = \hat{h}_{\mathrm{WS}} + G_{T=1}\hat{P}_1^{\dagger}\hat{P}_1 + G_{T=0}\hat{P}_0^{\dagger}\hat{P}_0 - \hbar\omega\hat{t}_x\,, \quad (2)$$

where $\hat{P}_1^{\dagger}$ and $\hat{P}_0^{\dagger}$ create isovector and isoscalar pairs, respectively. The model is similar to the one described in detail in Ref. [8] with the difference that the most general Bogolyubov transformation without any symmetry induced restrictions is employed. It is important to stress that our calculations are identical to the ones done in Ref. [7] to compute $T = 2$ excitations in e-e nuclei.

The Hamiltonian (2) is solved using the Lipkin-Nogami (LN) approximate number projection. The number projection serves here essentially as a source of *spontaneous* isospin symmetry breaking [8]. Because of this mechanism, LN mixes different pairing phases similar to the exact model solutions allowing, most likely, for a simulation of higher-order effects such as quartetting or α clustering [9]. Isospin symmetry can be restored subsequently, which is done here approximately by the isocranking method in complete analogy to the case of spherical symmetry breaking and spatial rotations.

In our previous Letter we showed that the cranked ground state configuration $|\mathrm{vac}\rangle$ with $T_x = \sqrt{6}\,[T_x = \sqrt{T(T+1)}]$ yields surprisingly accurate predictions for $\Delta E_{T=2}$. However, as discussed above, we cannot repeat this procedure for the $T = 1$ states and determine the frequency $\hbar\omega$ so that $T_x = \sqrt{2}$ since such a state does not break time-reversal symmetry. To properly describe the $T = 1$ states in the presence of pairing correlations implies that one has to start from a trial wave function that corresponds to the lowest elementary excitation, i.e., to the 2QP excitation, $\hat{\alpha}_1^{\dagger}\hat{\alpha}_2^{\dagger}|\mathrm{vac}\rangle$. Hence, we proceed as follows: (i) At each iteration step we perform the standard Hartree-Fock-Bogolyubov (HFB) transformation [10]

$$\begin{pmatrix}\mathbf{U}^{(k)}\\ \mathbf{V}^{(k)}\end{pmatrix} \rightarrow \begin{pmatrix}\mathbf{V}^{(k)\star}\\ \mathbf{U}^{(k)\star}\end{pmatrix} \quad (3)$$

for the two lowest quasiparticle states $k = 1, 2$. Moreover (ii) we impose a certain, very small, spatial cranking frequency $\hbar\omega_s \sim 0.01$ MeV to remove the degeneracies in the QP spectrum. This does not influence the excitation energy, $\Delta E_{T=1}$, and is further justified because the $T = 1$ states have, in general, $I \neq 0$. Finally, (iii) since, at isofrequency zero, the alignment $\langle 2qp|\hat{t}_x|2qp\rangle_{\omega=0} = 0$, we determine the cranking frequency $\hbar\omega$ so that our solution satisfies the condition of $T_x = 1$.

The results of our calculations are shown in Fig. 2. Isoscalar pairing plays a crucial and, interestingly, unexpected role regarding the nature of these states. In our previous Letter, it was shown that isorotations strongly reduce $T = 0$ pairing correlations and the $T = 2$ states are predicted to be purely isovector paired. Still, isoscalar correlations are vital in restoring the correct inertia parameter [7] and, hence, the excitation energy. In contrast, isorotation of the 2QP configuration results in a smooth increase of isoalignment and quenching of the weak isovector pairing (see Fig. 3). This puzzling result can be understood qualitatively by going to the so-called canonical basis [10] (see Ref. [11] for further details). In this basis, at low ω (i.e., for the mixed-phase solution), all canonical QP states have fractional occupation numbers. The structure of the canonical basis changes with increasing ω so that it approaches the limit of symmetric $|+\rangle$ or antisymmetric $|-\rangle$ combinations of the original WS states, as expected from the SP model discussed above. Simultaneously, the occupation numbers of the blocked states go to unity. Let us further observe that isovector and isoscalar pair creators are:

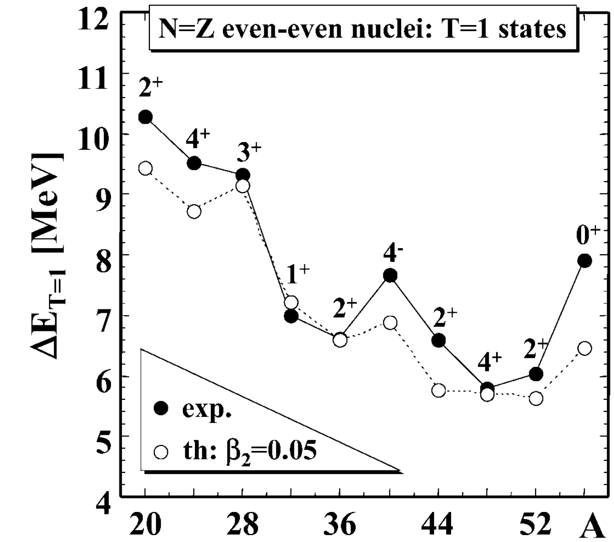

FIG. 2. Excitation energies, $\Delta E_{T=1}$, and angular momenta, I^{π}, of the lowest $T = 1$ states in e-e nuclei (•). The calculated results are marked by (∘).

$P^{\dagger}_{T=1} \sim a^{\dagger}_{+}\bar{a}^{\dagger}_{+} + a^{\dagger}_{-}\bar{a}^{\dagger}_{-}$ and $P^{\dagger}_{T=0} \sim a^{\dagger}_{+}\bar{a}^{\dagger}_{-} - a^{\dagger}_{-}\bar{a}^{\dagger}_{+}$, respectively, when expressed in the $|\pm\rangle$ basis. They correspond to entirely different scattering processes and will, apparently, react completely differently to blocking. Indeed, with increasing ω the contribution to the $\Delta_{T=1}$ gap coming from the lowest canonical QP states approaches $\sim U_{+}V^{*}_{+} \rightarrow 0$, while for the $T = 0$ field it corresponds to $\sim U_{-}V^{*}_{+} + U_{+}V^{*}_{-} \rightarrow 1$. Hence, with increasing ω, blocking becomes more and more effective in the $T = 1$ channel, whereas it does not affect the $T = 0$ correlations. Once the nucleus reaches the isoalignment of $T_x = 1$ the isosymmetry of the blocked pair is fully restored. This isovector pair decouples from the o-o $T = 0$ paired core and aligns along the cranking axis. The system becomes *trapped* in this state and the $T = 0$ pairing is destroyed by the isoCoriolis antipairing effect only at very high ω [7].

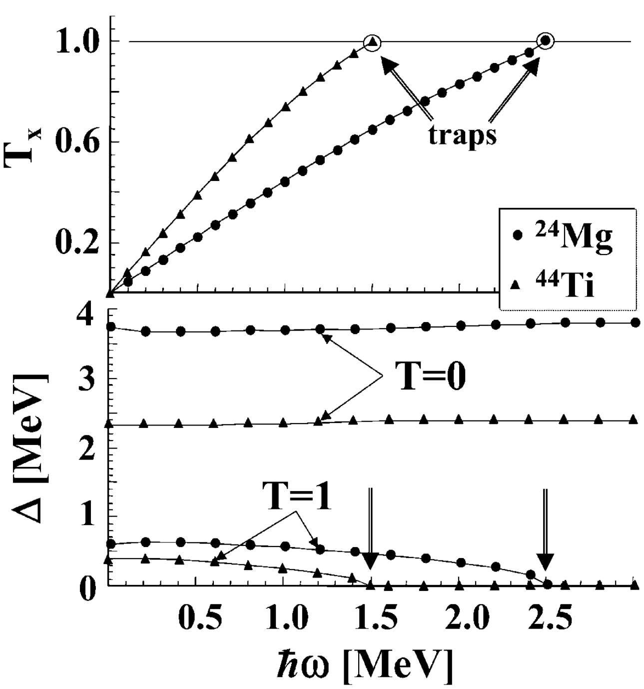

FIG. 3. Isospin T_x and isoscalar and isovector pairing gaps versus rotational frequency. Calculations have been done for ^{24}Mg and ^{44}Ti. The figure clearly indicates the collapse of isovector pairing correlations, giving rise to isospin traps.

Let us finally turn to the spectrum of o-o $N = Z$ nuclei. There, the ground state is determined by the competition between the $T = 1$ and $T = 0$ states. Several authors already pointed out that the structure of the ground state of o-o $N = Z$ nuclei reflects the delicate balance between the symmetry energy and pairing correlations, and that the energy difference may constitute a sensitive probe for the role of isovector and isoscalar pairing correlations [3,5,6,12]. To better understand the situation in $N = Z$ o-o nuclei let us come back to the extreme SP picture. In this model two valence nucleons can form either an isovector, $T = 1$, pair $(|+\rangle\overline{|+\rangle})$, giving rise to an isoaligned ground state configuration, or isoscalar pair $(|-\rangle|+\rangle)$, forming a $T = 0$ p-h excitation. Although the energy of both states is degenerate, the states have entirely different structures: The $T = 0$ state is time-odd and carries angular momentum, whereas the $T = 1$ is time-even and has zero angular momentum.

The crucial question is then how to describe these states in a realistic mean-field–based theory including pairing correlations. The ground state wave function in e-e nuclei is time-even. Likewise, the $T = 1$ state of the o-o $N = Z$ nucleus can be regarded as a linear combination of the isobaric analog states, i.e., the $(N + 1, Z - 1)$ and $(N - 1, Z + 1)$ e-e neighbors. It has the properties of an e-e–like vacuum, however, *excited in isospace*. Since we project on good $T_z = 0$, the e-e vacuum needs to be isocranked to yield the correct value of $T_x = \sqrt{2}$. No quasiparticle excitation is required to describe the $T = 1$ state and therefore there will be no reduction of isovector pairing correlations, but the isoscalar pairing will be suppressed due to the isoCoriolis antipairing effect [7].

On the other hand, the HFB ground state wave function has clearly the wrong symmetry (time-even) for the $T = 0$ state in o-o nuclei. Therefore, the only way to describe it, within a mean-field–based theory, is by means of the corresponding 2QP excitation, $\hat{\alpha}^{\dagger}_{1}\hat{\alpha}^{\dagger}_{2}|\text{vac}\rangle$. In this way all minimal-isospin $[T = |N - Z|/2]$ states, the ground states in o-o nuclei, are treated consistently as 2QP exciatations within the HFB approximation. The difference between the theoretical approach to calculate $T = 0$ and $T = 1$ states in o-o nuclei is shown schematically in the inset of Fig. 4, which elucidates the role played by 2QP excitation and isocranking, respectively.

To obtain a quantitative estimate for the energy difference of the $T = 0$ and $T = 1$ states, $\Delta E = \Delta E_{T=1} - \Delta E_{T=0}$, in o-o nuclei, we performed a set of calculations following the rules sketched above. The results are presented in Fig. 4. As mentioned above, to first order these two basically different states are almost degenerate in

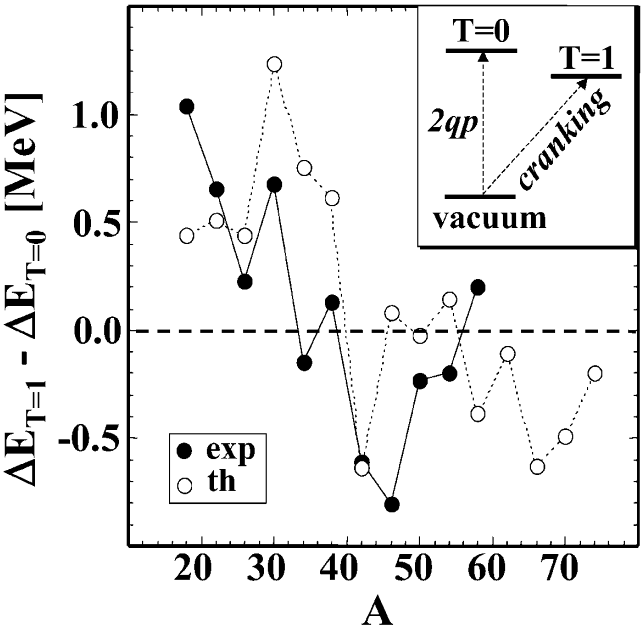

FIG. 4. Empirical (•) and calculated (∘) excitation energies, $\Delta E = \Delta E_{T=1} - \Delta E_{T=0}$, of the lowest $T = 0$ and $T = 1$ states in o-o $N = Z$ nuclei. The inset indicates schematically the two different excitation modes of the $T = 0$ and $T = 1$ states in our calculations (see text for more details).

experiment (•). Our calculations (∘) show the same trend. This is particularly interesting because it was claimed previously, that this degeneracy is proof of lacking $T = 0$ pairing correlations [6]. Evidently, these claims were based upon a poor understanding of the underlying structure of the elementary excitations allowed in the presence of proton-neutron pairing correlations. The $T = 0$ states in o-o nuclei are less bound than comparable e-e nuclei, not due to the lack of $T = 0$ correlations but due to the large $T = 0$ pair gap, which results in a comparable large 2QP excitation energy.

Our calculations not only show the near degeneracy but also the inversion of the sign of ΔE which, in agreement with experiment, takes place somewhere around the $f_{7/2}$ subshell. The inversion reflects basically the different mass dependence of the symmetry energy and the $T = 0$ pairing correlations. Since the value of $\Delta E_{T=1}$ is governed by the symmetry energy, it will decrease with mass as $\sim 1/A$. On the other hand, the value of $\Delta E_{T=0}$ is governed by pairing properties, i.e., depends on the size of the effective pairing gap including both $T = 0$ and $T = 1$ pairing correlations. Apparently, the pairing correlations do not fall off with mass as rapidly as $1/A$, giving rise to the inversion.

From our generalized HFB theory it is straightforward to understand the basic differences in the excitation energy pattern of e-e and o-o nuclei. In e-e nuclei, we need to consider both quasiparticle excitations *and* isospin cranking for the $T = 1$ excitation. Both are costly in energy. In addition the superfluidity of the $T = 0$ core reduces the moment of inertia and the excitation energy is rather high. In o-o nuclei, we simply deal with the competition between isocranking ($T = 1$) and 2QP excitation ($T = 0$). Energetically, to first approximation, these effects are very similar.

In summary, we have presented a consistent microscopic explanation of pairing phenomena in o-o and e-e $N = Z$ nuclei based on an extended *mean-field* approximation. Our model includes, in a self-consistent manner, both isoscalar and isovector pairing correlations, and takes into account projection onto good particle number (within the so-called Lipkin-Nogami approximation [8]), and isospin (within isospin cranking formalism [7]). In e-e $N = Z$ nuclei the $T = 1$ excitation corresponds to an isocranked 2QP configuration. With increasing isofrequency, the valence pair decouples from the isoscalar-paired odd-odd core and aligns along the x axis in isospace, forming a trap at $T_x = 1$.

In o-o $N = Z$ nuclei the $T = 1$ excitation is described by means of the isocranked o-o "false vacuum" with $T_x = \sqrt{2}$. Hence, this state represents a mixture of e-e neighbors ($Z - 1, N + 1$ and $Z + 1, N - 1$) in accordance with isospin and time-reversal symmetry. The $T = 0$ excitations in o-o $N = Z$ nuclei, on the other hand, are treated as 2QP excitations in accordance with time-reversal symmetry. This is consistent with standard self-consistent HFB treatment of all o-o $N \neq Z$ nuclei. The agreement between the data is more than satisfactory given the simplicity of our model. Moreover, because all parameters follow exactly those used for the calculations of the $T = 2$ states [7], we have a consistent scheme that accounts simultaneously for the mass excess (the Wigner energy), the $T = 1$, and $T = 2$ states in e-e $N = Z$ nuclei, and the near degeneracy as well as inversion of $T = 0$ and $T = 1$ states in o-o $N = Z$ nuclei.

This work was supported by the Göran Gustafsson Foundation, the Swedish Natural Science Research Council (NFR), and the Polish Committee for Scientific Research (KBN) under Contract No. 2 P03B 040 14.

[1] A. Bohr, B. R. Mottelson, and D. Pines, Phys. Rev. **110**, 936 (1958).
[2] S. T. Belyaev, special issue of Mat. Fys. Medd. Dan. Vid. Selsk. **31** (No. 11) (1959).
[3] J. Jänecke, Nucl. Phys. **73**, 97 (1965).
[4] N. Zeldes and S. Liran, Phys. Lett. **62B**, 12 (1976).
[5] P. Vogel, Nucl. Phys. **A662**, 148 (2000).
[6] A. O. Macchiavelli *et al.,* Phys. Rev. C **61**, 041303(R) (2000).
[7] W. Satuła and R. Wyss, Phys. Rev. Lett. **86**, 4488 (2001).
[8] W. Satuła and R. Wyss, Nucl. Phys. **A676**, 120 (2000).
[9] J. Dobes and S. Pittel, Phys. Rev. C **57**, 688 (1998).
[10] P. Ring and P. Schuck, *The Nuclear Many Body Problem* (Springer-Verlag, New York, 1980).
[11] W. Satuła and R. Wyss, nucl-th/0104015.
[12] S. Frauendorf and J. Sheikh, Nucl. Phys. **A645**, 509 (1999).