Pairing correlations. I. Description of odd nuclei in mean-field theories

T. Duguet, P. Bonche, P.-H. Heenen, J. Meyer

Pairing correlations. Part 1: description of odd nuclei in mean-field theories.

T. Duguet, P. Bonche,
Service de Physique Théorique, CEA Saclay,
91191 Gif sur Yvette Cedex, France
P.-H. Heenen,
Service de Physique Nucléaire Théorique, Université Libre de Bruxelles, C.P 229, B-1050 Bruxelles, Belgium
J. Meyer
Institut de Physique Nucléaire de Lyon,
CNRS-IN2P3 / Université Claude Bernard Lyon 1,
43, Bd. du 11.11.18, 69622 Villeurbanne Cedex, France

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Abstract

In order to extract informations on pairing correlations in nuclei from experimental masses, the different contributions to odd-even mass differences are investigated within the Skyrme HFB method. In

this first paper, the description of odd nuclei within HFB is discussed since it is the key point for the understanding of the above mentioned contributions. To go from an even nucleus to an odd one, the advantage of a two steps process is demonstrated and its physical content is discussed. New results concerning time-reversal symmetry breaking in odd-nuclei are also reported.

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1 Introduction

A proper description of odd nuclei by mean-field methods requires to break the time-reversal symmetry, making their study much harder than for even ones. Since this symmetry is broken by the unpaired nucleon, the BCS approximation is not anymore valid and has to be replaced by the Hartree-Fock-Bogolyubov (HFB) one. This symmetry breaking has also the consequence that the individual wave-functions are no longer doubly degenerate, doubling at least the computing task. Nevertheless, because of present computer capacities and of the development of new iteration schemes, it is now possible to describe even and odd nuclei on the same footing at the mean-field level of approximation.

Thanks to that, observables can be calculated along an isotopic or isotonic chain without uncertainties related to a different level of approximations for even and odd particle number. This is particularly important for differential quantities computed by finite difference formulae, as the odd-even mass staggering (OES). Such observables, directly related to experimental data,

*Corresponding author : duguet@spht.saclay.cea.fr

put into evidence the specificities of odd nuclei with respect to even ones and have been intensively used to adjust effective pairing interactions.

Their proper analysis is difficult as self-consistency mixes the different effects related to the addition of a nucleon, especially the modification of the chemical potential, the breaking of time-reversal symmetry and the weakening of pairing correlations. In order to isolate an interpret the different contributions to odd-even effects, it is essential to correctly formalize and understand the transition between even and odd quantum states. To give some insights on this question, a perturbative analysis is particularly adapted since one can a priori write analytical relations between neighbor nuclei in term of creation or annihilation operators.

The HF approximation provides a useful step in the understanding of this transition, since it does not involve pairing effects. In this case, the link [1] between even and odd states is perturbatively given by the creation of a particle on the first empty level in the state of the nucleus with one less nucleon. We shall however reconsider this simple case because, to be useful for the understanding of the more general HFB description of odd nuclei, the HF approximation has to be derived as the zero pairing limit of the HFB one.

When pairing is taken into account, a well-known successful perturbative procedure consists in describing an odd state as a one quasi-particle (qp) state on the even neighbor vacuum. However, this procedure suffers from an inconsistency with regard to the particle number [1]. It demands an ad hoc readjustment of the chemical potential. This is what is implicitly done when the theoretical BCS gap at the Fermi energy taken from the calculation of an even state is compared to experimental odd-even mass differences. This procedure is however quite satisfactory for energy predictions, and has been extensively used [2].

We shall show that these inconsistencies can eliminated by a redefinition of the vacuum on which the qp is created by perturbation. The two step prodedure which is introduced allows to analyse in details the description of odd nuclei by fully self-consistent calculations and in particular, to emphasize the changes brought about by pairing correlations when going from an even to an odd nucleus.

A similar two step picture to go from even to odd systems has been defined by Balian, Flocard and Veneroni [3, 4] for the density operator. They introduced it in terms of number-parity-projected BCS states in the more general context of Fermionic super-conducting systems at finite temperature. However, they have not extensively studied the implications of this prescription in the context of nuclear structure. This intermediate vacuum has also been used as a natural definition of the smooth part of the microscopic binding energy in a work dealing with the OES [5].

The present work is organized as follow. In section 2.1, the standard perturbative qp creation process in BCS theory is reviewed and analyzed in order to point out some important characteristics for the description of odd states. In section 2.2, we propose a slightly different prescription for a perturbative treatment of odd nuclei. In section 2.3, the zero pairing limit of our revised picture is performed in order to show how it matches with the usual HF one. In section 3 and 4, detailed HFB calculations are performed on even and odd Ce isotopes in order to illustrate the procedures discussed at the perturbative level in section 2. Conclusions are drawn in section 4.

2 Odd nuclei description in a mean-field theory including pairing

2.1 Perturbative nucleon addition process

Let us start with the BCS description of an even nucleus. For a given effective Hamiltonian $\hat{H}$, one determines the ground-state wave-function $\mid \Psi(\mathrm{N}) >$ with the constraint that it has a mean number of particles equal to N. This constraint is imposed by the chemical potential λ_N as Lagrange multiplier. A first approximation for the ground state of the odd neighbor with one more neutron [†] is obtained by a perturbative one qp creation $\mid \Psi_{\mathrm{k}} > \; = \alpha_k^\dagger \mid \Psi(\mathrm{N}) >$, where $\alpha_k^\dagger$ is a qp creation operator. The average particle number of the state $\mid \Psi_{\mathrm{k}} >$ is $N + u_k^2 - v_k^2$, where v_k^2 is the BCS occupation number of the state k. This average-number of particles is not necessarily equal to $N + 1$ and depends on the qp which has been selected [1]. The energy difference between the state $\mid \Psi_{\mathrm{k}} >$ and the even ground-state is:

$$\begin{aligned} < \Psi_{\mathrm{k}} \mid \hat{H} \mid \Psi_{\mathrm{k}} > - < \Psi(\mathrm{N}) \mid \hat{H} \mid \Psi(\mathrm{N}) > \; &= \; (u_k^2 - v_k^2)\lambda^N + E_k^N \\ &= \; \frac{e_k(e_k - \lambda^N) + {\Delta_k}^2}{\sqrt{(e_k - \lambda^N)^2 + {\Delta_k}^2}} \; , \end{aligned} \tag{1}$$

where the chemical potential λ^N and the qp energy $E_k^N = \sqrt{(e_k - \lambda^N)^2 + {\Delta_k}^2}$ are taken from the even ground-state.

If the qp corresponds to a state having an energy e_k close to λ^N ($u_k^2 - v_k^2 \approx 0$), the energy difference 1 is approximatively equal to E_k^N and is close to Δ_k. However, the mean particle number is close to N, and $\mid \Psi_{\mathrm{k}} >$ is not a good candidate to describe an odd nucleus. To ensure an odd average number of particles in $\mid \Psi_{\mathrm{k}} >$, one should create a qp such that $(e_k - \lambda^N)$ is much larger than Δ_k. In such a case, the energy difference is approximatively given by

[†] In what follows we limit ourselves to the case of an odd isotope with one more neutron. All what is presented can be easily transposed to the removal of a neutron, or to odd isotones.

$e_k \gg \lambda^N$. Once again, $\mid \Psi_{\rm k} >$ is not a good candidate for the ground state of the neighboring odd nucleus.

This analysis shows that an odd nucleus wave-function cannot be approximated by a perturbative one qp excitation on the ground state of an even nucleus. Such a treatment does lead either to a wrong particle number and/or to a bad energy.

To circumvent the problem, one can put artificially $u_k^2 - v_k^2 \approx \pm 1$ in Eq. 1 (see for instance ref. [1], Chap. 6.3.4) which leads to:

$$< \Psi_{\rm k} \mid \hat{H} \mid \Psi_{\rm k} > - < \Psi({\rm N}) \mid \hat{H} \mid \Psi({\rm N}) > = \pm \lambda^N + E_k^N \ . \qquad (2)$$

Such a procedure is satisfactory for the determination of energies. However, it does not provide a tool to calculate other observables as radii or deformation since the wave-function still does not have the right mean particle number.

Such a problem does not appear in self-consistent calculations since the one qp excitation is numerically performed together with a constraint on the correct average number of nucleons [‡]. The chemical potential is readjusted self-consistently whatever the starting point of the calculation is. However, to correct the inconsistencies of the perturbative picture is a necessary step to identify the various contributions to the transition from an even nucleus to its odd neighbor.

2.2 Revised perturbative scheme

To improve the perturbative analysis requires the definition of a new vacuum on which qp states are blocked in such a way that the choice of an energetically favorable qp leads to a state with a nearly correct particle number.

[‡]In BCS theory, it consists of solving the gap equation for an even number of particles excluding the state occupied by the odd nucleon.

A way to do that is to first determine the fully paired state having the right mean odd particle number. Let us denote that state by $\mid \Psi^{\mathrm{BCSE}}(\mathrm{N}+1) >$. The subscript BCSE means that the state is constructed as an *Even* vacuum without qp excitation and without breaking time-reversal invariance but with an odd average particle number. The lowest excitation energy with respect to this new reference vacuum will be generated by the qp with the lowest energy but the $\mid \Psi_{\mathrm{k}}^{\mathrm{BCS}} >$ will now have an odd mean number of particles with a good approximation. The energy difference $\Delta E(k)$ with the even neighbor becomes:

$$\begin{aligned} \Delta E(k) &= \underbrace{E^{BCSE}(N+1) - E^{BCS}(N)} + E_k^{N+1} \\ &\approx \frac{\partial E^{BCSE}}{\partial N} + E_k^{N+1} \quad , \end{aligned}$$

where E_k^{N+1} is the energy of the lowest qp in $\mid \Psi^{\mathrm{BCSE}}(\mathrm{N}+1) >$ and $E^{BCSE}(N)$ is the energy of the BCS fully paired vacuum with N particle (even or odd). This result is formally similar to that of Eq. 2. However, the qp excitation is now defined in the reference state $\mid \Psi^{\mathrm{BCSE}}(\mathrm{N}+1) >$ and no had hoc modification of the chemical potential is required.

This procedure, although not perfect as it remains perturbative, is now qualitatively satisfactory from all points of view and provides at the same time a good approximation for the energy and for the wave-function of an odd nucleus.

Such a perturbative qp creation on top of the odd fully paired state, instead of the even neighbor's one, has already been introduced by Ring *et. al* [6] and used with success in Ref. [7]. Its main justification was simplicity with respect to self-consistent blocking, but not the formal step achieved with respect to a perturbative qp creation performed on the even vacuum.

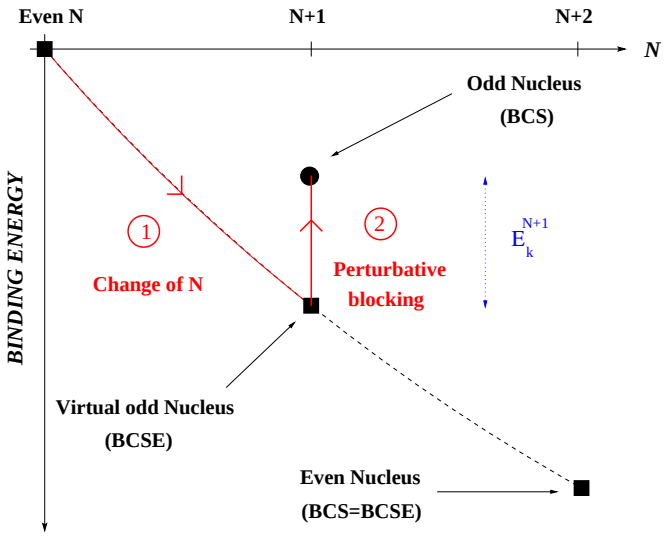

Figure 1: Schematic picture of the two step procedure proposed to determine the ground state of an odd isotope.

The introduction of an intermediate reference vacuum requires to study an odd nucleus in two steps. This procedure, illustrated on Fig. 1, eliminates the inconsistency between the addition of a nucleon and the creation of an energetically favorable qp excitation. From a mathematical point of view, it shows that the odd fully paired state is better grounded than an even neighbor ground-state as the zero-order reference for a perturbation theory of odd nuclei. In the rest of this paper, we will analyse these steps from a physical point of view and use them to separate self-consistent calculations in two identified processes.

2.3 Limit of zero-pairing

The description of an odd nucleus with respect to an even neighbor is at first sight less complicated in the absence of pairing. Indeed, there is no problem related to the particle number and an odd nucleus is simply obtained by adding a nucleon on the first empty level in the even neighbor's HF state. Two different approximations are used within this picture.

If time-reversal invariance is not broken, each single-particle state is at least doubly degenerate and the odd nucleon is added using the filling approximation: the first pair of empty levels in the even neighbor are identically occupied with probability 0.5 in the odd state[§].

If time-reversal symmetry breaking is properly taken into account and for a deformed configuration, all degeneracies are lifted and the first pair of empty levels in the even isotope are occupied with probability 1 and 0 in the odd neighbor[¶].

[§]For spherical nuclei, one adds $1/2j + 1$ particle in each state of the last degenerate j shell

[¶]For spherical nuclei, one orbital of the shell is completely filled, lifting the degeneracies. Several tries have to be done in order to get the lowest in energy.

Let us now analyze how the standard HF picture matches with the zero-pairing limit of the perturbative method described in section 2.2. Most of the developments presented in this section have straightforward zero-pairing limits. Let us look explicitly to the limit for odd states only.

The limit of the perturbative one qp BCS state with an odd particle number is:

$$\mid \Psi_{\rm n}^{\rm BCS}({\rm N+1}) > \;\; \rightarrow \;\; \mid \Psi_{\rm n}^{\rm HF}({\rm N+1}) > \;\; = \;\; a_n^\dagger \prod_{k=1}^{N/2} a_k^\dagger \, a_{\bar{k}}^\dagger |0\rangle \;, \qquad (3)$$

whereas the fully paired odd vacuum leads to:

$$\mid \Psi^{\rm BCSE}({\rm N+1}) > \;\; \rightarrow \;\; \mid \Psi^{\rm HFE}({\rm N+1}) > \;\; = \;\; \frac{1}{\sqrt{2}} \left(1 + a_n^\dagger \, a_{\bar{n}}^\dagger\right) \prod_{k=1}^{N/2} a_k^\dagger \, a_{\bar{k}}^\dagger |0\rangle \;. (4)$$

One can check that:

$$\mid \Psi_{\rm n}^{\rm HF}({\rm N+1}) > = \alpha_n^\dagger \mid \Psi^{\rm HFE}({\rm N+1}) > \qquad (5)$$

where $\alpha_n^\dagger = \frac{1}{\sqrt{2}}(a_n^\dagger - a_{\bar{n}})$ is the singular[‖] zero-pairing limit for the lowest qp creation operator.

The wave function $\mid \Psi^{\rm HFE}({\rm N+1}) >$ introduced as the limit of the BCSE state is none of the two currently used HF wave-functions. However it leads to the same one-body density matrix, and thus to the same energy as the HF wave-function [**] obtained using the filling approximation.

[‖] Other qp operators $\alpha_k^{(\dagger)}$ $(k \neq n, \bar{n})$ tend to standard particle creation or annihilation operators $a_k^{(\dagger)}$.

[**] The filling approximation is actually defined through a density operator which is a statistical mixture of the two Slater determinants where one of the two time-reversed orbitals at the Fermi energy is filled. The $\mid \Psi^{\rm HFE} >$ state 4 for odd nuclei is a linear combination of the two neighboring even HF states.

The HF ground-state for odd nuclei is now described by a *one qp excitation* on top of the HFE state and not as in the usual procedure directly on top of the HF wave function of an even neighbor through particle operators. The two-step picture defined in the BCS case is thus extended to the zero pairing limit and will allow an analysis of the OES for any pairing correlations intensity.

The zero pairing limit illustrates the physical content of the nucleon addition process. The nucleon is *added* in the HFE wave function by increasing the occupation of each state of the last couple of degenerate orbits by 0.5. For odd N, the qp excitation *specifies* which one of the two states will eventually be occupied by the single nucleon in the odd wave function. The only difference in presence of pairing is that the nucleon is added over the whole fermi sea in the BCSE wave function because of pair scattering, while the qp creation still specifies the state eventually occupied by the single nucleon.

2.4 Self-consistent HFB treatment of odd nuclei

Since time-reversal symmetry is broken in an odd nucleus, a proper treatment of pairing correlations requires the use of the HFB method and the introduction of time-odd components in the mean-field.

In this context, Eq. 3 is replaced by:

$$\begin{aligned} E^{HFB}(N) &= E^{HFBE}(N) + [E^{HFB}(N) - E^{HFBE}(N)] \\ &= E^{HFBE}(N) + \overbrace{E^{pol}(N) \quad + \quad \Delta(N)} \quad , \end{aligned} \tag{6}$$

where HFBE refers to fully paired states, $\Delta(N)$ is the positive contribution due to the self-consistent blocking of pairing correlations in odd nuclei due to the presence of a single nucleon. $E^{pol}(N)$ is the part of the binding energy related to polarisation effects in odd nuclei. First, it contains a static

deformation-polarisation of the core induced by the non-zero multipole moment of the odd nucleon density. Second, the breaking of the time-reversal symmetry by this odd nucleon brings about non-zero spin and current contributions. The sum $E^{pol}(N) + \Delta(N)$ can be viewed as the self-consistent qp energy to be compared to the perturbative one, E_k^{N+1}.

In a fully self-consistent calculation, HFE and HF states are defined as the self-consistent zero-pairing limit of HFBE and HFB states.

3 Results

3.1 Addition of a nucleon

In this section, we apply the decomposition of energy introduced in section 2 to a chain of cerium isotopes, from ^{118}Ce to ^{166}Ce. Our aim is to determine to which extent this decomposition allows to decouple both effects related to the addition of a nucleon.

We have performed Hartree-Fock-Bogolyubov plus Lipkin-Nogami (HFBLN) calculations with the formalism and forces in the particle-hole (SLy4 Skyrme force) and particle-particle (zero-range density dependent pairing force) channels described in ref [8, 9]. Each odd nucleus is calculated twice: first, as a HFBLN fully paired vacuum with an odd average number of neutrons (HFBE state) and then with the fully self-consistent HFBLN scheme (HFB state). In this case, several qp configurations are investigated to determine the one corresponding to the ground state.

Cerium isotopes have been chosen because of their intermediate masses and also because their axial mean quadrupole deformation evolves regularly along the whole chain from sphericity to large deformations.

Fig. 2 displays the chemical potential as a function of mass from ^{150}Ce to

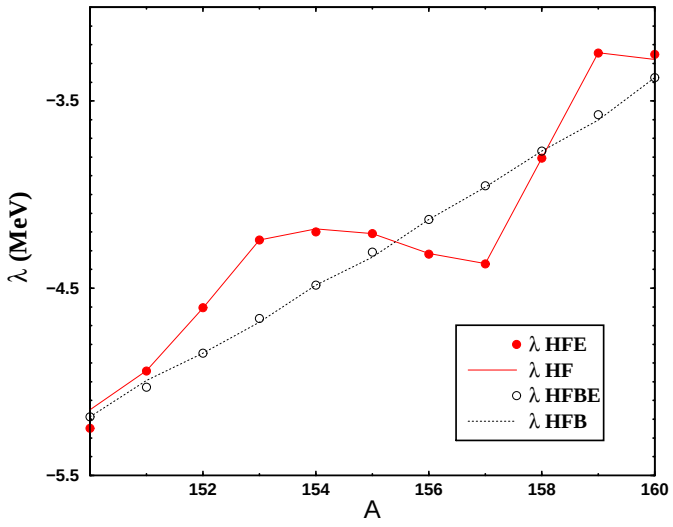

Figure 2: Chemical potential along the cerium isotopic line between ^{150}Ce and ^{160}Ce for HFE, HF, HFBE and HFB calculations.

^{160}Ce for HFE, HF, HFBE and HFB calculations. The chemical potentials in HF(E) [††] states are well defined in the zero-pairing limit of HFB(E) ones.

The results are represented for a sub-zone which is representative of the full cerium isotopic line that we have calculated. The figure shows that the change of Fermi level due to the addition of a nucleon is fully taken into account by introducing only a constraint on an odd particle number (HF(B)E calculations) and is not affected by the self-consistent blocking in the final state. It proves that the qp creation carries no additional particle with respect to the reference vacuum HF(B)E, as expected from the perturbative picture. This justifies from a quantitative point of view the decoupling of the single nucleon addition in the fully paired vacuum and its blocking in the full HF(B) odd state.

The evolution of λ with N depends on the underlying mean-field as well as on the occupation numbers. On Fig. 3 are shown the neutron single-particle spectra obtained in the HFBE and HFB calculations. For odd nuclei, the double degeneracy of the single-particle energies is lifted in the HFB calculation, leading to an odd-even staggering of these single-particle energies. However, if one takes the mean energy between the states of a doublet, the HFBE and HFB single-particle spectra are identical. Fig. 4 displays the single-particle neutron spectra for HF(E) calculations and shows that the same remark remains valid in the zero-pairing limit.

We can conclude from these comparisons that constraining the HF(B)E state to an odd number of particles without creating a qp excitation lead to the same mean-field as the full HF(B) state, except for small polarisation effects due to the breaking of time-reversal invariance.

[††]The parenthesis in HFB(E) means that the corresponding sentence deals with "HFB *and* HFBE". Identically, HF(B)E means "HFE and HFBE" and HF(E) means "HF and HFE".

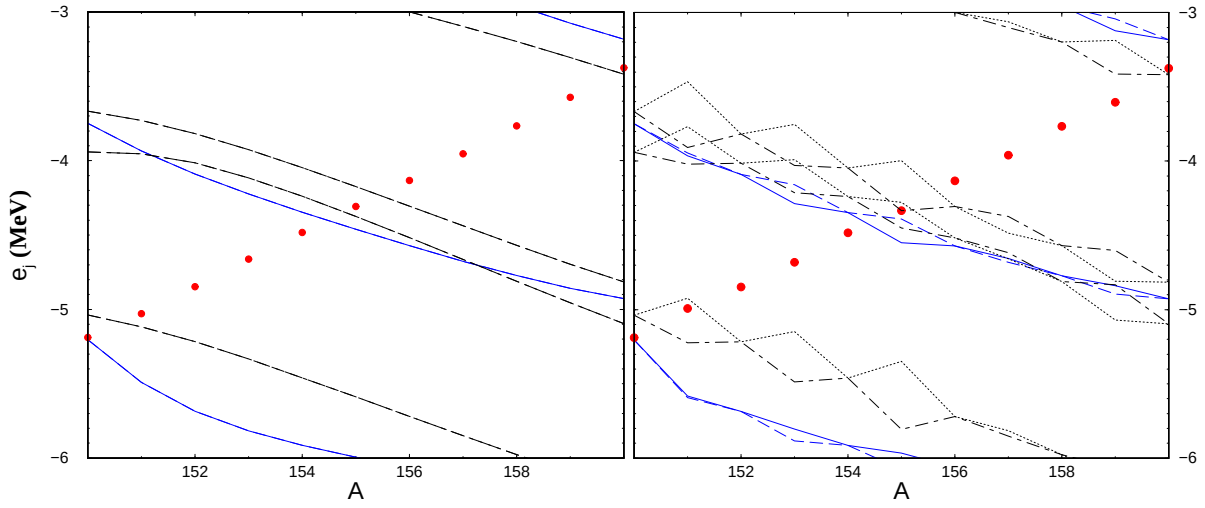

Figure 3: Single-particle spectrum as a function of the mass number A between ^{150}Ce and ^{160}Ce. The left panel corresponds to the HFBE case, the right one to the HFB one. The conventions for (parity, signature) are : (+,+)=solid line, (+,-)=long-dashed line, (-,+)=dotted line, (-,-)=dot-dashed line. Circles are for the chemical potential.

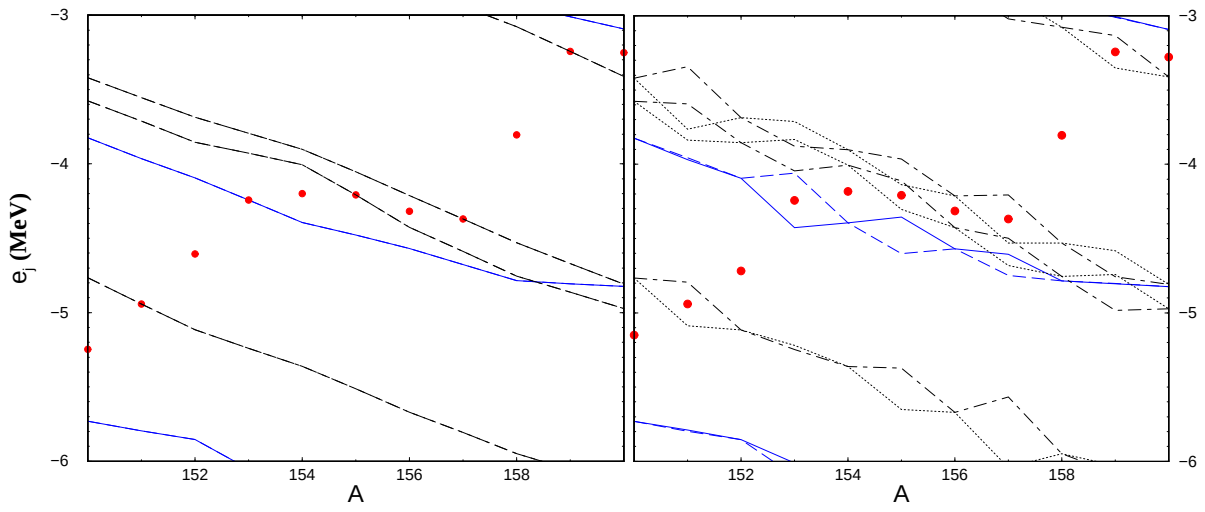

Figure 4: Same as Fig. 3 for the HFE and HF cases respectively.

We will therefore take $E^{HF(B)E}$ as the "Mean-Field" part of the binding energy. In the zero-pairing limit, this definition reduces to the time-reversal invariant part of the interaction. When pairing correlations are present, this energy includes also the part of the pairing energy which is not related to the blocking effect and which varies smoothly with the particle number.

Even if the previous conclusions are valid in both the HF(E) and HFB(E) cases, the situation differs depending whether pairing correlations are included or not. The left panels of Fig. 3 and 4 show that the single-particle spectra are different in the two cases. In addition, Fig. 2 shows the smoother behavior for $\lambda_{HFB(E)}$ as compared to $\lambda_{HF(E)}$. This proves that the inclusion of the pairing is not a perturbative effect and deeply modifies the wave-function.

The fundamental difference between $\mid \Psi^{\mathrm{HFBE}} >$ and $\mid \Psi^{\mathrm{HFE}} >$ is related to the way a nucleon is added in both cases: while it is added on a specific pair of time reversed orbits in the HFE case as discussed in section 2.3, it is

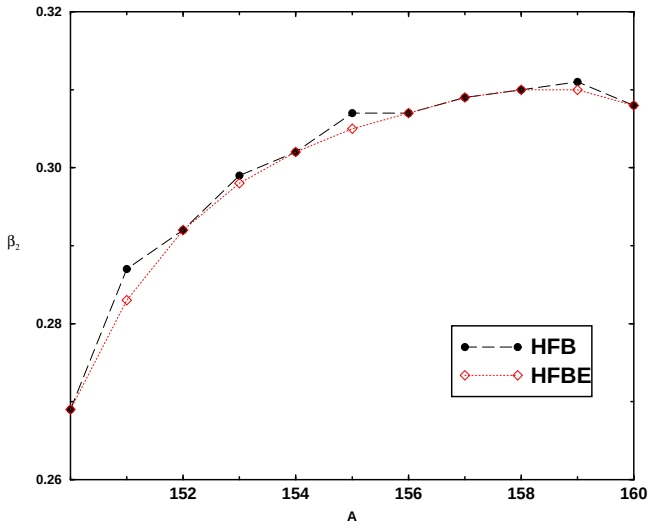

Figure 5: HFB and HFBE axial quadrupole deformation parameters $\beta_2 = \sqrt{\frac{\pi}{5}}\frac{<\hat{Q}_{20}>}{A<r^2>}$ along the cerium isotopic line between ^{150}Ce and ^{160}Ce.

spread out on several orbits around the Fermi level in the HFBE case because of pair scattering, making the variation of $\lambda_{HFB(E)}$ smoother with A.

The same type of analysis is valid for other observables. Fig. 5 gives the mass number dependence of the axial quadrupole moment. The smooth variation related to the modification of the mean-field is fully taken into account in the HFBE state. In the HFB calculation of odd nuclei, a tiny additional change of deformation appears due to the qp creation. The proposed scheme allows to decouple the two contributions.

3.2 Qp creation effect without pairing

We have studied the process of the addition of one nucleon through the definition of $\mid \Psi^{\mathrm{HF(B)E}} >$ as a reference vacuum. Let us focus now on the blocking of this added nucleon. We propose a simple tool to disentangle the two components of the qp creation process: the breaking of time-reversal invariance and the quenching of pairing. First, the zero-pairing case is treated because it contains one of the two effects only.

The energy difference E^{HF} - E^{HFE} displayed on Fig. 6 gives a direct information on polarisation effects brought by the odd nucleon, especially through the breaking of the time-reversal symmetry. This symmetry breaking removes the degeneracy between signature partners (see Fig. 3 and 4). As noticed in previous works [10, 11], this effect is the largest for signature partners corresponding to the qp which is created. Fig. 6 shows that the net effect is repulsive and of the order of a few hundreds keV. Along the cerium isotopic line, it ranges from 48 keV for ^{155}Ce to 223 keV for ^{147}Ce.

The polarisation effects obtained with the Sly4 interaction have been found attractive on average in ref [12] for light nuclei. The difference with our results may be related either to a mass dependence of the effect or to a competition between isovector and isoscalar effects [13]. The effect of the

isovector terms of the interaction is indeed very weak in the study of N ≈ Z nuclei of Ref. [12] while it is not the case in the present study of Ce isotopes.

In appendix A is derived an approximate expression for the difference between HF and HFE energies. It is based on the assumption that the HF and HFE single-particle wave-functions are identical, leading to the same matrix elements for the two-body force; the two N-body wave-functions only differing through individual occupation numbers. This assumes that the deformation-polarisation of the core induced by the blocked nucleon is very weak.

This perturbative calculation for the polarisation effect in absence of pairing gives:

$$E^{pol} = E^{HF} - E^{HFE} \approx \frac{\tilde{e}_n - \tilde{e}_{\bar{n}}}{4} \quad . \tag{7}$$

where $\tilde{e}_n$ and $\tilde{e}_{\bar{n}}$ are the split orbits in the HF wave-function having occupation numbers 1 and 0 respectively.

The results obtained using this approximation are also plotted on Fig. 6 and are in very good agreement with the full polarisation effect along the whole cerium isotopic line. This justifies that the individual wave-functions are marginally modified by the qp creation and shows that core deformation-polarisation effects are weak.

The energy difference 7 can be rewritten in terms of a single unperturbed diagonal particle-hole matrix element of the two-body force between the blocked time-reversed states:

$$E^{pol} \approx -\frac{\bar{V}^{p-h}_{n\bar{n}n\bar{n}}}{4} \quad . \tag{8}$$

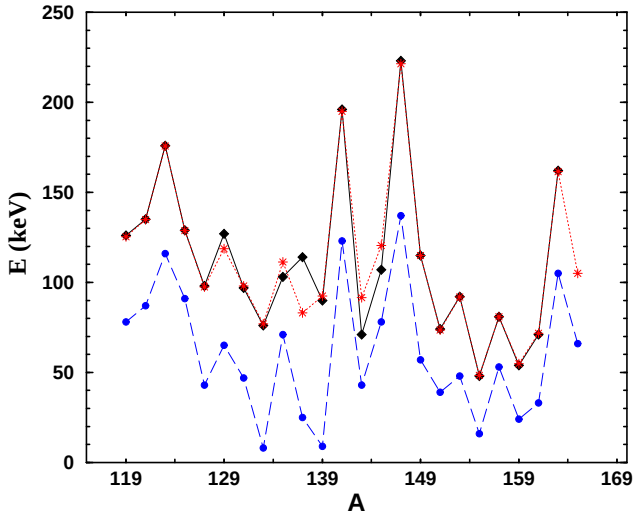

Figure 6: Diamonds: energy difference E^{HF} - E^{HFE} (see text) along the cerium isotopic line. Stars: approximation $[\tilde{e}_n^{HF} - \tilde{e}_{\bar{n}}^{HF}]/4$ for the polarisation effect in odd nuclei. Circles: time-odd mean-field terms contribution $-\bar{V}^{odd}_{n\bar{n}n\bar{n}}/4$ to the time-reversal symmetry breaking effect.

On Fig. 6 is also plotted the contribution of the time-odd terms of the interaction $-\bar{V}^{odd}_{n\bar{n}n\bar{n}}/4$ to E^{pol}. The explicit expression of $\bar{V}^{odd}_{n\bar{n}n\bar{n}}$ can be worked out from Ref. [14]. One can see that the time-odd terms are roughly responsible for 2/3 of the time-reversal symmetry breaking effect for all isotopes. The erratic behavior of the polarisation effect as a function A is directly related to these terms, while the time-even terms seem to be less sensitive to the characteristics of the blocked orbits.

Eq. 7 and 8 allow to extract the polarisation effect in a simple way from a single calculation. Either one performs a full HF calculation and evaluates the polarisation effect in term of the single-particle energy splitting, or one performs a simpler HFE calculation and evaluates the polarisation effect by extracting the relevant matrix element.

The single-particle character of the polarisation energy illustrated by Eq. 7 and 8 has been pointed out in ref. [12] where it has been shown that:

$$E^{pol}(N-Z=2n) = E^{pol}(N-Z=2n+1) + E^{pol}(N-Z=2n-1) \quad . \quad (9)$$

The fact that the polarisation energy is shown to be related to the splitting of a single pair of states or a single matrix element simplifies the analysis.

One can therefore relate the magnitude of the polarisation energy in an odd nucleus with three properties of the blocked orbital. In decreasing order of importance they are: a small j_z component on the deformation axis (K quantum number), a down-slopping behavior of the individual energy with A and a large total angular momentum j for the spherical shell from which the orbit originates. That orbitals with these characteristics have large polarisation effects is not surprising since the same orbitals are known to be very sensitive to rotation which is also an effect related to time-odd terms of the mean-field. The large energy difference that can be seen on Fig. 6

for ^{147}Ce is associated with the blocking of the very down-slopping Nilsson orbital [660]1/2, originating from the $1i13/2$ shell. In ^{123}Ce and in ^{141}Ce, the large polarisation corresponds to the [541]1/2 blocked orbitals coming from the $2f7/2$ spherical shell. These last two nuclei are of particular interest because although they have different masses and very different deformations (see Fig. 5), their large polarisation energy is of the same order of magnitude since it is related to the matrix element involving the same pair of Nilsson blocked states. This demonstrates that K is a relevant quantum number in order to characterize the magnitude of E^{pol}. These conclusions are valid along the whole cerium isotopic line.

3.3 Qp creation effect with pairing

When pairing correlations are included, the energy difference E^{HFB} - E^{HFBE} mixes both the effect of the blocking of pairing and the polarisation effect and cannot be used to extract one of them only. However, it is shown in Appendix A that the approximation 7 for the polarisation effect still holds for HFB calculations.

As a consequence, E^{pol} has the same order of magnitude in average in HF and HFB cases although it can be significantly different for a given nucleus as it can be seen on Fig. 7. Polarisation energies in the non zero pairing case are given on Fig. 7 only for nuclei for which the assumption of a perturbative calculation is valid.

Due to self consistency, the ordering of the qp levels may be different in the HFE and HFBE calculations. On Table 1 are listed the Nilsson labels of the orbitals corresponding to the qp created for each odd cerium isotopes in the HF and HFB calculations. The differences that can be seen on Fig. 7 between both calculations are related to the different qp corresponding to the ground states of ^{123,145,147,155,163,165}Ce. For ^{161,163,165}Ce, the difference is due

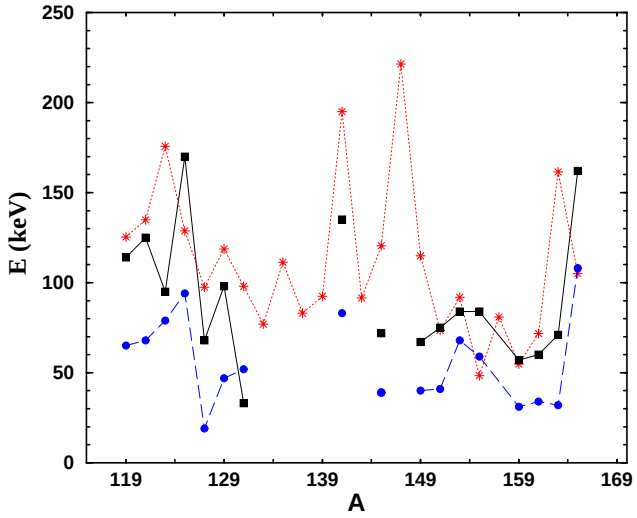

Figure 7: Stars: approximation $[\tilde{e}_n^{HF} - \tilde{e}_{\bar{n}}^{HF}]/4$ for polarisation effect in odd nuclei. Squares: same as stars for the HFB calculation. Circles: time-odd mean-field terms contribution $-\bar{V}_{n\bar{n}n\bar{n}}^{odd}/4$ to the polarisation effect.

to a shift by two neutron units for the blocked qp. Thus, the polarisation energies in ^{163}Ce and^{165}Ce with pairing included are respectively equal to those of ^{161}Ce and ^{163}Ce without pairing.

¿From ^{141}Ce to ^{163}Ce the polarisation energy has a smoother behavior when pairing is included. In the HF calculation, the lowest qp automatically changes from one odd nucleus to next, while the same qp may remain the lowest in energy in several neighboring nuclei in the HFB case, making the effect smoother with A.

There are only eight nuclei for which the created qp excitation is identical in both calculations. For five of them, ^{119,129,151,159}Ce, the polarisation effect is not significantly modified by the inclusion of pairing. However, for three others, ^{125,131,141}Ce, the self-consistency between the mean-field and the pairing field in the HFB calculation is large enough to induce a significant modification of the energy splitting $\tilde{e}_n - \tilde{e}_{\bar{n}}$.

As in zero-pairing case, the contribution of time-odd terms, plotted on Fig. 7, contributes to approximately 2/3 of the full polarisation energy and follows the average behavior of E^{pol}. This illustrates the sensitivity of time-odd components of the interaction to the (j_z, j) quantum numbers of the created qp.

The polarisation energies have been calculated for the tin isotopic line in Ref. [15] within the framework of relativistic mean-field theory. Pairing correlations were treated in the BCS approximation. It was found attractive by about 300 keV for two different parametrizations of the force. We have performed a similar study within our approach and we have found that the polarisation energy for the same isotopes is repulsive by approximately 100 keV. These contradicting results show the necessity of further analysis on the dependency of the polarisation effect on self-consistent models and forces that are used. The main source of uncertainty is due to the fact that the time-odd

terms of the phenomenological forces have only been indirectly constrained through time-even ones [16]. The possibility to associate the polarisation effect with a specific matrix element of the force could open a way for the inclusion of a constraint on these terms in the standard fitting procedures.

4 Conclusions

In this paper, we have re-analyzed the way odd nuclei are described in self-consistent mean-field calculations with a double goal. We wanted to focus on the nucleon addition process in the nuclear mean-field wave-function and on its energetic consequences when going from one nucleus to the neighbor. We also wanted to define a procedure such that the HF treatment of odd nuclei is the zero-pairing limit of the HFB treatment. To achieve these goals, we have defined a two steps procedure.

The first step corresponds to the description of odd nuclei as even ones, by an appropriate constraint on the particle number. This has required a modification of the usual HF filling approximation. It has been shown that this pseudo even state takes into account the variation of the mean-field with mass number.

In the second step, a qp is created on top of this odd vacuum. This does not modify the position of the Fermi level whatever the characteristics of the created qp (shell, spin, parity). Thus, the physical effect of the addition of a nucleon is contained in this fully paired state while the qp creation brings the extra polarisation and the modification of pairing correlations due to the non pairing of this added odd nucleon.

An application to the Ce isotopic line has illustrated the relevance of this decoupling and the possibility to remove a smooth behavior of physical observables like energies and quadrupole moments thanks to this pseudo even

structure.

Thus, the creation of a qp has two effects on binding energy of odd nuclei. The first is related to the breaking of time-reversal invariance while the second is due to the non pairing of a nucleon. In the HF case, we have shown that the first effect can be related with an excellent accuracy to the lift of the Kramers degeneracy of the conjugate pair of orbits in the single-particle spectrum having occupation 1 and 0. This effect is also present with pairing correlations and can still be related to the same Kramers degeneracy. In this case, its energetic effect is dominated by the quenching of pairing in the qp creation process. We have also shown that the first effect can be associated with a single matrix element in the particle-hole channel. This result is promising for the necessary inclusion of a constraint on the mean-field time-odd terms in the standard fitting procedure of phenomenological two-body forces. In the present study, this result has allowed us to isolate the specific contributions of these time-odd terms which have been shown to account for 2/3 of the time-reversal symmetry breaking effect in odd cerium isotopes when using SLy4.

In the second part of this work, we will use the above analysis of odd nuclei in order to understand the different contributions to the odd-even mass fomulas currently used to approximate the pairing gap [17, 18].

APPENDIX: Perturbative calculation of the qp creation effect

The energy of an HFB state can be expressed in the canonical basis and is given by:

$$E^{HFB} = \sum_k \left(e_k - \frac{1}{2} \sum_{k'} \bar{V}^{p-h}_{kk'kk'} \, v^2_{k'} \right) v^2_k - \frac{1}{4} \sum_{k,l} \bar{V}^{p-p}_{k\bar{k}l\bar{l}} \, u_k \, v_k \, u_l \, v_l \quad , \qquad (10)$$

where $\bar{V}^{p-h}_{kk'kk'}$ and $\bar{V}^{p-p}_{k\bar{k}l\bar{l}}$ are the antisymmetrised matrix elements of the two-body force, v_k^2 are the eigenvalues ($u_k^2 = 1 - v_k^2$) of the density matrix and e_k the diagonal matrix elements of the Hartree-Fock field in the canonical basis:

$$e_k \;\; = \;\; t_k + \sum_{k'} \bar{V}^{p-h}_{kk'kk'}\, v^2_{k'} \quad , \tag{11}$$

where t_k is the diagonal matrix element of the kinetic energy operator for an individual wave-function ϕ_k in the canonical basis. We use the convention that k and $\bar{k}$ are paired partners. If not specified, the sum runs over all individual states. For simplicity, the rearrangement terms in the mean-field due to the density dependence of the Skyrme interaction are not included. However, their introduction does not modify the final expression for the polarisation energy.

The diagonal matrix element of the pairing field can also be defined by:

$$\Delta_k = -\frac{1}{2} \sum_l \bar{V}^{p-p}_{k\bar{k}l\bar{l}}\, u_l\, v_l \tag{12}$$

Let us consider two approximations a and b [‡‡] of the exact HFB state of a given nucleus. To evaluate the difference between the energies obtained with these two approximations, we will suppose that one has only to take into account the changes in occupation v_k^2 and that changes in the canonical basis wave functions can be neglected in the calculation of the matrix elements of the interaction.

Let us take as state a a time-reversal invariant HFB state. One has then $e_k = e_{\bar{k}}$. The differences between the individual energy e_k in the state a and

[‡‡] All quantities referring to the case b will be upper-lined with a tilde.

the energies $\tilde{e}_k$ and $\tilde{e}_{\bar{k}}$ in the state b are given by:

$$\begin{aligned} \tilde{e}_k - e_k &= \sum_{k'} \bar{V}^{p-h}_{kk'kk'} \left(\tilde{v}^2_{k'} - v^2_{k'} \right) \quad , \\ \tilde{e}_{\bar{k}} - e_k &= \sum_{k'} \bar{V}^{p-h}_{\bar{k}k'\bar{k}k'} \left(\tilde{v}^2_{k'} - v^2_{k'} \right) \quad , \end{aligned} \tag{13}$$

Using the relations $\bar{V}^{p-h}_{kk'kk'} = \bar{V}^{p-h}_{k'kk'k}$ and $\sum_{k'} \bar{V}^{p-h}_{kk'kk'} v^2_{k'} = \sum_{k'} \bar{V}^{p-h}_{k\bar{k}'k\bar{k}'} v^2_{k'}$, one can derive the following expression:

$$E^b - E^a = \frac{1}{2} \sum_k \left[(e_k + \tilde{e}_k) \left(\tilde{v}^2_k - v^2_k \right) - \tilde{\Delta}_k \tilde{u}_k \tilde{v}_k + \Delta_k u_k v_k \right] \tag{14}$$

A Without pairing

Let us take for a the HFE wave-function and for b the HF one. The energy difference $E_b - E_a$ is due to time-reversal symmetry breaking and is equal to the polarisation energy E^{Pol}. The occupation numbers of all individual states below the Fermi level λ^{odd} are 1, and 0 for all states above, except for the pair of states with energies just above λ^{odd} which are 1/2 for a and 1 and 0 for b.

The energy difference given by Eq. 14 becomes:

$$\begin{aligned} E^{Pol} = E^{HF} - E^{HFE} &= (\tilde{e}_n - \tilde{e}_{\bar{n}}) \,/\, 4 \quad , \\ &= -\bar{V}^{p-h}_{n\bar{n}n\bar{n}} \,/\, 4 \quad , \end{aligned} \tag{15}$$

the second expression being obtained using Eq. 13 and the cancelation of the antisymmetrised matrix element $\bar{V}^{p-h}_{nnnn}$.

B With pairing

In the presence of pairing correlations, the energy difference (E^{HFB} - E^{HFBE}) contains contributions coming from the blocking of pairing and from polarisation effects due to the breaking of time-reversal invariance. This energy difference is calculated in two steps. First, the polarisation effects are eliminated by performing a filling approximation. This means that starting from the fully paired HFBE state, the occupation probabilities in the canonical basis are changed from v_k^2 to $\tilde{\tilde{v}}_k^2$ for all states, except for two of them close to the Fermi energy for which the occupations $\tilde{\tilde{v}}_n^2$ and $\tilde{\tilde{v}}_{\bar{n}}^2$ are set to 1/2. The blocking of pairing is taken into account by excluding these two states n and $\bar{n}$ from the calculation of Δ. Second, we consider the fully blocked state, for which the occupation probabilities are denoted by $\tilde{v}_k^2$, the state n and $\bar{n}$ having an occupation 1 and 0 respectively.

We have checked numerically that it is a fair approximation to take the occupation probabilities $\tilde{v}_k^2$ and $\tilde{\tilde{v}}_k^2$ and the pairing gaps $\tilde{\tilde{\Delta}}_k$ and $\tilde{\Delta}_k$ equal for all k and $\bar{k}$ except for n and $\bar{n}$.

Using this assumption, one can show that:

$$\begin{aligned} \tilde{\tilde{e}}_k \;=\; \tilde{\tilde{e}}_{\bar{k}} \;&=\; \tilde{e}_k - \left(\bar{V}^{p-h}_{knkn} - \bar{V}^{p-h}_{k\bar{n}k\bar{n}}\right) / 2 \quad , \\ &= \qquad (\tilde{e}_k + \tilde{e}_{\bar{k}}) \,/\, 2 \quad . \end{aligned} \tag{16}$$

The two successive energy differences can now be given in terms of the full blocked state variables (variables defined with one tilde on top of them) using Eq. 14:

$$E^{\tilde{\tilde{H}}FB} - E^{HFBE} = \frac{1}{2}\sum_{k\neq n,\bar{n}}\left(e_k + \frac{\tilde{e}_k+\tilde{e}_{\bar{k}}}{2}\right)(\tilde{v}_k^2 - v_k^2) + \left(e_n + \frac{\tilde{e}_n+\tilde{e}_{\bar{n}}}{2}\right)\left(\frac{1}{2} - v_n^2\right) \quad ,$$

$$- \frac{1}{2}\sum_k \left(\tilde{\Delta}_k\,\tilde{u}_k\,\tilde{v}_k \;-\; \Delta_k\,u_k\,v_k\right)$$

$$E^{\tilde{H}FB} - E^{HFBE} = \frac{1}{2}\sum_k \Big[\,(e_k + \tilde{e}_k)\,(\tilde{v}_k^2 - v_k^2) \;-\; \tilde{\Delta}_k\,\tilde{u}_k\,\tilde{v}_k \;+\; \Delta_k\,u_k\,v_k\Big] \quad .$$

We approximate the pure polarisation effect in the presence of pairing correlations by the energy difference $E^{\tilde{H}FB} - E^{\tilde{\tilde{H}}FB}$. Using the last two equations, we obtain:

$$E^{Pol} = \frac{\tilde{e}_n - \tilde{e}_{\bar{n}}}{4} \quad , \tag{17}$$

(18)

This result is formally identical to the HF result.

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Table 1: Nilsson numbers of created qp in odd cerium isotopes for zero as well as for realistic neutron pairing intensity (in MeV.fm^{-3}). Numbers are not reported when the created qp mixes several Nilsson states.

Cerium	$V_n^{p-p}=0$	$V_n^{p-p}=1250$
	K[Nn$_z\Lambda$]	
^{119}Ce	3/2[422]	3/2[422]
^{121}Ce	3/2[422]	5/2[532]
^{123}Ce	1/2[541]	5/2[413]
^{125}Ce	1/2[411]	1/2[411]
^{127}Ce	7/2[523]	5/2[402]
^{129}Ce	7/2[523]	7/2[523]
^{131}Ce	7/2[404]	7/2[404]
^{133}Ce	9/2[514]	
^{135}Ce	3/2[402]	
^{137}Ce	9/2[514]	
^{139}Ce	11/2[505]	
^{141}Ce	1/2[541]	1/2[541]
^{143}Ce	3/2[532]	3/2[532]
^{145}Ce	1/2[530]	3/2[532]
^{147}Ce	1/2[660]	
^{149}Ce	3/2[651]	3/2[521]
^{151}Ce	3/2[521]	3/2[521]
^{153}Ce	5/2[642]	3/2[521]
^{155}Ce	5/2[523]	1/2[521]
^{157}Ce	1/2[521]	
^{159}Ce	5/2[512]	5/2[512]
^{161}Ce	7/2[633]	5/2[512]
^{163}Ce	1/2[600]	7/2[633]
^{165}Ce	1/2[510]	1/2[600]