Effect of core polarization on magnetic dipole moments in deformed odd-mass nuclei

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Magnetic properties of deformed odd-mass nuclei are studied within a nonrelativistic mean-field-plus-pairing approach, namely the Skyrme-Hartree-Fock-BCS approach with self-consistent blocking. For an odd number of nucleons these approaches lead to the breaking of the time-reversal invariance. The deviation from the Schmidt values of the isoscalar magnetic dipole moment is known to result from a subtle balance between core-polarization effects and meson-exchange current effects. However, the former are usually calculated in the random phase approximation without time-reversal symmetry breaking at the mean-field level. In this work we show that if one takes into account this symmetry breaking already in the mean-field solution, the correction from core polarization yields a significant contribution to the empirical quenching of the spin gyromagnetic ratios as compared to the free values in deformed odd-mass nuclei. Moreover, we calculate magnetic dipole moments in the Bohr and Mottelson unified-model description with self-consistent blocked mean-field intrinsic states. The obtained results in the $A \sim 100$ and $A \sim 180$ mass regions as well as for three actinide nuclei compare favorably with experimental data.

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I. INTRODUCTION

It has been recognized for a very long time (see, e.g., Refs. [1,2] for an in-depth analysis) that the usual description of magnetic properties in deformed odd-mass nuclei merely due to the geometrical coupling of an unpaired (dubbed in what follows as "last") nucleon with an even-even core must be corrected. Two corrective effects are generally considered. The first and most important one is the coupling of the dynamics of the last nucleon with the core nucleon dynamics through time-reversal symmetry-breaking parts of the mean field. This coupling generates the appearance of a spin-vector component in that part of the one-body reduced density matrix which is due to the core nucleons. It results also in the existence of nonvanishing currents in the core. In deformed nuclei, as described within the so-called unified model of Bohr and Mottelson [3], this polarization manifests itself phenomenologically as a quenching of the spin gyromagnetic factors, g_s, from their free values by about 30% [2]. Note, en passant, that in this model approach, the totality of the deviation of magnetic moments from their pure single-particle values is merely attributed to a core polarization, within which only spin degrees of freedom play a role. The second correction, resorting to explicit mesonic degrees of freedom, is deemed to be less important (see, e.g., Ref. [4]). It is not directly accessible under the nonrelativistic reduction of the nucleonic interactions because it represents the contribution to the magnetic properties of the currents of the charged virtual mesons responsible for the neutron-proton interaction. This effect cannot be considered here in our microscopic approach using a nonrelativistic effective nucleon-nucleon interaction of the Skyrme type [5,6].

In the present paper, to study the magnetic effect of the core polarization induced by the last nucleon, we work within the Hartree-Fock-BCS (HFBCS) framework with a self-consistent blocking of the last nucleon. We consider eleven well-deformed nuclei (five odd-N and six odd-Z nuclei) as typical examples in the $A \sim 100$, $A \sim 180$, and actinide mass regions, assuming axial and intrinsic parity symmetries.

A direct comparison of the results of such microscopic calculations in well-deformed nuclei with the spectroscopic data may be performed using the unified-model framework [3] as done, e.g., in Ref. [7]. This allows one to generate nuclear states of a given spin and parity through the coupling of the intrinsic and rotational degrees of freedom approximately treated within this model. In such a treatment, the Coriolis coupling may influence the nuclear spectroscopic properties and in particular the magnetic ones which are the subject of the present study. Nevertheless, we have checked for the seventeen bandheads considered below and found that this coupling could be operative in only one single case—the $7/2^-$ state in the ^{175}Yb nucleus. For all other nuclei, no neighboring bandheads with a K value differing by ± 1 appear close enough in energy to allow for this coupling in the first order of perturbation theory. Consequently, the Coriolis coupling is neglected here.

The nuclear interaction that we use is the standard Skyrme interaction without inclusion, at this stage, of its tensor part. Strictly speaking, this is rather an energy-density functional because of the density dependence introduced in place of the zero-range three-body potential initially proposed by Skyrme [8]. Indeed, Stringari and collaborators showed that the SIII parameter set with the three-body potential yields isoscalar

spin instability in several subshell-closed, spin-unsaturated nuclei [9], and Lipparini and collaborators showed that the replacement with a two-body, density-independent term cures this instability [10].

The reason we discard the tensor part of the Skyrme interaction is because no parametrization which includes it and is free from finite-size spin instabilities is available yet [11]. Actually, it was recognized that, at least at the perturbative level, the tensor interaction plays within the energy-density functional framework a minor or simply corrective role for the ground-state mean-field characteristics [12] as well as for recently examined excitation modes as high-spin superdeformed rotation states [11] and isovector giant dipole resonances [13].

Having acknowledged the limitations of our current approach—ignoring the Coriolis coupling, tensor interaction, mesonic currents—and discussed their expected minor impact on our specific investigation carried out in the present study, we come to the point of this paper. We show that the self-consistent mean-field description offers a physical mechanism which accounts for the core-polarization effect induced by the presence of the unpaired (last) nucleon and that this description yields a fair reproduction of the experimentally observed magnetic dipole moments.

In the next section we present the theoretical framework, namely the Skyrme-HFBCS approach with self-consistent blocking, and the calculation of the spin quenching factor and total magnetic dipole moment. Then we present the calculation settings and the obtained results, and we provide a detailed analysis and interpretation of the latter. In the last section, we draw conclusions from the obtained results and propose some extensions of this study.

II. THEORETICAL FRAMEWORK

A. Self-consistent mean-field solutions with time-reversal symmetry breaking

Self-consistent mean-field ground-state solutions are obtained in the Skyrme-Hartree-Fock-BCS framework, briefly recalled below with an emphasis on the approximations made and the peculiarities stemming from the time-reversal symmetry breaking at the one-body level.

The nuclear Hamiltonian $\hat{H}$ considered is the sum of the intrinsic kinetic energy $\hat{K}$, the nuclear interaction $\hat{V}$, and the Coulomb interaction between protons. As often done, we make the approximation that neutrons and protons have the same mass m and neglect the two-body contribution to $\hat{K}$, so that the intrinsic kinetic energy becomes a one-body operator written as [14]

$$\hat{K} = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{\hat{\mathbf{p}}_i^2}{2m}. \tag{1}$$

The nuclear interaction $\hat{V}$ is chosen to be the Skyrme density-dependent local two-body interaction defined by the sum of the central $\hat{V}_{\rm c}$, density-dependent $\hat{V}_{\rm DD}$ (to mock up three-body effects) and spin-orbit $\hat{V}_{\rm s.o.}$ contributions given, in coordinate representation, by

$$\begin{aligned} V_{\rm c}(\mathbf{r}_1,\mathbf{r}_2) = {} & t_0(1 + x_0 P_\sigma)\,\delta(\mathbf{r}_1 - \mathbf{r}_2) \\ & + \frac{t_1}{2}(1 + x_1 P_\sigma)\,[\delta(\mathbf{r}_1 - \mathbf{r}_2)\,\mathbf{k}^2 + \text{H.c.}] \\ & + t_2(1 + x_2 P_\sigma)\,\mathbf{k}^\dagger \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2)\,\mathbf{k}\,, \end{aligned} \tag{2}$$

where $P_\sigma = \frac{1}{2}(1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)$ is the spin-exchange operator, $\mathbf{k} = \frac{i}{2}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)$, and H.c. denotes the Hermitian conjugate of the preceding term in the bracket,

$$V_{\rm DD}(\mathbf{r}_1,\mathbf{r}_2) = \frac{t_3}{6}(1 + x_3 P_\sigma)\,\rho^\alpha\left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2}\right)\delta(\mathbf{r}_1 - \mathbf{r}_2), \tag{3}$$

where ρ is the nucleon density,

$$V_{\rm s.o.}(\mathbf{r}_1,\mathbf{r}_2) = i\,W_0\,(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{k}^\dagger \times \delta(\mathbf{r}_1 - \mathbf{r}_2)\mathbf{k}\,. \tag{4}$$

In the context of time-reversal symmetry-breaking calculations, it should be noted that the two-body density-dependent interaction $V_{\rm DD}$ is not equivalent to a three-body zero-range interaction, as discussed earlier by various authors (see, e.g., Ref. [10]).

As is well known, the expectation value E of the above Hamiltonian $\hat{H}$ calculated for a normalized Slater determinant $|\Phi\rangle$ is a time-even functional

$$E = \int d\mathbf{r}\,(\mathcal{H}_{\rm kin}(\mathbf{r}) + \mathcal{H}_{\rm c}(\mathbf{r}) + \mathcal{H}_{\rm DD} + \mathcal{H}_{\rm s.o.}(\mathbf{r}) + \mathcal{H}_{\rm Coul}(\mathbf{r})) \tag{5}$$

of local densities, where $\mathcal{H}_{\rm kin}(\mathbf{r})$, $\mathcal{H}_{\rm c}(\mathbf{r})$, $\mathcal{H}_{\rm DD}(\mathbf{r})$, $\mathcal{H}_{\rm s.o.}(\mathbf{r})$, and $\mathcal{H}_{\rm Coul}(\mathbf{r})$ are the kinetic, central, density-dependent, spin-orbit, and Coulomb energy-density contributions. These local densities are classified in two categories according to their behavior under time-reversal symmetry, represented by an antiunitary operator $\mathcal{T}$:

(1) time-even densities, which commute with $\mathcal{T}$ and are scalar or rank-2 tensor quantities: nucleon density $\rho_t(\mathbf{r})$, kinetic-energy density $\tau_t(\mathbf{r})$, spin-current tensor $\mathbf{J}_t^{\mu\nu}(\mathbf{r})$;
(2) time-odd densities, which anticommute with $\mathcal{T}$ and are vector quantities: spin density $\mathbf{s}_t(\mathbf{r})$, current (or momentum) density $\mathbf{j}_t(\mathbf{r})$, spin-kinetic-energy density $\mathbf{T}_t(\mathbf{r})$.

The subscript t denotes the considered charge state, namely $t = n$ for neutrons and $t = p$ for protons. It is omitted when the sum of neutron and proton contributions is implied. The definition of the above listed densities can be found, e.g., in Refs. [6,11,15,16] but are explicated in Appendix A—together with the above energy-density contributions—to make this paper self-contained. Note that additional densities come into play when the nuclear interaction includes tensor terms (see, e.g., Ref. [12]).

Because we study here well-deformed nuclei (in order for their mean-field description to be relevant) with axial and left-right symmetric shapes in their ground state, the single-particle states denoted hereafter as $|i\rangle$ have a definite projection Ω_i of the angular momentum on the symmetry axis and a definite parity π_i. On the other hand, the suppression

of the Kramers degeneracy does not allow us in principle to define pairs of states having respectively $\Omega_i > 0$ and $\Omega_i < 0$ values, as this is the case when the time-reversal symmetry is present. In the BCS treatment of pairing correlations, this poses the problem of properly defining the notion of pairs. In this work we define the conjugate state $|\tilde{i}\rangle$ of a given neutron or proton single-particle state $|i\rangle$ as the one that has the same charge state and the largest overlap in absolute value with the time-reversed state $|\tilde{i}\rangle = \mathcal{T}|i\rangle$ (for the space-spin part of the states). In practice, it turns out that this overlap is equal to 1 within 1% or less for all cases encountered. One can similarly define a neutron-proton pair without ambiguity. Thus, due to the perturbative character of the polarization effects which we have above alluded to, it is generally possible to assign unambiguously single-particle states of a given $(|\Omega|,\pi)$ subspace into well-defined pairs which will be dubbed below as quasidegenerate pairs.

In the well-deformed nuclei the unified-model picture for the ground state (see Eq. (4-19) of Ref. [17]) applies and allows one to equate the total angular momentum I and parity π in the ground state with the angular-momentum projection on the symmetry axis $K = \Omega_i$ and parity π_i of the last nucleon, namely $I = K$ and $\pi = \pi_i$ in the absence of Coriolis coupling effects.

When solving the Hartree-Fock-BCS equations, we start from a converged solution for an underlying even-even core (assuming axial and left-right symmetries) and implement the self-consistent blocking procedure. A priori, there is an ambiguity in the definition of such a core stemming from the possibility of considering the last nucleon as a hole or a particle state in one of the two relevant cores. In practice, provided that the two cores have roughly the same deformation, such an ambiguous choice has no practical consequence, due to the self-consistent treatment to be performed from either starting point. In practice, in what follows, we will take as core nuclei the isotopes having one neutron or one proton less than the studied odd nuclei. Then the single-particle state which has the desired quantum numbers K and π and the lowest energy above the underlying even-even core is imposed to have an occupation factor equal to 1 and does not participate in pair excitations. The BCS equations are thus solved for the remaining single-particle spectrum.

B. Choice of the Skyrme parametrization

Two points of view can be adopted to determine the Skyrme parametrization:

(1) interaction point of view: the independent parameters to be considered are those entering the various parts of the nuclear interaction Eqs. (2) to (4);
(2) functional point of view: the parameters to be considered are the B_i coupling constants appearing in the expression of the hamiltonian density (see Appendix A), subject to Galilean invariance.

In the first point of view, all terms corresponding to the coupling constants B_i should be taken into account, whereas in the second point of view one can choose to discard some of the B_i terms (see Appendix A). In either approach the adjustment of parameters is traditionally performed in even-even nuclei so that the terms involving time-odd local densities identically vanish. Therefore these terms are not constrained and may yield spin instabilities in nuclear matter. This is the case for SLy4, SLy5, and all TIJ parameter sets [11], but not for the more recent parametrization SLy5* [18] built from SLy5 [19] with the additional constraint not to yield finite-size spin instabilities in nuclear matter.

In finite nuclei the appearance of instabilities depends particularly on the strength of the B_{18} and B_{19} coupling constants, which drive the $\mathbf{\Delta s}$ and $\mathbf{\Delta s}_t$ contributions to the Hamiltonian density and Hartree-Fock Hamiltonian, but also on the numerical implementation of the Hartree-Fock equations. Here we employ a matrix representation of the Hartree-Fock Hamiltonian using the cylindrical harmonic-oscillator basis and we evaluate all integrals by a Gauss-type quadrature (Gauss-Hermite along the symmetry axis z and Gauss-Laguerre in the perpendicular plane). We have found no instability with SLy4 and SLy5, and so did we using SIII [20], SkM* [21], and SLyIII.0.8 [22].

The various parameter sets can be split into different categories according to (i) the power α of the density dependence:

(1) α is integer: this is the case of SIII and SLyIII.xx for which $\alpha = 1$; these functionals can be regularized when used in configuration-mixing calculations such as the generator coordinate method or symmetry restoration [23];
(2) α is noninteger, usually fractional: this is the case of SkM*, SLy4, SLy5, and TIJ, which cannot be regularized;

(ii) according to the neglect or the inclusion of the $\overleftrightarrow{\mathbf{J}}^2$ terms:

(1) $\overleftrightarrow{\mathbf{J}}^2$ terms neglected: SIII, SkM*, SLy4, etc.;
(2) $\overleftrightarrow{\mathbf{J}}^2$ terms taken into account: SLy5, SLy5*, SLyIII.xx, TIJ, etc.;

(iii) or according to the presence or absence of the tensor interaction:

(1) tensor interaction taken into account: TIJ;
(2) no tensor interaction: SIII, SkM*, SLy4, SLy5, SLy5*, SLyIII.xx, etc.

Since by now no parametrization is yet available that includes the tensor part of the Skyrme interaction and is, at the same time, free from finite-size spin instabilities, we consider here only the central and spin-orbit parts. Moreover, we have to restrict to parametrizations in which the center-of-mass correction is treated in the above-mentioned way, namely the one-body contribution to the binding energy and effective-mass field [defined in Eq. (A30)] only is taken into account in the adjustment procedure.

In this context, and for the sake of making in our study meaningful comparisons between interactions and with data, we retain two parameter sets satisfying the following three conditions: (i) they are free from finite-size spin instabilities, (ii) they have the same power α of the density dependence,

and (iii) one is fitted with the $\overleftrightarrow{J}^2$ terms taken into account and the other is without these terms. The only choice left among the above quoted (and frequently used) parametrizations is SIII and SLyIII.xx. More precisely we use here the SLyIII.0.8 parameter set as recommended in Ref. [22].

When using SIII interaction, the Coulomb direct and exchange (approximated à la Slater) contributions are taken care of as discussed in Appendix A [see Eq. (A3)]. On the contrary, the SLyIII.0.8 interaction parameters have been fitted by neglecting completely the Coulomb exchange contribution, thus preserving the regularizable character of this energy functional.

In the calculations performed with SIII, we neglect the $\overleftrightarrow{J}^2$ terms as well as the $\mathbf{s}\cdot\boldsymbol{\Delta}\mathbf{s}$ terms in the energy-density functional, and all the contributions they produce in the Hartree-Fock Hamiltonian. In particular, the only time-odd fields are the spin field $\mathbf{S}(\mathbf{r})$ and the current field $\mathbf{A}(\mathbf{r})$. We call this framework the minimal scheme. In contrast, when using the SLyIII.0.8 parametrization, all terms in the energy-density functional and in the Hartree-Fock Hamiltonian produced by the central and spin-orbit parts of the Skyrme interaction are taken into account. In addition to the above two time-odd fields we also have the spin-gradient field $\mathbf{C}(\mathbf{r})$, which can be considered as a spin-dependent effective-mass field. This framework is called here the full scheme.

C. Magnetic dipole moment

In the unified model of Bohr and Mottelson, the magnetic dipole moment $\mu_{\rm tot}$ of the axially symmetric ground state of an odd-mass nucleus is the sum of an intrinsic contribution $\mu_{\rm intr}$ and a contribution from the collective degrees of freedom $\mu_{\rm coll}$ (see Eq. (4-86) of Ref. [17]).

For $\boldsymbol{K \neq 1/2}$, the former is proportional to the expectation value (for the microscopic state) of the projection $\hat{\mu}_z$ of the magnetic dipole moment operator on the symmetry axis (chosen to be the z axis) according to

$$\mu_{\rm intr} = \frac{K}{K+1}\,\langle\Psi|\hat{\mu}_z|\Psi\rangle, \tag{6}$$

where $|\Psi\rangle$ is the normalized nuclear state with good quantum numbers K and π. The one-body operator $\hat{\mu}_z$ is defined by

$$\hat{\mu}_z = g_\ell\hat{\ell}_z + g_s\hat{s}_z, \tag{7}$$

where $\hat{\ell}_z$ and $\hat{s}_z$ are the corresponding projections of the single-particle orbital and spin angular-momentum operators. Because $\hat{\mu}_z$ is a one-body operator, $\langle\Psi|\hat{\mu}_z|\Psi\rangle$ can be written in the same form as in the independent-particle model (where core polarization is absent). This allows us to define an effective spin gyromagnetic ratio $g_s^{\rm (eff)}$ by the relation

$$\langle\Psi|\hat{\mu}_z|\Psi\rangle = g_\ell^{(q)}\langle\hat{\ell}_z\rangle_{\rm odd} + g_s^{\rm (eff)}s_{\rm odd}, \tag{8}$$

where q is the charge state of the odd nucleon (the other charge state being denoted by $\overline{q}$) and $\langle\hat{\ell}_z\rangle_{\rm odd}$ (resp. $s_{\rm odd}$) is the expectation value of $\hat{\ell}_z$ (respectively, $\hat{s}_z$) for the odd nucleon. The ratio $g_s^{\rm (eff)}/g_s^{(q)}$ is called the spin quenching factor. According to Eqs. (7) and (8) this ratio takes the following expression:

$$\frac{g_s^{\rm (eff)}}{g_s^{(q)}} = \frac{\langle\Psi|\hat{\mu}_z|\Psi\rangle - g_\ell^{(q)}(K - s_{\rm odd})}{g_s^{(q)}s_{\rm odd}}\,. \tag{9}$$

To exhibit explicitly the core-polarization effect on the quenching factor we rewrite $g_s^{\rm (eff)}/g_s^{(q)}$ as

$$\frac{g_s^{\rm (eff)}}{g_s^{(q)}} = 1 - \delta\,, \tag{10}$$

where

$$\delta = \sum_t \frac{\left(g_\ell^{(t)} - g_s^{(t)}\right)\langle\Psi|\hat{s}_z|\Psi\rangle_{\rm core}^{(t)}}{g_s^{(q)}s_{\rm odd}} \tag{11}$$

represents the core-polarization contribution to the spin quenching factor. In Eq. (10) the minus sign has been chosen because the empirical value of $g_s^{\rm (eff)}/g_s^{(q)}$ is smaller than 1.

The collective contribution $\mu_{\rm coll}$, on the other hand, is proportional to the collective gyromagnetic ratio g_R according to

$$\mu_{\rm coll} = \frac{K}{K+1}\,g_R\,. \tag{12}$$

In this work we calculate g_R microscopically within the Inglis-Belyaev approximation in the underlying even-even nucleus, which gives the "unpolarized" value $g_R^{\rm (unpol)}$, and we compare it with the "polarized" value $g_R^{\rm (pol)}$ obtained with the same expression using the single-particle states, occupation factors, and quasiparticle energies resulting from the HFBCS calculation with blocking.[1] In both cases we can use the following expression deduced from that of Ref. [24],

$$g_R = \frac{\sum_{k,\ell}\langle\ell|\hat{\mu}_-|k\rangle\langle k|\hat{j}_+|\ell\rangle\,(u_k v_\ell - u_\ell v_k)^2/(E_k + E_\ell)}{\sum_{k,\ell}\langle\ell|\hat{j}_-|k\rangle\langle k|\hat{j}_+|\ell\rangle\,(u_k v_\ell - u_\ell v_k)^2/(E_k + E_\ell)}, \tag{13}$$

where the sums run over all Hartree-Fock-BCS single-particle states, except the blocked state when the polarized value is computed. The operators $\hat{j}_\pm = \hat{j}_x \pm i\,\hat{j}_y$ are the usual angular-momentum raising and lowering operators (similar expressions hold for $\hat{\mu}_\pm$), E_k is the quasiparticle energy of the single-particle state $|k\rangle$, and u_k and v_k are the usual BCS vacancy and occupation amplitudes for the single-particle state $|k\rangle$. It is worth noting that the free g_s value is used in the $\hat{\mu}_-$ operator. This enables to assess the impact of the core-polarization mechanism studied here on this quantity, especially in view of the earlier finding that the effect of core polarization on g_R translates into different effective g_s factors in $\hat{\mu}_z$ and $\hat{\mu}_\pm$ matrix elements [25,26].

III. RESULTS AND DISCUSSION

A. Calculations settings

We apply the above theoretical formalism to examine the magnetic properties of the following nuclei: ^{99}Sr, ^{99}Y, ^{103}Mo,

[1]The time-reversed conjugate states are thus replaced with the conjugate states defined in Subsec. II A.

TABLE I. Harmonic-oscillator basis parameters b (in fm^{-1}) and q (dimensionless) optimized with 13 major shells for SIII and SLyIII.0.8 parametrizations of the Skyrme functional. The strengths of the seniority force used for the optimizations are given in Table II.

Nucleus	SIII		SLyIII.0.8	
	b	q	b	q
^{98}Sr	0.507	1.37	0.514	1.16
^{102}Mo	0.502	1.24	0.511	1.12
^{174}Yb	0.528	1.57	0.497	1.59
^{178}Hf	0.520	1.45	0.498	1.58
^{234}U	0.506	1.32	0.518	1.22
^{236}U	0.505	1.32	0.518	1.22

^{103}Tc, ^{175}Yb, ^{175}Lu, ^{179}Hf, ^{179}Ta, ^{235}U, ^{235}Np, and ^{237}Np. They are representative nuclei of three deformation regions, namely $A \sim 100$, $A \sim 180$, and actinide nuclei, for which some experimental data are available.

We choose the SIII and SLyIII.0.8 Skyrme parameter sets as argued in Subsec. II B. For each parametrization the cylindrical harmonic-oscillator basis parameters are optimized for the core even-even nucleus by minimizing the binding energy. The definitions of the size parameter b and the deformation parameter q is to be found in Ref. [27]. The truncated harmonic-oscillator basis contains thirteen major shells. In Table I we report the obtained values of b and q.

For each charge state, the single-particle states participating in the BCS treatment lie up to 6 MeV above the Fermi level. As usual (see Ref. [28] for a precise definition) a smoothing factor is attached to each single-particle state to suppress sudden variations in the configuration-space content. It is defined by a width parameter $\mu = 0.2$ MeV. For such a configuration space, the strengths of the seniority force in BCS have been calibrated in each mass region against experimental three-point mass formulas (centered on the odd nuclei as suggested in Ref. [29]). With the standard notation $G_0^{(t)}$ of the constant pairing parameter for the charge state t (such that the corresponding matrix element of the residual interaction is given by $G^{(t)} = G_0^{(t)}/(N^{(t)} + 11)$, where $N^{(t)}$ is the number of nucleons in this charge state), the calculation procedure is denoted as HFBCS(G). Table II displays the calibrated values of $G_0^{(t)}$ for the various mass regions.

Finally the numbers of the Gauss integration points used in the z direction and in the perpendicular plane are $N_G^{(z)} = 50$ (25 points for $z > 0$ because parity symmetry is assumed) and $N_G^{(r)} = 20$, respectively.

TABLE II. Seniority force strengths for neutrons $G_0^{(n)}$ and protons $G_0^{(p)}$ (in MeV) calibrated for each Skyrme parametrization and each mass region.

Mass region	SIII		SLyIII.0.8	
	$G_0^{(n)}$	$G_0^{(p)}$	$G_0^{(n)}$	$G_0^{(p)}$
$A \sim 100$	−17.9	−19.5	−18.6	−20.8
$A \sim 176$	−18.1	−16.5	−18.1	−16.8
$A \sim 234$	−18.2	−16.9	−17.0	−13.5

B. Mechanism of the time-reversal symmetry breaking and core-polarization effect

Let us outline the physical mechanism for the time-reversal symmetry breaking in the mean field and the appearance of the core-polarization effect in odd-mass nuclei. The presence of an unpaired neutron or proton on top of the even-even core leads to the appearance of uncompensated time-odd fields in the Hartree-Fock Hamiltonian (A29), which cause a suppression of the Kramers degeneracy in the single-particle spectrum. In the beginning of the iterative procedure these fields are equal to the mere contribution of the last nucleon, which we write with the subscript "odd." The expressions of the time-odd fields for the charge states q and $\overline{q}$ (defined in Subsec. II C) thus become

$$\mathbf{A}_q = -2(B_3 + B_4)\,\mathbf{j}_{\rm odd} + 2B_9\,\boldsymbol{\nabla} \times \mathbf{s}_{\rm odd}, \tag{14}$$

$$\mathbf{A}_{\overline{q}} = -2B_3\,\mathbf{j}_{\rm odd} + B_9\boldsymbol{\nabla} \times \mathbf{s}_{\rm odd}, \tag{15}$$

$$\mathbf{S}_q = 2B_9\boldsymbol{\nabla} \times \mathbf{j}_{\rm odd} + 2[B_{10} + B_{11} + \rho^{\alpha}(B_{12} + B_{13})]\mathbf{s}_{\rm odd} - (B_{14} + B_{15})\,\mathbf{T}_{\rm odd} + 2(B_{18} + B_{19})\boldsymbol{\Delta}\mathbf{s}_{\rm odd}, \tag{16}$$

$$\mathbf{S}_{\overline{q}} = B_9\,\boldsymbol{\nabla} \times \mathbf{j}_{\rm odd} + 2(B_{10} + \rho^{\alpha} B_{12})\,\mathbf{s}_{\rm odd} \tag{17}$$

$$\mathbf{C}_q = -(B_{14} + B_{15})\,\mathbf{s}_{\rm odd} \tag{18}$$

$$\mathbf{C}_{\overline{q}} = -B_{14}\,\mathbf{s}_{\rm odd}. \tag{19}$$

As substantiated in Sec. III, the main part of the converged fields $\mathbf{S}_q$, $\mathbf{A}_q$, and $\mathbf{C}_q$ consists of these "initial" values, which are merely due to the last nucleon. The differences between the actual $\mathbf{S}_q$, $\mathbf{A}_q$, and $\mathbf{C}_q$ fields and their initial values, or between the whole $\mathbf{S}_{\bar{q}}$, $\mathbf{A}_{\bar{q}}$, and $\mathbf{C}_{\overline{q}}$ fields and zero, correspond only to perturbative corrections. These corrective terms yield, as a result of the mean-field iteration process, a core polarization affecting currents and spin-vector densities. In such a way, at the end of the self-consistent procedure, the single-particle spectrum does not possess the Kramers degeneracy anymore. This effect is similar to a magnetic core polarization.

C. Intrinsic magnetic moments

We perform HFBCS(G) calculations with SIII and SLyIII.0.8 Skyrme parametrizations using the corresponding parameters listed in Tables I and II by blocking the constrained K^{π} orbital. The ground-state results obtained are given in Table III, with a straightforward notation. Let us simply mention that the rank in the given K^{π} single-particle subspace—sorted by increasing single-particle energy—is the number of the single-particle state closest to the Fermi level[2] and that the Q_{20} values correspond to the quadrupole moment of the total (mass) distribution. Here in addition to the g_s quenching factors we display in nuclear magneton μ_N units the expectation value of the $\hat{\mu}_z$ operator denoted by $\langle\hat{\mu}_z\rangle$.

[2]We define the Fermi energy as the arithmetic mean of the N_tth and $(N_t + 1)$th single-particle energies for the charge state t, sorted by increasing order.

TABLE III. HFBCS(G) ground-state results using SIII and SLyIII.0.8 (abbreviated SLyIII below) with the corresponding parameters of Tables I and II. The energy E is the binding energy, Q_{20} is the mass quadrupole moment, $s_{\rm odd}$ is the expectation value (in $\hbar$ units) of the $\hat{s}_z$ operator for the blocked state, $\langle\hat{\mu}_z\rangle$ is the expectation value (in nuclear magneton μ_N units) of the $\hat{\mu}_z$ operator for the nuclear state, and $g_s^{(\rm eff)}/g_s^{(q)}$ is the spin quenching factor. The superscript q denotes the charge state of the last nucleon.

Nucleus	K^π(rank)	E (MeV)		Q_{20} (fm^2)		$s_{\rm odd}$		$\langle\hat{\mu}_z\rangle$		$g_s^{(\rm eff)}/g_s^{(q)}$	
		SIII	SLyIII	SIII	SLyIII	SIII	SLyIII	SIII	SLyIII	SIII	SLyIII
^{99}Sr	$5/2^-(3)$	−829.267	−828.052	1010.1	874.7	0.380	0.370	−1.054	−1.203	0.725	0.851
	$3/2^+(5)$	−829.281	−828.664	961.5	807.3	0.342	0.328	−1.050	−1.172	0.803	0.935
^{99}Y	$5/2^+(2)$	−836.410	−836.302	985.3	743.3	0.427	0.410	4.097	4.196	0.848	0.920
^{103}Mo	$3/2^+(5)$	−876.726	−877.652	866.5	581.5	0.346	0.285	−1.041	−1.018	0.786	0.935
	$5/2^-(3)$	−876.561	−876.928	949.3	660.8	0.369	0.335	−1.028	−1.069	0.728	0.835
^{103}Tc	$5/2^+(2)$	−879.088	−881.418	692.2	438.1	0.398	0.370	3.935	3.996	0.825	0.902
	$3/2^-(4)$	−879.244	−880.745	796.7	572.8	0.489	0.487	3.270	3.393	0.827	0.876
^{175}Yb	$7/2^-(3)$	−1405.205	−1404.961	1882.9	1820.2	−0.417	−0.421	1.139	1.307	0.713	0.811
^{175}Lu	$7/2^+(2)$	−1405.158	−1405.588	1855.8	1779.2	−0.478	−0.478	1.866	1.681	0.791	0.861
^{179}Hf	$9/2^+(2)$	−1432.423	−1432.221	1750.2	1709.2	0.435	0.437	−1.222	−1.445	0.734	0.865
^{179}Ta	$7/2^+(2)$	−1431.325	−1431.787	1811.3	1771.5	−0.479	−0.479	1.877	1.687	0.786	0.857
	$9/2^-(1)$	−1431.651	−1431.940	1727.3	1680.9	0.478	0.479	6.202	6.428	0.816	0.900
^{235}U	$7/2^-(5)$	−1774.887	−1770.228	2572.6	2477.1	0.351	0.357	−0.987	−1.196	0.735	0.876
^{235}Np	$5/2^+(5)$	−1773.765	−1770.160	2619.5	2527.4	0.341	0.346	3.729	3.887	0.824	0.896
	$5/2^-(4)$	−1773.885	−1770.583	2608.6	2531.7	−0.384	−0.383	1.167	1.024	0.801	0.868
^{237}Np	$5/2^+(5)$	−1786.173	−1781.834	2698.0	2611.7	0.339	0.344	3.722	3.879	0.825	0.897
	$5/2^-(4)$	−1786.212	−1782.170	2693.7	2620.0	−0.386	−0.386	1.163	1.019	0.799	0.866

The intrinsic magnetic moment can be deduced from $\langle\hat{\mu}_z\rangle$ by multiplying it by $K/(K+1)$.

Overall the calculated quenching factor is smaller—corresponding to a stronger quenching effect—when using the SIII parameter set than with the SLyIII.0.8 parametrization. It typically falls in the 0.70–0.85 range with the former and 0.80–0.95 with the latter. Even though the empirical value of the order of 0.7 is even smaller, the calculated results show that at least half of the observed quenching can be accounted for by a core-polarization effect. The mechanism responsible for this effect can be analyzed thanks to the above-mentioned perturbative character of the time-odd fields.

Indeed, to a good approximation the values obtained for the g_s quenching factor can be reproduced within a perturbative approach to the time-odd part $\hat{h}^{(t)}_{\rm odd}$ of the Hartree-Fock potential using both Skyrme parametrizations considered here. In this approach we calculate at first order in $\hat{h}^{(t)}_{\rm odd}$ the core-polarization contribution δ to the spin quenching factor after one iteration starting from the HFBCS(G) solution for the core even-even nucleus. Details of calculations are given in Appendix B.

Let us first discuss the results obtained with the SLyIII.0.8 parametrization because all terms generated in the energy and one-body fields by the central part of the Skyrme interaction are taken into account. As visible from Table IV, there is a good agreement between the perturbative and the self-consistent calculations of δ. The former tend in most cases to produce only a slight overestimation of the core-polarization effect. This validates the qualitative description of the mechanism of time-reversal symmetry breaking presented in Subsec. III B and allows us to provide a fine analysis of this effect on the spin quenching factor.

At first order of perturbation it is possible to express δ as a sum of contributions from the three time-odd Hartree-Fock fields

$$\delta = \delta_S + \delta_A + \delta_C, \tag{20}$$

where the indices S, A, and C refer to the spin field **S**, current field **A**, and the spin-gradient field **C**, respectively. Table IV shows that the core-polarization effect on the spin quenching factor is driven by a competition between the spin field and the spin-gradient field. More precisely the dominant contribution to δ is δ_S and is partly counterbalanced by δ_C, with the contribution from the current field playing a weak role.

TABLE IV. Calculated values of δ. The "Exact" columns refer to the self-consistent HFBCS(G) calculations. In the perturbative calculations, the contributions from each time-odd Hartree-Fock fields are also reported. The SLyIII.0.8 parametrization has been used. See the text for details.

Nucleus	K^π	Exact		Perturbative			
		$s_{\rm odd}$	δ	δ	δ_S	δ_A	δ_C
^{99}Sr	$3/2^+$	0.328	0.065	0.039	0.181	−0.033	−0.109
^{99}Y	$5/2^+$	0.410	0.080	0.101	0.188	−0.027	−0.061
^{179}Hf	$9/2^+$	0.437	0.135	0.159	0.273	−0.022	−0.092
^{179}Ta	$7/2^+$	−0.479	0.143	0.187	0.246	0.010	−0.069
	$9/2^-$	0.479	0.100	0.122	0.202	−0.015	−0.065
^{235}U	$7/2^-$	0.357	0.124	0.143	0.244	−0.011	−0.090
^{235}Np	$5/2^+$	0.346	0.104	0.122	0.195	−0.012	−0.060
	$5/2^-$	−0.383	0.132	0.157	0.210	0.013	−0.066

TABLE V. Contributions to δ from each Skyrme parameter using the SLyIII.0.8 parametrization.

Nucleus	K^π	Exact		Perturbative									
		$s_{\rm odd}$	δ	δ	δ_{t_0}	$\delta_{t_0x_0}$	δ_{t_1}	$\delta_{t_1x_1}$	δ_{t_2}	$\delta_{t_2x_2}$	δ_{t_3}	$\delta_{t_3x_3}$	δ_{W_0}
^{99}Sr	$3/2^+$	0.328	0.065	0.039	0.546	−0.153	−0.178	0.019	−0.110	0.037	−0.155	0.055	−0.021
^{99}Y	$5/2^+$	0.410	0.080	0.101	0.319	0.079	−0.103	−0.020	−0.031	−0.008	−0.076	−0.024	−0.034
^{179}Hf	$9/2^+$	0.437	0.135	0.159	0.546	0.004	−0.166	−0.009	−0.086	0.020	−0.127	−0.006	−0.016
^{179}Ta	$7/2^+$	−0.479	0.143	0.187	0.402	−0.005	−0.087	0.005	−0.030	−0.015	−0.107	0.004	0.022
	$9/2^-$	0.479	0.100	0.122	0.381	0.015	−0.100	−0.010	−0.049	0.003	−0.096	−0.002	−0.022
^{235}U	$7/2^-$	0.357	0.124	0.143	0.588	−0.059	−0.170	0.001	−0.099	0.031	−0.136	0.016	−0.029
^{235}Np	$5/2^+$	0.346	0.104	0.122	0.342	0.058	−0.096	−0.015	−0.036	−0.007	−0.086	−0.018	−0.019
	$5/2^-$	−0.383	0.132	0.157	0.336	0.020	−0.065	0.001	−0.037	−0.013	−0.090	−0.007	0.011

Moreover, the matrix elements $\langle\phi_{k'}|\hat{h}^{(t)}_{\rm odd}|\phi_k\rangle$ entering the expression (B9) of δ can be viewed as linear functions of the Skyrme parameters t_i, t_ix_i, and W_0 in the interaction point of view or linear functions of the coupling constants B_i in the functional point of view. Therefore, each of the three time-odd field contributions can be broken down in terms generated by the Skyrme parameters or the coupling constants. We can thus write δ as the following sums:

$$\delta = \sum_{i=0}^{3}\left(\delta_{t_i} + \delta_{t_ix_i}\right) + \delta_{W_0} \tag{21}$$

and

$$\delta = \sum_i \left(\delta_S^{(B_i)} + \delta_A^{(B_i)} + \delta_C^{(B_i)}\right), \tag{22}$$

where the sum over i in Eq. (22) involves the retained coupling constants (namely B_1 to B_{15}, B_{18} and B_{19} in the full scheme, and B_1 to B_{13} in the minimal scheme). The contribution to δ from a given Skyrme parameter in Eq. (21) represents the value of δ when all the other parameters are set to 0 in $h^{(t)}_{\rm odd}$ when computing $\delta^{(t)}$ from Eq. (B9). Moreover the decompositions (20) and (22) thus imply, for example, $\delta_S = \sum_i \delta_S^{(B_i)}$. The values of each contribution in Eq. (21) are displayed in Table V for SLyIII.0.8. It is found that the dominant term is δ_{t_0} and that this term is counterbalanced by δ_{t_1} and δ_{t_2}. Overall the $\delta_{t_ix_i}$ contribution is much smaller than δ_{t_i} for all values of i. Finally, even if δ_{W_0} is always smaller than the δ_{t_i} terms, we find without exception that the sign of δ_{W_0} is opposite to the sign of $s_{\rm odd}$. For positive values of $s_{\rm odd}$, which is most often the case in our selected sample of nuclei, the spin-orbit term yields a slight reduction of the spin quenching factor.

Let us now turn to the SIII parametrization. As explained in Subsec. II B, it has to be used without the $\overleftrightarrow{\mathrm{J}}^2$ terms. In the minimal scheme considered here, the $\mathbf{s}\cdot\mathbf{\Delta s}$ terms are also discarded. Therefore, we have by definition $\delta_C = \delta_{t_1} = \delta_{t_1x_1} = \delta_{t_2} = \delta_{t_2x_2} = 0$. In this case we still find that the δ_S contribution to δ is much larger than δ_A for all considered nuclei. With the $3/2^+$ solution in ^{99}Sr as a representative example, we obtain the results reported in the first line of Table VI.

In order to compare with the results obtained using SLyIII.0.8, let us also consider each parameter set in the scheme appropriate to the other set. The results obtained with SIII in the full scheme and those obtained with SLyIII.0.8 in the minimal scheme are reported in the second and third lines of Table VI. For both parametrizations we observe that the exact value of δ drops when going from the minimal scheme to the full scheme. This drop is reproduced in the perturbative approach, which allows us to investigate the reasons for this strong decrease in the light of the decomposition of δ given by Eq. (20). As can be seen in Table VI, the inclusion of all time-odd terms not only leads to a significant, negative value of δ_C, but also decreases the δ_S contribution. In both schemes the spin-current contribution δ_A is small and its variation does not contribute to the observed drop of δ.

To understand the decrease of δ_S from the minimal scheme to the full scheme, we need to decompose δ_S in terms of the coupling constants B_9 to B_{15}, B_{18}, and B_{19} appearing in Eq. (A35). The results for the $K^\pi = 3/2^+$ solution of the ^{99}Sr nucleus are displayed in Table VII. In the four calculations the spin-orbit contribution δ_{S,B_9} is found to be negligible. From the first and third lines of Table VII it is clear that, in the absence of the B_{14}, B_{15}, B_{18}, and B_{19} terms, the value of δ_S results from a competition between $\delta_S^{(B_{11})}$ and $\delta_S^{(B_{12})}$ on the one

TABLE VI. Perturbative analysis of the core-polarization contribution δ to the g_s quenching factor for the $K^\pi = 3/2^+$ solution in ^{99}Sr with SIII and SLyIII.0.8 (abbreviated SLyIII) parametrizations in the minimal or full scheme (see Subsec. II C for definition).

Parameter set	Scheme	Exact		Perturbative			
		$s_{\rm odd}$	δ	δ	δ_S	δ_A	δ_C
SIII	Min.	0.342	0.197	0.266	0.287	−0.021	0
	Full	0.383	0.085	0.094	0.190	−0.013	−0.083
SLyIII	Min.	0.286	0.206	0.241	0.277	−0.036	0
	Full	0.328	0.065	0.039	0.181	−0.033	−0.109

TABLE VII. Detailed perturbative analysis of the spin-field contribution to δ_S in the $K^\pi = 3/2^+$ solution of the ^{99}Sr nucleus with SIII and SLyIII.0.8 parametrizations with all or selected time-odd terms.

Parameter set	Scheme	δ_S	$\delta_S^{(B_9)}$	$\delta_S^{(B_{10})}$	$\delta_S^{(B_{11})}$	$\delta_S^{(B_{12})}$	$\delta_S^{(B_{13})}$	$\delta_S^{(B_{14})}$	$\delta_S^{(B_{15})}$	$\delta_S^{(B_{18})}$	$\delta_S^{(B_{19})}$
SIII	Min.	0.275	−0.004	−0.103	0.448	0.058	−0.124	0	0	0	0
	Full	0.190	−0.006	−0.078	0.428	0.042	−0.114	0	−0.086	0	0.004
SLyIII.0.8	Min.	0.274	−0.007	−0.152	0.537	0.054	−0.155	0	0	0	0
	Full	0.183	−0.006	−0.155	0.549	0.056	−0.155	0.025	−0.144	0.003	0.010

hand and $\delta_S^{(B_{10})}$ and $\delta_S^{(B_{13})}$ on the other hand. The sum of the former contributions dominates but is counterbalanced by the sum of the latter. When the B_{14}, B_{15}, B_{18}, and B_{19} terms are taken into account, we find that $\delta_S^{(B_{10})}$, $\delta_S^{(B_{11})}$, $\delta_S^{(B_{12})}$, and $\delta_S^{(B_{13})}$ do not change significantly and that $\delta_S^{(B_{15})}$ acquires a rather large, negative value. Therefore the decrease of δ_S when going from the minimal scheme to the full scheme is essentially caused by the appearance of the negative $\delta_S^{(B_{15})}$ term generated by the $\sum_t(\overleftrightarrow{\mathbf{J}}_t^2 - \mathbf{s}_t \cdot \mathbf{T}_t)$ contribution to the central part of the Hamiltonian density.

Finally it is worth noting that, despite a different treatment of the Coulomb interaction (as discussed), the SIII and SLyIII.0.8 parametrizations give comparable values of δ when they are used in the same scheme. This has been checked to be the case also for other nuclear states than the one considered in Table VII. We can explain this similarity by the facts that these parametrizations contain the same density dependence, namely a linear dependence in $\rho(\mathbf{r})$ (except for the small Coulomb exchange contribution in the case of the SIII parametrization), and that their parameters contributing most to δ, namely t_0, t_0x_0, t_1, t_3, and t_3x_3, have comparable values. We can thus conclude that the spin quenching factor is not sensitive to the change from one considered approximate treatment of the Coulomb interaction to the other.

D. Total magnetic moments

The total magnetic moments μ_{tot} of the nuclei under study are simply given by

$$\mu_{\text{tot}} = \mu_{\text{intr}} + \mu_{\text{coll}}, \tag{23}$$

where the collective contribution μ_{coll} requires the evaluation of the collective gyromagnetic ratio g_R. This evaluation is done using Eq. (13) for the underlying even-even nucleus without and with core polarization, which gives the values denoted by $g_R^{(\text{unpol})}$ and $g_R^{(\text{pol})}$ respectively. The calculated values of $g_R^{(\text{unpol})}$ are found to be 10–15% smaller than the crude Z/A approximation and can be significantly different from the values of $g_R^{(\text{pol})}$. The μ_{tot} values obtained with SIII and SLyIII.0.8 in the considered states are given in Tables VIII and IX, respectively, in comparison with available experimental values [30].

TABLE VIII. Magnetic moments (in μ_N units) with the SIII parametrization: intrinsic contribution μ_{intr}, collective gyromagnetic ratio $g_R^{(\text{unpol})}$ calculated without core polarization, corresponding total magnetic moment $\mu_{\text{tot}}^{(\text{unpol})}$, collective gyromagnetic ratio $g_R^{(\text{pol})}$ calculated with core polarization, corresponding total magnetic moment $\mu_{\text{tot}}^{(\text{pol})}$, and experimental μ_{exp} values taken from Ref. [30] (by convention, the most recent value is retained when several entries appear).

Nucleus	K^π	μ_{intr}	$g_R^{(\text{unpol})}$	$\mu_{\text{tot}}^{(\text{unpol})}$	$g_R^{(\text{pol})}$	$\mu_{\text{tot}}^{(\text{pol})}$	μ_{exp}
^{99}Sr	$5/2^-$	−0.753	0.262	−0.566	0.302	−0.537	
	$3/2^+$	−0.630		−0.473	0.305	−0.447	−0.261(5)
^{99}Y	$5/2^+$	2.927	0.262	3.114	0.285	3.131	
^{103}Mo	$3/2^+$	−0.624	0.249	−0.475	0.251	−0.473	
	$5/2^-$	−0.734		−0.556	0.213	−0.582	
^{103}Tc	$5/2^+$	2.811	0.249	2.989	0.450	3.132	
	$3/2^-$	1.962		2.111	0.303	2.144	
^{175}Yb	$7/2^-$	0.886	0.338	1.149	0.361	1.167	0.768(8)
^{175}Lu	$7/2^+$	1.452	0.338	1.715	0.352	1.726	2.2323(11)
^{179}Hf	$9/2^+$	−1.000	0.345	−0.718	0.327	−0.732	–0.6409(13)
^{179}Ta	$7/2^+$	1.460	0.345	1.728	0.335	1.721	2.289(9)
	$9/2^-$	5.075		5.357	0.351	5.362	
^{235}U	$7/2^-$	−0.768	0.324	−0.516	0.289	−0.543	–0.38(3)
^{235}Np	$5/2^+$	2.663	0.324	2.894	0.407	2.954	
	$5/2^-$	0.833		1.064	0.354	1.086	
^{237}Np	$5/2^+$	2.744	0.318	2.971	0.407	3.035	3.14(4)
	$5/2^-$	0.831		1.058	0.348	1.080	1.68(8)

TABLE IX. Same as Table VIII for SLyIII.0.8.

Nucleus	K^π	$\mu_{\rm intr}$	$g_R^{\rm (unpol)}$	$\mu_{\rm tot}^{\rm (unpol)}$	$g_R^{\rm (pol)}$	$\mu_{\rm tot}^{\rm (pol)}$	$\mu_{\rm exp}$
^{99}Sr	$5/2^-$	−0.859	0.301	−0.644	0.276	−0.662	
	$3/2^+$	−0.703		−0.523	0.310	−0.517	−0.261(5)
^{99}Y	$5/2^+$	2.997	0.301	3.212	0.412	3.291	
^{103}Mo	$3/2^+$	−0.611	0.341	−0.406	0.270	−0.449	
	$5/2^-$	−0.763		−0.520	0.227	−0.601	
^{103}Tc	$5/2^+$	2.854	0.341	3.098	0.701	3.355	
	$3/2^-$	2.036		2.241	0.403	2.278	
^{175}Yb	$7/2^-$	1.017	0.352	1.291	0.369	1.304	0.768(8)
^{175}Lu	$7/2^+$	1.308	0.352	1.582	0.367	1.593	2.2323(11)
^{179}Hf	$9/2^+$	−1.182	0.347	−0.898	0.318	−0.922	−0.6409(13)
^{179}Ta	$7/2^+$	1.312	0.347	1.583	0.347	1.583	2.289(9)
	$9/2^-$	5.259		5.543	0.366	5.558	
^{235}U	$7/2^-$	−0.931	0.478	−0.559	0.441	−0.588	−0.38(3)
^{235}Np	$5/2^+$	2.776	0.478	3.117	0.468	3.110	
	$5/2^-$	0.731		1.073	0.499	1.087	
^{237}Np	$5/2^+$	2.771	0.479	3.113	0.477	3.112	3.14(4)
	$5/2^-$	0.728		1.070	0.500	1.085	1.68(8)

Overall the difference between calculated and measured values of $\mu_{\rm tot}$ is of the order of a few tenths of μ_N, so we can consider that we obtain a reasonable agreement given that, for a given effective interaction, there is not a single free parameter in our approach. A closer comparison reveals a better agreement using the SIII parametrization (in the minimal scheme) than with SLyIII.0.8 (in the full scheme). One finds that the root mean square deviation of our results (in μ_N units) from data is 0.44 for the former and 0.53 for the latter when $g_R^{\rm (unpol)}$ is used, whereas it is 0.42 for SIII and 0.52 for SLyIII.0.8 when using $g_R^{\rm (pol)}$. Despite the large differences between $g_R^{\rm (unpol)}$ and $g_R^{\rm (pol)}$ in some cases, both values yield a similar agreement with data. The difference in the root mean square deviation between the two parametrizations could be related to the smaller spin quenching factor when taking into account all time-odd terms in the Hartree-Fock mean field, making the SIII results closer to the phenomenologically retained value of about 30% for the quenching of the spin gyromagnetic factor. One could thus argue that the magnetic moment is an observable that could be used to add in the fitting protocol a constraint on the coupling constants driving the Hartree-Fock fields to which the magnetic moment is sensitive (essentially B_{14} and B_{15}).

IV. CONCLUSIONS AND PERSPECTIVES

In this work we have explored, within the Skyrme-Hartree-Fock-BCS framework, the mechanism of response of an even-even core to the time-reversal breaking perturbation brought by the presence of an extra nucleon in the odd-mass nuclei. Assuming that the orbital gyromagnetic ratio is unaffected, we have found that the addition of this nucleon treated in the self-consistent blocking approach yields a sizable contribution to the quenching of the spin gyromagnetic factor away from its free value.

Moreover, we have shown that this core-polarization effect is of order 1 in the time-odd part of the Hartree-Fock Hamiltonian. This effect is driven by the spin field but is partly counterbalanced by the spin-gradient field—which adds a spin-dependent contribution to the effective-mass field—when it is taken into account in the corresponding Skyrme parametrization. In particular, the SIII parametrization yields a quenching factor close to the empirical one, whereas the SLyIII.0.8 parametrization provides a weaker effect. This suggests that the magnetic moment could be used in constraining the Skyrme parameters (in the interaction point of view) or the coupling constants (in the functional point of view) in the fitting protocol.

Finally, when including the collective contribution to magnetic moments, we have obtained a reasonable overall agreement with experimental data for well-deformed odd-mass nuclei in mass regions $A \sim 100$, rare-earth nuclei around $A \sim 180$, and actinide nuclei (around $A = 236$). This is all the more encouraging because, for a given effective interaction (or energy-density functional depending on the point of view), we have no free parameters. Moreover, the selected parametrizations did not include the magnetic moments in their fitting protocol.

A natural extension of this work is the calculation of magnetic moments in $N \sim Z$ nuclei where the neutron-proton pairing is at work and is expected to noticeably affect the intrinsic magnetic moment (see Ref. [31]). In these nuclei a consistent treatment of $T = 1$ and $T = 0$ pairing correlations is required and the highly truncated diagonalization approach, described, for example, in Ref. [32], is a tool of choice.

Another direction of extension of the present work is the study of more complex blocked configurations known as multiquasiparticle bandheads, in even-even, odd-mass as well as odd-odd deformed nuclei. This could be of special interest in regards to a recently initiated study of magnetic moments and deformations in nuclear high-K isomeric states [33].

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APPENDIX A: ENERGY-DENSITY FUNCTIONAL AND HARTREE-FOCK FIELDS AS FUNCTIONS OF LOCAL DENSITIES

We give here the expressions of the kinetic, central, density-dependent, spin-orbit, and Coulomb terms of the energy-density functional as functions of the local densities (the $\mathbf{r}$ dependence of which is omitted to alleviate the expressions) in an arbitrary coordinate system $\{x^\mu, \mu = 1,2,3\}$

$$\mathcal{H}_{\rm kin}(\mathbf{r}) = \left(1 - \frac{1}{A}\right)\frac{\hbar^2}{2m}\tau, \tag{A1}$$

$$\mathcal{H}_{\rm c}(\mathbf{r}) = B_1\,\rho^2 + B_{10}\,\mathbf{s}^2 + B_3\,(\rho\,\tau - \mathbf{j}^2) + B_{14}\,(\overleftrightarrow{\mathbf{J}}^2 - \mathbf{s}\cdot\mathbf{T}) + B_5\,\rho\,\Delta\rho + B_{18}\,\mathbf{s}\cdot\Delta\mathbf{s} + \sum_t \left\{B_2\,\rho_t^2 + B_{11}\,\mathbf{s}_t^2 + B_4\left(\rho_t\tau_t - \mathbf{j}_t^2\right) + B_{15}(\overleftrightarrow{\mathbf{J}}_t^2 - \mathbf{s}_t\cdot\mathbf{T}_t) + B_6\,\rho_t\,\Delta\rho_t + B_{19}\,\mathbf{s}_t\cdot\Delta\mathbf{s}_t\right\}, \tag{A2}$$

$$\mathcal{H}_{\rm DD}(\mathbf{r}) = \rho^\alpha\left[B_7\,\rho^2 + B_{12}\,\mathbf{s}^2 + \sum_t\left(B_8\,\rho_t^2 + B_{13}\,\mathbf{s}_t^2\right)\right], \tag{A3}$$

$$\mathcal{H}_{\rm s.o.}(\mathbf{r}) = B_9\left[\rho\,\boldsymbol{\nabla}\cdot\mathbf{J} + \mathbf{j}\cdot\boldsymbol{\nabla}\times\mathbf{s} + \sum_t(\rho_t\,\boldsymbol{\nabla}\cdot\mathbf{J}_t + \mathbf{j}_t\cdot\boldsymbol{\nabla}\times\mathbf{s}_t)\right], \tag{A4}$$

$$\mathcal{H}_{\rm Coul}(\mathbf{r}) \approx \frac{1}{2}\,\rho_p\,V_{\rm CD}(\mathbf{r}) - \frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\rho_p^{\frac{4}{3}}, \tag{A5}$$

where the index t in local densities is the charge state n or p. In the expression of $\mathcal{H}_{\rm Coul}(\mathbf{r})$, the direct Coulomb potential $V_{\rm CD}(\mathbf{r})$ is given by $V_{\rm CD}(\mathbf{r}) = e^2\int d^3\mathbf{r}'\frac{\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}$. To evaluate the contribution of the Coulomb exchange term, the Slater approximation is used [34] (and consistently in the Hartree-Fock Hamiltonian). In Eq. (A3) $\overleftrightarrow{\mathbf{J}}_t^2 = \mathrm{J}_{t,\mu\nu}\mathrm{J}_t^{\mu\nu}$ (using Einstein's summation convention) and in Eq. (A4) $\mathbf{J}_t$ denotes the antisymmetric part of the spin-current tensor $\mathrm{J}_t^{\mu\nu}$ [15]. The coefficients B_i appearing in Eqs. (A1) to (A4) are constants. In Eq. (A3) the symbol $\Delta \equiv \nabla_\mu\partial^\mu$ represents the Laplace operator (acting on a scalar or vector function), ∇_μ being the covariant derivative associated with the arbitrary coordinate system and $\partial_\mu = \frac{\partial}{\partial x^\mu}$. Vector quantities with an upper index are contravariant components in the natural basis $\boldsymbol{\epsilon}_\mu = \partial_\mu\mathbf{r}$, such that $\boldsymbol{\epsilon}_\mu\cdot\boldsymbol{\epsilon}_\nu$ is equal to the metric tensor $g_{\mu\nu}$, whereas lower indices refer to the covariant components in the reciprocal basis $\boldsymbol{\epsilon}^\mu$ such that $\boldsymbol{\epsilon}_\mu\cdot\boldsymbol{\epsilon}^\nu = \delta_\mu^\nu$. When acting on a vector function, the Laplace operator is written in bold.

The basic time-even local densities $\rho(\mathbf{r})$, $\tau(\mathbf{r})$, and $\mathrm{J}_{\mu\nu}(\mathbf{r})$ generated by the central and spin-orbit parts of the interaction are defined by

$$\rho(\mathbf{r}) = \sum_k v_k^2\,[\phi_k]^\dagger(\mathbf{r})[\phi_k](\mathbf{r}), \tag{A6}$$

$$\tau(\mathbf{r}) = \sum_k v_k^2(\boldsymbol{\nabla}[\phi_k]^\dagger(\mathbf{r}))\cdot\boldsymbol{\nabla}[\phi_k](\mathbf{r}), \tag{A7}$$

$$\mathrm{J}_{\mu\nu}(\mathbf{r}) = \frac{1}{2i}\sum_k v_k^2\{[\phi_k]^\dagger(\mathbf{r})\,\sigma_\nu\partial_\mu[\phi_k](\mathbf{r}) - (\partial_\mu[\phi_k]^\dagger(\mathbf{r}))\,\sigma_\nu[\phi_k](\mathbf{r})\}, \tag{A8}$$

whereas the relevant time-odd densities $\mathbf{s}(\mathbf{r})$, $T_\mu(\mathbf{r})$, and $\mathbf{j}(\mathbf{r})$ respectively read

$$\mathbf{s}(\mathbf{r}) = \sum_k v_k^2\,[\phi_k]^\dagger(\mathbf{r})\,\boldsymbol{\sigma}[\phi_k](\mathbf{r}), \tag{A9}$$

$$T_\mu(\mathbf{r}) = \sum_k v_k^2(\boldsymbol{\nabla}[\phi_k]^\dagger(\mathbf{r}))\cdot\sigma_\mu\boldsymbol{\nabla}[\phi_k](\mathbf{r}), \tag{A10}$$

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2i}\sum_k v_k^2\{(\boldsymbol{\nabla}[\phi_k]^\dagger(\mathbf{r}))[\phi_k](\mathbf{r}) - [\phi_k]^\dagger(\mathbf{r})\boldsymbol{\nabla}[\phi_k](\mathbf{r})\}. \tag{A11}$$

In the interaction point of view, the coupling constants B_i are combinations of the Skyrme parameters. Those entering the central contribution to the energy-density functional are

(1) from the t_0 term of the Skyrme interaction:

$$B_1 = \frac{t_0}{2}\left(1 + \frac{x_0}{2}\right), \tag{A12}$$

$$B_2 = -\frac{t_0}{2}\left(\frac{1}{2} + x_0\right), \tag{A13}$$

$$B_{10} = \frac{1}{4}\,t_0x_0, \tag{A14}$$

$$B_{11} = -\frac{1}{4}\,t_0, \tag{A15}$$

(2) from the t_1 and t_2 terms:

$$B_3 = \frac{1}{4}\left[t_1\left(1+\frac{x_1}{2}\right) + t_2\left(1+\frac{x_2}{2}\right)\right], \tag{A16}$$

$$B_4 = -\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right) - t_2\left(\frac{1}{2}+x_2\right)\right], \tag{A17}$$

$$B_5 = -\frac{1}{16}\left[3t_1\left(1+\frac{x_1}{2}\right) - t_2\left(1+\frac{x_2}{2}\right)\right], \tag{A18}$$

$$B_6 = \frac{1}{16}\left[3t_1\left(\frac{1}{2}+x_1\right) + t_2\left(\frac{1}{2}+x_2\right)\right], \tag{A19}$$

$$B_{14} = -\frac{1}{8}(t_1 x_1 + t_2 x_2), \tag{A20}$$

$$B_{15} = \frac{1}{8}(t_1 - t_2), \tag{A21}$$

$$B_{18} = -\frac{1}{32}(3t_1 x_1 - t_2 x_2), \tag{A22}$$

$$B_{19} = \frac{1}{32}(3t_1 + t_2). \tag{A23}$$

Because $|x_1|$ and $|x_2|$ are usually smaller than 1 (they are even 0 for SIII and SkM* parametrizations, for instance), the coupling constants B_{14} and B_{18} play a less important role than their respective counterparts B_{15} and B_{19} do. Finally, the coupling constants appearing in the density-dependent contribution $\mathcal{H}_{\rm DD}$ are defined as

$$B_7 = \frac{t_3}{12}\left(1+\frac{x_3}{2}\right), \tag{A24}$$

$$B_8 = -\frac{t_3}{12}\left(\frac{1}{2}+x_3\right), \tag{A25}$$

$$B_{12} = \frac{1}{24}t_3 x_3, \tag{A26}$$

$$B_{13} = -\frac{t_3}{24}, \tag{A27}$$

and the spin-orbit coupling constant is

$$B_9 = -\frac{W_0}{2}\,. \tag{A28}$$

The pairing correlations are then included in the many-body ground state within the BCS framework. As explained in detail in Ref. [6], this amounts to simply extending the definition of the local densities by incorporating the BCS occupation factors and adding the so-called pairing energy to the energy-density functional given by Eq. (5). The resulting energy is then varied with respect to the single-particle wave functions (in terms of which the local densities are expressed), with a normalization constraint enforced by Lagrange multipliers interpreted as single-particle energies e_k, and with respect to the occupation factors. The former variation yields the Hartree-Fock equations $\hat{h}^{(t)}_{\rm HF}|\phi_k\rangle = e_k|\phi_k\rangle$ with a Hartree-Fock one-body Hamiltonian $\hat{h}^{(t)}_{\rm HF}$ of the following form in coordinate representation for the charge state t

$$\begin{aligned}\langle \mathbf{r}|\hat{h}^{(t)}_{\rm HF}|\phi_k\rangle = &-\boldsymbol{\nabla}\cdot\left[\left(\frac{\hbar^2}{2m^*_t(\mathbf{r})} + \mathbf{C}_t(\mathbf{r})\cdot\boldsymbol{\sigma}\right)\boldsymbol{\nabla}[\phi_k](\mathbf{r})\right] \\ &+ (U_t(\mathbf{r}) + \delta_{tp}\,V_{\rm Coul}(\mathbf{r}))[\phi_k](\mathbf{r}) \\ &+ i\,\mathbf{W}_t(\mathbf{r})\cdot(\boldsymbol{\sigma}\times\boldsymbol{\nabla}[\phi_k](\mathbf{r})) \\ &- i\big[W^{\mu\nu}_t(\mathbf{r})\sigma_\nu\partial_\mu[\phi_k](\mathbf{r}) \\ &+ \nabla_\mu\big(W^{\mu\nu}_t(\mathbf{r})\sigma_\nu[\phi_k](\mathbf{r})\big)\big] \\ &- i\,\mathbf{A}_t(\mathbf{r})\cdot\boldsymbol{\nabla}[\phi_k](\mathbf{r}) + \mathbf{S}_t(\mathbf{r})\cdot\boldsymbol{\sigma}[\phi_k](\mathbf{r}),\end{aligned} \tag{A29}$$

where $[\phi_k](\mathbf{r})$ is the spinor notation for the wave function in coordinate representation. In Eq. (A29) we have used the property $\boldsymbol{\nabla}\cdot\mathbf{A}_t(\mathbf{r}) = 0$ which holds in this time-independent context. The time-even fields $m^*_t(\mathbf{r})$, $U_t(\mathbf{r})$, $V_{\rm Coul}(\mathbf{r})$, $\mathbf{W}_t(\mathbf{r})$, and $W_{t,\mu\nu}(\mathbf{r})$ denote the effective mass, the central-plus-density-dependent field, the Coulomb field, the spin-orbit field, and the spin-current field respectively, whereas $\mathbf{S}_t(\mathbf{r})$, $\mathbf{A}_t(\mathbf{r})$, and $\mathbf{C}_t(\mathbf{r})$ are time-odd fields. They are functions of the above local densities. In the following we call $\mathbf{S}_t(\mathbf{r})$ the spin field and $\mathbf{C}_t(\mathbf{r})$ the spin-gradient field. The expressions of the time-even fields are

$$\frac{\hbar^2}{2m^*_t(\mathbf{r})} = \left(1-\frac{1}{A}\right)\frac{\hbar^2}{2m} + B_3\,\rho + B_4\,\rho_t, \tag{A30}$$

$$\begin{aligned}U_t(\mathbf{r}) = &\,2\,(B_1\,\rho + B_2\,\rho_t) + B_3\,\tau + B_4\,\tau_t \\ &+ 2\,(B_5\,\Delta\rho + B_6\,\Delta\rho_t) \\ &+ \rho^{\alpha-1}\big[(2+\alpha)B_7\rho^2 + B_8\alpha\big(\rho_n^2+\rho_p^2+2\rho\,\rho_t\big)\big] \\ &+ B_9\,(\boldsymbol{\nabla}\cdot\mathbf{J} + \boldsymbol{\nabla}\cdot\mathbf{J}_t),\end{aligned} \tag{A31}$$

$$V_{\rm Coul}(\mathbf{r}) \approx V_{\rm CD}(\mathbf{r}) - \left(\frac{3}{\pi}\right)^{\frac{1}{3}} e^2\,\rho_p^{\frac{1}{3}}, \tag{A32}$$

$$\mathbf{W}_t(\mathbf{r}) = -B_9(\boldsymbol{\nabla}\rho + \boldsymbol{\nabla}\rho_t), \tag{A33}$$

$$W_{t,\mu\nu}(\mathbf{r}) = B_{14}\mathrm{J}_{\mu\nu} + B_{15}\mathrm{J}_{t,\mu\nu}, \tag{A34}$$

where the second contribution to $V_{\rm Coul}(\mathbf{r})$ is the exchange term in the Slater approximation, and the time-odd fields are given by

$$\begin{aligned}\mathbf{S}_t(\mathbf{r}) = &\,2(B_{10}+B_{12}\,\rho^\alpha)\mathbf{s} + 2(B_{11}+B_{13}\,\rho^\alpha)\mathbf{s}_t \\ &- B_9\,\boldsymbol{\nabla}\times(\mathbf{j}+\mathbf{j}_t) - B_{14}\,\mathbf{T} - B_{15}\,\mathbf{T}_t \\ &+ 2\,(B_{18}\,\boldsymbol{\Delta}\mathbf{s} + B_{19}\,\boldsymbol{\Delta}\mathbf{s}_t),\end{aligned} \tag{A35}$$

$$\mathbf{A}_t(\mathbf{r}) = -2(B_3\,\mathbf{j} + B_4\,\mathbf{j}_t) + B_9\,\boldsymbol{\nabla}\times(\mathbf{s}+\mathbf{s}_t), \tag{A36}$$

$$\mathbf{C}_t(\mathbf{r}) = -B_{14}\,\mathbf{s} - B_{15}\,\mathbf{s}_t, \tag{A37}$$

where the vector Laplacian of $\mathbf{s}$ is related to the spin-kinetic density through

$$\begin{aligned}\boldsymbol{\Delta}\mathbf{s}(\mathbf{r}) = &\,2\,\mathbf{T}(\mathbf{r}) + \sum_k v_k^2\{(\Delta[\phi_k]^\dagger(\mathbf{r}))\boldsymbol{\sigma}[\phi_k](\mathbf{r}) \\ &+ [\phi_k]^\dagger(\mathbf{r})\boldsymbol{\sigma}\,\Delta[\phi_k](\mathbf{r})\}\,.\end{aligned} \tag{A38}$$

The Hartree-Fock equations are solved by diagonalization of the $\hat{h}^{(t)}_{\rm HF}$ one-body Hamiltonian in the cylindrical harmonic-oscillator basis. The matrix elements of $\hat{h}^{(t)}_{\rm HF}$ are calculated by

integration in coordinate space as follows:

$$\langle a|\hat{h}^{(t)}_{\rm HF}|b\rangle = \int d^3\mathbf{r}\left\{(\boldsymbol{\nabla}[\phi_a]^\dagger(\mathbf{r}))\cdot\left(\frac{\hbar^2}{2m^*_t(\mathbf{r})}+\mathbf{C}_t(\mathbf{r})\cdot\boldsymbol{\sigma}\right)\boldsymbol{\nabla}[\phi_b](\mathbf{r})+(U_t(\mathbf{r})+\delta_{q\,p}\,V_{\rm Coul}(\mathbf{r}))\,[\phi_a]^\dagger(\mathbf{r})[\phi_b](\mathbf{r})\right.$$
$$+i\,[\phi_a]^\dagger(\mathbf{r})\,\mathbf{W}_t(\mathbf{r})\cdot(\boldsymbol{\sigma}\times\boldsymbol{\nabla}[\phi_b](\mathbf{r}))-i\,W_t^{\mu\nu}(\mathbf{r})\,[[\phi_a]^\dagger(\mathbf{r})\sigma_\nu\partial_\mu[\phi_b](\mathbf{r})-(\partial_\mu[\phi_a]^\dagger(\mathbf{r}))\sigma_\nu[\phi_b](\mathbf{r})]$$
$$\left.-\,i\,[\phi_a]^\dagger(\mathbf{r})\,\mathbf{A}_t(\mathbf{r})\cdot\boldsymbol{\nabla}[\phi_b](\mathbf{r})+[\phi_a]^\dagger(\mathbf{r})\,\mathbf{S}_t(\mathbf{r})\cdot\boldsymbol{\sigma}\,[\phi_b](\mathbf{r})\right\}. \tag{A39}$$

To derive Eq. (A39) we have used integration by parts over the whole coordinate space and the property of the field $\mathbf{A}_t(\mathbf{r})$ to have a vanishing divergence.

APPENDIX B: PERTURBATIVE TREATMENT OF THE CORE POLARIZATION

Let us consider the eigenstates $|\phi_k\rangle$ (normalized to unity) and eigenvalues e_k of the time-even part of the Hartree-Fock Hamiltonian $\hat{h}^{(t)}_{\rm even}$ for the nucleons of charge state t

$$\hat{h}^{(t)}_{\rm even}|\phi_k\rangle = e_k\,|\phi_k\rangle. \tag{B1}$$

This Hamiltonian is invariant under time-reversal, intrinsic parity, and axial symmetries. In the subspace of eigenvectors common to $\hat{h}^{(t)}_{\rm even}$, $\hat{\pi}$, and $\hat{j}_z$ the eigenvalues of $\hat{h}^{(t)}_{\rm even}$ are not degenerate. Therefore, we can use nondegenerate perturbation theory to express the eigenstates of the Hartree-Fock Hamiltonian $\hat{h}^{(t)}_{\rm HF}=\hat{h}^{(t)}_{\rm even}+\hat{h}^{(t)}_{\rm odd}$ at first order in $\hat{h}^{(t)}_{\rm odd}$

$$|\psi_k\rangle = |\phi_k\rangle + \sum_{k'\neq k}\frac{\langle\phi_{k'}|\hat{h}^{(t)}_{\rm odd}|\phi_k\rangle}{e_k-e_{k'}}\,|\phi_{k'}\rangle. \tag{B2}$$

By convention and to alleviate the notation, the index k implicitly contains the isospin quantum number.

Then the perturbed many-body state $|\Psi\rangle$ is the BCS state built with the single-particle states $|\psi_k\rangle$ and the occupation numbers calculated by solving the BCS equations with blocking from the single-particle states $|\phi_k\rangle$. The expectation value of the $\hat{s}_z$ operator in the state $|\Psi\rangle$ is thus given, at first order in $\hat{h}^{(t)}_{\rm odd}$, by

$$\langle\Psi|\hat{s}_z|\Psi\rangle = \sum_t\sum_k v_k^2\,\langle\psi_k|\hat{s}_z|\psi_k\rangle = \sum_t\left\{\sum_k v_k^2\,\langle\phi_k|\hat{s}_z|\phi_k\rangle + 2\sum_{\substack{k,k'\\k'\neq k}} v_k^2\,\frac{\mathrm{Re}\big(\langle\phi_k|\hat{s}_z|\phi_{k'}\rangle\,\langle\phi_{k'}|\hat{h}^{(t)}_{\rm odd}|\phi_k\rangle\big)}{e_k-e_{k'}}\right\}$$
$$= \langle\phi_i|\hat{s}_z|\phi_i\rangle + \sum_t\left\{\sum_{k\neq i} v_k^2\,\langle\phi_k|\hat{s}_z|\phi_k\rangle + 2\sum_{\substack{k,k'\\k'\neq k}} v_k^2\,\frac{\langle\phi_k|\hat{s}_z|\phi_{k'}\rangle\,\langle\phi_{k'}|\hat{h}^{(t)}_{\rm odd}|\phi_k\rangle}{e_k-e_{k'}}\right\}, \tag{B3}$$

where $|\phi_i\rangle$ is the blocked state (of charge state q). The second term of Eq. (B3) represents the even-even core contribution to the expectation value of the $\hat{s}_z$ operator. It can be explicitly written as

$$\sum_{k\neq i} v_k^2\,\langle\phi_k|\hat{s}_z|\phi_k\rangle = \sum_{\substack{k>0\\k\neq i,\bar{k}\neq i}} v_k^2(\langle\phi_k|\hat{s}_z|\phi_k\rangle + \langle\overline{\phi_k}|\hat{s}_z|\overline{\phi_k}\rangle), \tag{B4}$$

where $|\overline{\phi_k}\rangle$ is the time-reversal conjugate state of $|\phi_k\rangle$ and the notation $k>0, k\neq i, \bar{k}\neq i$ means that we restrict the summation to pairs of time-reversal conjugate states other than the blocked state. Because $\hat{s}_z$ anticommutes with the time-reversal operator, we find that

$$\sum_{k\neq i} v_k^2\,\langle\phi_k|\hat{s}_z|\phi_k\rangle = 0. \tag{B5}$$

Considering a basis $\{|\phi_k\rangle\}$ which yields a real representation of the Hartree-Fock Hamiltonian, we thus obtain

$$\langle\Psi|\hat{s}_z|\Psi\rangle = s_{\rm odd} + \sum_{t=q,\bar{q}}\langle\Psi|\hat{s}_z|\Psi\rangle^{(t)}_{\rm core}, \tag{B6}$$

where $s_{\rm odd}$ represents the expectation value of $\hat{s}_z$ in the perturbed blocked state and is given at first order by

$$s_{\rm odd} = \langle\phi_i|\hat{s}_z|\phi_i\rangle + 2\sum_{k\neq i}\frac{\langle\phi_i|\hat{s}_z|\phi_k\rangle\,\langle\phi_k|\hat{h}^{(q)}_{\rm odd}|\phi_i\rangle}{e_i-e_k}, \tag{B7}$$

and where $\langle\Psi|\hat{s}_z|\Psi\rangle^{(t)}_{\rm core}$ denotes the core contribution to $\langle\Psi|\hat{s}_z|\Psi\rangle$ for the charge state t, defined by

$$\langle\Psi|\hat{s}_z|\Psi\rangle^{(t)}_{\rm core} = 2\sum_{k\neq i}\sum_{k'\neq k}\frac{\langle\phi_k|\hat{s}_z|\phi_{k'}\rangle\,\langle\phi_{k'}|\hat{h}^{(t)}_{\rm odd}|\phi_k\rangle}{e_k-e_{k'}}. \tag{B8}$$

Then according to Eqs. (10), (11), (B6), and (B8), we can write the core-polarization contribution δ to the g_s quenching factor as $\delta = \sum_{t=q,\bar{q}} \delta^{(t)}$ with

$$\delta^{(t)} = 2\,\frac{g_\ell^{(t)} - g_s^{(t)}}{g_s^{(q)}} \sum_{k\neq i} \sum_{k'\neq k} \frac{\langle \phi_k | \hat{s}_z | \phi_{k'} \rangle}{s_{\rm odd}} \, \frac{\langle \phi_{k'} | \hat{h}_{\rm odd}^{(t)} | \phi_k \rangle}{e_k - e_{k'}}. \tag{B9}$$

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