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Spin constraints on nuclear energy density functionals

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The Gallagher-Moszkowski rule in the spectroscopy of odd-odd nuclei imposes a new spin constraint on the energy functionals for self-consistent mean field theory. The commonly used parametrization of the effective three-body interaction in the Gogny and Skyrme families of energy functionals is ill suited to satisfy the spin constraint. In particular, the Gogny parametrization of the three-body interaction has the spin dependence opposite to that required by the observed spectra. The two-body part has a correct sign, but in combination the rule is violated as often as not. We conclude that a new functional form is needed for the effective three-body interaction that can take into better account the different spin-isospin channels of the interaction.

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Nuclear energy density functionals have been very successful for describing the ground-state properties of nuclei, particularly the heavier nuclei with even numbers of neutrons and protons. On the other hand, the theory has been more difficult for nuclei with odd numbers of protons and/or neutrons. Even-even nuclear ground states invariably have nucleons paired off in the Kramers-degenerate orbitals, but odd-nucleon systems require consideration of spin densities and other time-odd densities in the functional. In condensed matter physics, time-odd states such as odd-electron systems are treated with extensions of the usual density functional theory (DFT) to include spin densities [1] and currents [2]. In nuclear physics, the situation is somewhat different in that fundamental guidance on the energy functional is weaker. Functionals are parameterized with the inclusion of spin-dependent terms but one relies heavily on phenomenology to determine the parameters. Up to now, the focus on even-even nuclei has left aspects of the spin and current dependence of the functionals less well tested. Namely, the self-consistent fields generated by the densities are even under time reversal, so the time-odd fields that are present in systems with odd number of nucleons are not controlled at all. Since roughly 75% of all nuclei have odd nucleon number and thus unpaired spins, it is important to find a reliable DFT or an alternative to treat them.

Some aspects of the time-odd fields have been examined in the literature [3–7], but important experimental information has been ignored in determining the parameters in the functionals. In particular, the spin dependence of the neutron-proton interaction is crucial to determine ground-state spins of odd-odd nuclei. We show in this communication that an energy functional from the Gogny family of functionals strongly violates an empirical rule for the determination of ground-state spins. The Gogny functional has a very specific form for an effective three-body interaction which automatically has the wrong sign for the spin dependence. The other leading family of functionals, based on Skyrme's parametrization, has the same form for the spatial dependence of the effective three-body interaction, and is likely to have the similar difficulties. Indeed, it was shown long ago that the contact parametrization could lead to instabilities in nuclear Hartree-Fock theory [4]; see also Ref. [8].

The rule that should be respected was formulated by Gallagher and Moszkowski (GM) [9] for the quasiparticle angular momentum couplings in strongly deformed odd-odd nuclei. Under those conditions the components of the angular momentum K_p, K_n of the odd nucleons along the symmetry axis are good quantum numbers. The two possible relative spin orientations, $K_p + K_n$ and $|K_p - K_n|$, give rise to two separate rotational bands having band-head angular momentum $J = |K_p \pm K_n|$. According to the rule [9,10], the orientation with parallel intrinsic spins is the lower energy band. As documented in a review of the GM rule [10], there are only rare exceptions.

We have developed a computer code to find the Hartree-Fock-Bogoliubov minima of the Gogny functional in axially symmetric nuclei, treating time-odd fields including the spin-dependent ones [11]. Applying the code to spin splittings in deformed nuclei, we found that the predicted splittings violated the GM rule more often than not. In retrospect, the result is not too surprising because as stated earlier none of the energy functionals in common use have been fitted to spin-dependent properties.

We now examine the origin of the results. It is useful to distinguish the two-body and three-body interactions that are present in the functionals. In principle there are enough degrees of freedom in the parametrization of the two-body interaction to take into account the GM splittings. However, the three-body interaction is essential for nuclear saturation and, for computational simplicity, it has a very constrained

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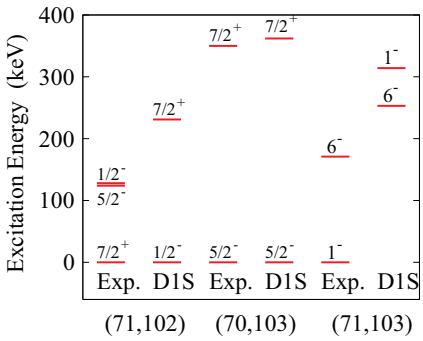

FIG. 1. (Color online) Low-lying band heads in the spectra of the nucleus ^{174}Lu and odd-A neighbors: ^{173}Lu (left), ^{173}Yb (center), and ^{174}Lu (right). Due to the inversion of the lowest proton quasiparticle energies, the ground-state doublet in ^{174}Lu is not the lowest two-quasiparticle configuration in the calculated spectrum. Lower energy calculated configurations are not shown.

parametrization. Namely, it is a density-dependent contact interaction in both the Skyrme and Gogny functionals of the form

$$t_3(1 + x_0\hat{P}_\sigma)\delta(\vec{r}_1 - \vec{r}_2)\rho((\vec{r}_1 + \vec{r}_2)/2)^\alpha \qquad (1)$$

in the standard notation [12]. It is further restricted to the parallel-spin interaction ($x_0 = 1$) in the Gogny functionals. It must be repulsive to saturate nuclear matter, but it cannot have a significant antiparallel-spin component because that channel requires an attractive interaction overall to produce BCS pairing.

We first illustrate the problem with a well-known example, the nucleus ^{174}Lu. The odd nucleons in its ground band have angular momenta and parities $(K_p, K_n) = (7/2^+, 5/2^-)$ for the proton and neutron respectively. These correspond to Nilsson orbitals $[404]\downarrow_p$ and $[512]\uparrow_n$. The spins are parallel for antiparallel orbital angular momentum, i.e., $K = |K_p - K_n|$. Indeed, the ground-state band has $K^\pi = 1^-$ in agreement with the Gallagher-Moszkowski rule. The other coupling of angular momenta, $K = K_p + K_n = 6^-$, is associated with an excited band with a band head at 171-keV excitation. The experimental levels are compared with the HFB calculations in Fig. 1. We first show the spectra of neighboring odd-A nuclei on the left-hand and middle panels. In the middle one, the theory confirmed the ground-band assignment of a quasiparticle in the $[512]\uparrow_n$ Nilsson orbital. However, the theory does not predict the correct ordering of the proton quasiparticle energies, shown in the left-hand panel. As a consequence, the $[404]\downarrow_p$ $[512]\uparrow_n$ appear as excited states in the theoretical spectrum of the ^{174}Lu, shown in the right-hand panel. One sees that the level ordering is opposite to the experimental, with the 6^- band head below the 1^-, thus violating the GM rule.

To understand the theoretical splittings in more detail, we separate three contributions:

(i) the spin dependence of the two-body interaction, treating the interaction in first-order perturbation theory;

(ii) the spin dependence of the density-dependent interaction, again treating it perturbatively;

(iii) the many-body rearrangement effects associated with the wave function modifications in the two-quasiparticle state.

TABLE I. Theoretical spin splittings of neutron-proton configurations for odd-odd nuclei in the rare-earth region. For each nucleus, two-quasiparticle states were constructed, taking 10 to 15 proton quasiparticle orbitals and a like number of neutron quasiparticle orbitals. The table shows the percentages of the cases in which the calculated splitting agrees with the GM rule, combining the results for several isotopes of each element. Columns labeled 2BP, 3BP, and FP show the perturbative results for the two-body interaction alone, the three-body interaction alone, and the full interaction treated perturbatively. The last column shows the results of the fully self-consistent calculation of the HFB minima. The table shows the results for the D1S interaction [13]. We also have calculated splittings with the D1M interaction [14] and found similar results.

	2BP (%)	3BP (%)	FP (%)	Self-consistent (%)
$^{164-168}$Ho	93	8	28	45
$^{168-172}$Tm	97	4	26	41
$^{172-176}$Lu	97	4	28	40
$^{180-184}$Ta	97	5	37	30
$^{184-188}$Lu	97	3	36	28

The two- and three-body perturbative contributions are $+188$ and -291 keV, respectively. The rearrangement contribution is $+44$ keV, giving a total splitting of -61 keV as shown in the level scheme in Fig. 1. This should be compared with an empirical value of $+114$, which is what is left of the observed splitting of $+171$ after the rotational effects have been removed [10]. Thus, as claimed earlier, the three-body contribution has a bad sign and in this case it overwhelms the good sign of the two-body contribution.

We carried out this analysis on 100–225 doublets in each of 15 nuclei in the deformed rare-earth region. All of these nuclei have strong prolate deformations. The results are shown in Table I. A histogram of calculated GM splittings for for the Lu isotopes is provided in the Supplemental Material [16]. These results confirm the statements made earlier that the two-body interaction has a correct sign, the three-body interaction has the wrong sign, and the net sign with all the contributions is variable and inconsistent with a general GM rule.

To gain a better understanding of the origin of the problem we briefly review how the interaction energies are calculated using the one-body densities of Hartree-Fock-Bogoliubov (HFB) theory. When time-reversal symmetry is broken the one body-density matrix can be decomposed as the sum of a time-even density and a time-odd density. In the expression of the total energy there is a contribution which is quadratic in the time-odd term. Starting from an even-even HFB reference state, the creation of a quasiparticle leads to a nonzero time-odd density matrix. The blocking of the time-reversed state leads to the same time-odd density but with opposite sign. To build the two configurations defining a GM pair, a proton quasiparticle with quantum number K_p and a neutron one with K_n are

blocked to obtain one of the states. The other corresponds to blocking $(-K_p, K_n)$. Among the different terms contributing to the energy in the Gogny interaction there are a few that do not contribute to the splitting, namely the Wigner term of the central potential, the Coulomb potential, and the pairing channel of the central potential. Among the remaining terms, the spin-orbit contribution is much smaller than the other two and will be omitted in the discussion. Tensor potentials are not common either in Gogny or Skyrme interactions but they may be required to improve the single-particle spectrum in some cases [15,17]. It was shown in Ref. [10] that the tensor contribution to the GM splitting has in most of the cases the same sign as the central one and is typically much smaller in magnitude. Its inclusion is not expected to modify our conclusions; we only consider the contributions of central two-body and three-body interactions in the following.

We first calculate the perturbative contribution to the splitting, taking the expectation value of the energy functional in the two-quasiparticle states formed by applying the Bogoliubov quasiparticle creation operators to the HFB ground state of a neighboring even-even nucleus. The formula for the energy difference due to the three-body interaction is very simple if the quasiparticle spins are perfectly aligned along the symmetry axis. Namely, the contribution of the three-body term Δv^{3b} is

$$\begin{aligned}\Delta v^{3b} &= v^{3b}(K_p, K_n) - v^{3b}(-K_p, K_n) \\ &= 4t_3 \int d^3\vec{r}\,\rho^{\alpha}\left(\rho^{p,o}_{1/2,1/2}\rho^{n,o}_{1/2,1/2} + \bar{\rho}^{p,o}_{1/2,-1/2}\bar{\rho}^{n,o}_{1/2,-1/2}\right),\end{aligned} \tag{2}$$

where ρ is the ordinary density, and $\rho^{\tau,t}_{s,s'}(\vec{r}) = \sum_{ll'} \rho^{\tau,t}_{qs,q's'}\varphi^{*}_{q'}(\vec{r})\varphi_q(\vec{r})$ represent the different components of the density, depending on nucleon type τ, spin projections s and s', and the time-reversal behavior $t = \pm 1$ (even, odd) of the density matrix elements $\rho^{\tau,t}_{qs,q's'}$. The bar denotes the modulus of a (complex) density. If the blocked quasiparticle is BCS-like (i.e., linear combinations of creation and annihilation canonical basis states) then the time-odd density matrix $\rho^{\tau,o}_{qs,q's'}$ is diagonal in the canonical basis with zeros in the diagonal except for the blocked orbital quantum number, where it takes the value $\pm 1/2$ according to the direction of the spin σ of the blocked orbital. In this very specific case only taking place at the first iteration (first order), the density $\rho^{\tau,o}_{1/2,-1/2}$ is zero and the sign of $\rho^{\tau,o}_{1/2,1/2}$ equals $(-1)^{\sigma-1/2}$. Therefore Δv^{3b} is positive for parallel spins and negative for antiparallel ones, just the opposite of the GM rule.[1] Since all of the quantities in the integrand as well as t_3 are positive, the contribution to the splitting is repulsive, i.e., the wrong sign.

It is also of interest to examine the various interactions in a momentum space representation, taking the two-quasiparticle wave function as $|\vec{k}_n s_n, \vec{k}_p s_p\rangle$ with $\vec{k}$ as the nucleon's momentum and s as its spin quantum number.[2] The two-body interaction energy in the Gogny functional depends on the relative momentum $|\vec{k}_n - \vec{k}_p|$. Taking the two particles on the Fermi surface, the relative momentum is given by $q_{\pm} = k_F\sqrt{1 \pm \cos\theta}$ with $\cos\theta = \vec{k}_n \cdot \vec{k}_p / k_n k_p$. The contribution to the GM splitting,

$$\Delta v^{2b} = \langle q_+ \uparrow_n \uparrow_p |v| q_+ \uparrow_n \uparrow_p\rangle - \langle q_- \uparrow_n \downarrow_p |v| q_- \uparrow_n \downarrow_p\rangle, \tag{3}$$

is shown in the left-hand panel of Fig. 2 as the solid line. The three-body contribution, given by

$$\Delta v^{3b} = t_3 \rho^{\alpha}, \tag{4}$$

is shown as the dashed line. One sees that the two components have opposite sign. They are added together in the plot on the

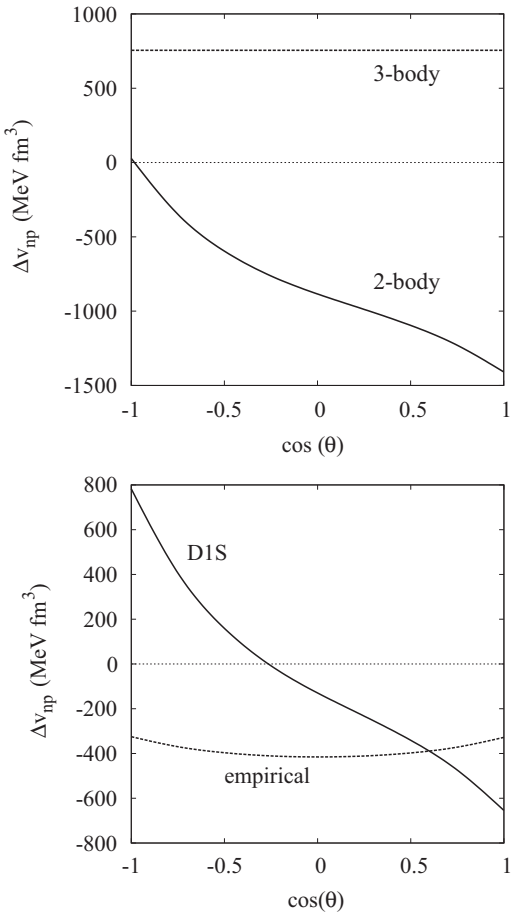

FIG. 2. Matrix elements of the effective neutron-proton interaction from the D1S Gogny energy functional at nuclear matter density, $\rho = 0.16$ fm^{-3}. In the upper panel, the individual contributions of the two- and three-body terms from Eqs. (3) and (4) are shown. In the lower panel, the total for the D1S is shown in comparison to the empirical Δv_{np} discussed in Refs. [10,18].

[1] In the actual HFB calculation the blocked quasiparticle may have a mixture of the two spin orientations and the simple argument given above may fail. This occurs for some configurations treated in Table I.

[2] See Supplemental Material for specific formulas in terms of the Gogny parameters [16].

right. Both signs of the GM splitting are possible, depending on the angle θ. In that plot we also show an empirical neutron-proton interaction, constructed to fit the data on the GM multiplets [10,18]. The interactions are in rough agreement when the momenta in the parallel-spin state are also parallel but strongly disagree when the momenta are antiparallel in that state.

The nuclear matter results also have implications for the Landau parameters of the system. The connection is discussed in the Supplemental Material [16].

We conclude with some remarks about the construction of a better three-body interaction. It seems clear that the contact nature of the Gogny (and Skyrme) interactions is at the root of the problem of reproducing the empirical spin dependence of the neutron-proton interaction. There have been proposals in the literature to generalize the three-body interaction by including derivative terms [19,20] as in the Skyrme two-body interaction. Unfortunately the expansion in powers of the derivatives gives rise to many terms and it is difficult from a purely empirical point of view to determine the coefficients. The interaction arises both from the subnucleon degrees of freedom that are missing from theory as well as from the correlations that are missing from the mean-field treatment of the nucleon degrees of freedom. The latter, called the induced three-body interaction, has a long range [21] and a nonlocality [22] that is impossible to account for in a contact interaction. It should also be mentioned that taking the three-body interaction as an energy functional rather than an effective Hamiltonian can give rise to serious difficulties with broken symmetries and correlation effects [23,24]. The high computational cost of a three-body Hamiltonian can perhaps be mitigated by using separable parametrizations or hypercontraction [25].

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