Effects of tensor forces in nuclear spin–orbit splittings from ab initio calculations

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ABSTRACT

A systematic and specific pattern due to the effects of the tensor forces is found in the evolution of spin–orbit splittings in neutron drops. This result is obtained from relativistic Brueckner–Hartree–Fock theory using the bare nucleon–nucleon interaction. It forms an important guide for future microscopic derivations of relativistic and nonrelativistic nuclear energy density functionals.

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The understanding of nuclear density functionals in terms of the nucleon–nucleon (NN) interaction is one of the present frontiers in nuclear physics. As manifested by the quadrupole moment of the deuteron [1], the tensor force is an important component in the NN interaction. In the form of the two pion exchange the tensor force also provides the main part of the nuclear attraction [2], which is taken into account by the scalar σ meson in phenomenological models [3]. However, the role of the tensor force on the spin properties in finite nuclei is much less clear.

In configuration interaction (CI) calculations it has been found that the tensor force plays an important role in the shell structure far away from stability [4]. On the other side, in nearly all of the successful applications of phenomenological nuclear energy density functionals [5], tensor forces have been neglected for many years.

This has changed recently and much work has been done to investigate the impact of tensor forces in phenomenological nonrelativistic [6–24], and relativistic density functionals [25–33]. Still, it is difficult to find significant features in experimental data which are only connected to tensor forces and therefore suitable for an adjustment of their parameters. In a fit to nuclear masses and radii, for example, with relativistic density functional theory [29], one obtains the best fit for vanishing tensor forces. On the other hand it has been found, that the single particle energies [4,7,34] depend in a sensitive way on tensor forces. However, in the context of density functional theory, single particle energies are only defined as auxiliary quantities [35]. In experiment they are often fragmented and therefore only indirectly accessible. The fragmentation is caused by effects going beyond mean field, i.e., by the admixture of complicated configurations, such as the coupling to low-lying surface vibrations [36–41].

Obviously, the attempts to determine precise values for the strength parameters of the tensor forces in universal nuclear energy density functionals by a phenomenological fit to experimental data in finite nuclei is still a difficult problem [15]. In such a situation we propose to determine these strength parameters from microscopic ab initio calculations based on the well known bare nucleon–nucleon forces. In fact, much progress has been achieved in the microscopic description of nuclear structure in recent years [42–50]. However, these are calculations of extreme numerical complexity and therefore they could be applied, so far, only in the region of light nuclei or for nuclei close to magic configurations.

For the investigation of heavy nuclei all over the periodic table, one is still bound to various versions of phenomenological nuclear density functionals and their extensions beyond mean field [51–53]. Of course the ultimate goal is an ab initio derivation of such functionals. At present, such attempts are in their infancy [54–56]. In Coulombic systems, where there exist very successful microscopically derived density functionals, one starts from the

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E-mail address: meng@pku.edu.cn (J. Meng).
The coupled system of RBHF equations (4), (5), and (6) is solved by iteration. The initial basis is a Dirac Woods–Saxon basis [74] obtained by solving the spherical Dirac equation in a box with the size $R_{\text{box}} = 8$ fm and a mesh size $dr = 0.05$ fm. During the RBHF iteration it is gradually transformed to the self-consistent RHF basis as explained in Ref. [50]. The Bethe–Goldstone equation (4) is solved in the same way as in Ref. [50], except that now only the isospin channel $T_z = 1$ is included.

Fig. 1 shows the total energy $E$ in units of $\hbar\omega N^{4/3}$ and the radii of $N$-neutron drops (with $N$ from 4 to 50) in a HO trap calculated by the RBHF theory using the bare interaction Bonn A [73]. For the cases of open shells, the filling approximation is used.

The results are compared with the quantum Monte-Carlo (QMC) calculations [64,66] based on the 2N interaction AV18 [80] (without and with the 3N forces UX1 and IL7), with the no-core shell model (NCSM) calculations [66,67] based on the chiral 2N + 3N forces, and the force JISP16. The factor $\hbar\omega N^{4/3}$ takes into consideration that in the Thomas–Fermi approximation [81] the total energy for a non-interacting $N$-Fermion system in a HO trap is given by

$$E = \frac{3^{4/3}}{4} \hbar\omega N^{4/3} \approx 1.082 \hbar\omega N^{4/3}.$$

With increasing neutron number of the drops we observe a saturation of $E/\hbar\omega N^{4/3}$ for $N \geq 20$, in contrast to the nuclear case where the binding energy per nucleon saturates for large mass number $A$. The matrix elements of the bare nucleon–nucleon interaction are very large and difficult to be used directly in nuclear many-body theory. Within Brueckner theory, the bare interaction is therefore replaced by an effective interaction in the nuclear medium, the $G$-matrix. It takes into account the short-range correlations by summing up all the ladder diagrams of the bare interaction [75,76] and it is deduced from the Bethe–Goldstone equation [77],

$$\tilde{G}_{abc}^{\alpha}(W) = \tilde{V}_{abc} + \frac{1}{2} \sum_{cd} \tilde{V}_{abcd} \tilde{G}_{cd}^{\beta}(W),$$

where in the RBHF theory $|a\rangle, |b\rangle$ are solutions of the relativistic Hartree–Fock (RHF) equations, $\tilde{V}_{abc}$ are the anti-symmetrized two-body matrix elements (3) and $W$ is the starting energy. The intermediate states $c, d$ run over all states above the Fermi surface with $\varepsilon_c, \varepsilon_d > \varepsilon_F$. The single-particle motion fulfills the RHF equation in the external field of a harmonic oscillator (HO):

$$(T + U + \frac{1}{2} M \omega^2 r^2)|a\rangle = \varepsilon_a |a\rangle,$$

where $\varepsilon_a = \varepsilon_a + M$ is the single-particle energy with the rest mass of the nucleon $M$ and $\hbar \omega = 10$ MeV. The self-consistent single-particle potential $U$ is defined by the $G$-matrix [50,78,79]:

$$\langle a|U|b\rangle = \sum_{c=1}^{N} (ac|\tilde{G}|bc),$$

where the index $c$ runs over the occupied states in the Fermi sea (no-sea approximation). In contrast to the RBHF calculations for self-bound nuclei in Refs. [49,50], a center of mass correction is not necessary in the external field.

The coupled system of RBHF equations (4), (5), and (6) is solved by iteration. The initial basis is a Dirac Woods–Saxon basis [74] obtained by solving the spherical Dirac equation in a box with the size $R_{\text{box}} = 8$ fm and a mesh size $dr = 0.05$ fm. During the RBHF iteration it is gradually transformed to the self-consistent RHF basis as explained in Ref. [50]. The Bethe–Goldstone equation (4) is solved in the same way as in Ref. [50], except that now only the isospin channel $T_z = 1$ is included.

The mixed $V_{\alpha}$ contains the exchange contributions of different mesons $\alpha = \sigma, \delta, \omega, \rho, \eta, \pi$. The interaction vertices $\Gamma_\alpha$ for particles 1 and 2 contain the corresponding $\gamma$-matrices for scalar ($\sigma, \delta$), vector ($\omega, \rho$), and pseudoscalar ($\eta, \pi$) couplings and the isospin matrices $\tilde{\tau}$ for the isovector mesons $\lambda, \rho$, and $\pi$. For the Bonn interaction [73], a form factor of monopole-type is attached to each vertex and $D_{\alpha\beta}(r_1, r_2)$ represents the corresponding meson propagator. Retardation effects were deemed to be small and were ignored from the beginning. Further details are found in Ref. [50].

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By comparing with the QMC and NCSM calculations in panel (a), the results of the RBHF with the interaction Bonn A are similar to those obtained with the JISP16 interaction. For \( N \leq 14 \), Bonn A is also similar to AV8’ + IL7, but getting closer to AV8’ afterwards. This result is favorable as JISP16 is a phenomenological nonlocal NN interaction which reproduces the scattering data as well as it gives a good description for light nuclei [82,83]. On the other hand, AV8’ + IL7 gives a much better description for light nuclei up to \( A = 12 \) than AV8’ or AV8’ + UIX, but the three-pion rings included in IL7 give too much over-binding for pure neutron matter at higher densities [66,84].

Panel (b) of Fig. 1 shows the corresponding radii. While the energies of RBHF with Bonn A are similar to those of the JISP16 interaction, the radii of RBHF are smaller. In comparison with the results of AV8’ + UIX and chiral force, the energies and radii of RBHF with Bonn A are smaller, except when \( N \) approaches 18, where the radii become close to chiral 2N + 3N results.

In Fig. 2, we show the SO splittings of \( N \)-neutron drops for 1p, 1d, 1f, and 2p in a HO trap calculated by the RBHF theory using the Bonn A interaction. They are compared with results obtained by various phenomenological relativistic mean-field (RMF) density functionals, including the nonlinear meson-exchange models NL3 [85] and PK1 [86], the density-dependent meson-exchange models DD-ME2 [87] and PKDD [86], and the nonlinear point-coupling model PC-PK1 [88]. This figure shows the evolution of the various SO splittings with neutron number. For the microscopic RBHF results we find a clear pattern: The SO splitting of a specific orbit with orbital angular momentum \( l \) decreases as the next higher \( j = j_z = l + 1/2 \) orbit is filled and reaches a minimum when this orbit is fully occupied. As the number of neutron continues to increase, the \( j = j_z = l - 1/2 \) orbit begins to be occupied and the SO splitting increases.

Otsuka et al. [4] have found a similar effect between neutron and proton in nuclei. They explained it in terms of the monopole effect of the tensor force, which produces an attractive interaction between a proton in a SO aligned orbit with \( j = j_z = l + 1/2 \) and a neutron in a SO anti-aligned orbit with \( j' = j'_z = l' - 1/2 \) and a repulsive interaction between the same proton and a neutron in a SO aligned orbit with \( j = j_z = l + 1/2 \).

As discussed in Ref. [4] a similar mechanism, but with smaller amplitude, exists also for the tensor interaction between neutrons with \( T = 1 \). Therefore we can explain the behavior of the SO splitting in Fig. 2 in a qualitative way: we consider, for instance, the decrease of the 1d SO splitting if we go from \( N = 20 \) to \( N = 28 \). Because of the interaction with the neutrons filling the 1f\(_{3/2}\) shell above \( N = 20 \), the 1d\(_{5/2}\) orbit is shifted upward and the 1d\(_{3/2}\) is shifted downward, thus reducing the 1d SO splitting. Above \( N = 28 \) we fill in neutrons into 2p\(_{3/2}\) and 1f\(_{5/2}\). They interact with the 1d-neutrons in the opposite way and increase the SO-splitting for the 1d configuration.

On the other hand, this specific evolution of SO splitting is not significant for any of the phenomenological RMF density functionals in Fig. 2, which do not include a tensor term. In order to verify that this specific pattern is indeed caused by the tensor term, we show in Fig. 3 the same calculation but with the RHF density functional PKO1 [25], which includes the tensor force induced by the pion coupling through the exchange term. Without readjusting the other parameters of this functional, we have multiplied a factor \( \lambda \) in front of the pion coupling to investigate the effects of the tensor forces. It is remarkable to see that the evolution of the SO splitting is strongly influenced by the strengths of the tensor forces significantly. For \( \lambda = 1 \) we have the results of the density functional PKO1. They show already the right pattern, but the size of the effect is somewhat too small. This can be understood by the fact, that it is difficult to fit the strengths of the tensor forces just to bulk properties such as binding energies and radii [29]. The general feature of these SO splittings found in our RBHF calculations with Bonn A can be well reproduced with PKO1 simply by multiplying a factor \( \lambda = 1.3 \) in front of the pion coupling. One may wonder if the tensor force discussed here is too strong, as the orig-
that the SO splitting decreases as the next \( j = l + 1/2 \) orbit being occupied, and increases again as the next \( j = l - 1/2 \) orbit being occupied. This is similar to the effects of tensor forces between neutron and proton as has been found in Ref. [4]. The pattern of the evolution of SO splittings cannot be reproduced by the RMF density functionals, while it can be well reproduced with the RHF density functional PK01 which includes tensor forces. This implies that the strengths of tensor forces in neutron drops can be derived from \textit{ab initio} calculations and used as a guide for future \textit{ab initio} derivations of nuclear density functionals.

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Fig. 3. (Color online) Similar to Fig. 2, but in comparison with the RHF density functional PK01 [25] with different strength of pion coupling characterized by \( \lambda \).

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