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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.

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 non-relativistic [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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infinite system and the exact solution of an electron gas [57]. In nuclei, there are attempts to proceed in a similar way and to derive in a first step semi-microscopic functionals. Modern relativistic and nonrelativistic *ab initio* descriptions of symmetric nuclear matter at various densities are used as meta-data in order to reduce the number of phenomenological parameters of the density functionals considerably [58–60]. However, microscopic calculations of nuclear matter give us no information about the effective tensor force in the nuclear medium, because this is a spin-saturated system and their influence is therefore negligible. In order to learn the tensor force we propose in this letter to start from meta-data for a finite system, neutron drops confined in an external potential to keep the neutrons bound.

A neutron drop provides an ideal and simple system to investigate the neutron-rich environment. Because of the missing proton–neutron interaction, the equations for neutron drops are much easier to be solved than those for finite nuclei. Therefore they have been investigated in the literature by many different *ab initio* methods [61–68] and also by phenomenological density functional theory [69].

Starting from bare nuclear forces, Brueckner–Hartree–Fock (BHF) theory provides the G-matrix, a density dependent effective interaction in the nuclear medium and the basis of phenomenological density functional theory in nuclei [70]. As an *ab initio* theory, the nonrelativistic version of BHF with 2N forces failed [71] because of the missing 3N forces, but it has been shown that the relativistic version allows to derive the saturation properties of infinite nuclear matter from bare 2N forces only [72].

In this Letter we use the relativistic Brueckner–Hartree–Fock (RBHF) theory to study the effects of tensor forces in neutron drops. This theory has recently been developed to describe finite nuclei self-consistently [49,50] with results in much better agreement with experimental data than the nonrelativistic calculations based on 2N forces only.

We start from the relativistic bare nucleon–nucleon interaction Bonn A [73] and investigate neutron drops confined in an external harmonic oscillator potential using the RBHF theory. We study drops with an even number of neutrons from $N = 4$ to 50 and compare their energies and radii with other nonrelativistic *ab initio* calculations. Special attention is paid on the possible signature of the tensor force in the neutron–neutron interaction, that is, the evolution of spin–orbit (SO) splitting with neutron number.

We start with a relativistic one-boson-exchange NN interaction which describes the NN scattering data [73]. The Hamiltonian can be expressed as:

$$H = \sum_{kk'} \langle k|T|k'\rangle b_k^\dagger b_{k'} + \frac{1}{2}\sum_{klk'l'} \langle kl|V|k'l'\rangle b_k^\dagger b_l^\dagger b_{l'} b_{k'}, \tag{1}$$

where the relativistic matrix elements are given by

$$\langle k|T|k'\rangle = \int d^3r\, \bar\psi_k(\mathbf{r})\,(-i\boldsymbol{\gamma}\cdot\nabla + M)\,\psi_{k'}(\mathbf{r}), \tag{2}$$

$$\langle kl|V_\alpha|k'l'\rangle = \int d^3r_1 d^3r_2\, \bar\psi_k(\mathbf{r}_1)\Gamma_\alpha^{(1)}\psi_{k'}(\mathbf{r}_1) \times D_\alpha(\mathbf{r}_1,\mathbf{r}_2)\bar\psi_l(\mathbf{r}_2)\Gamma_\alpha^{(2)}\psi_{l'}(\mathbf{r}_2). \tag{3}$$

The indices k, l run over a complete basis of Dirac spinors with positive and negative energies, as, for instance, over the eigensolutions of a Dirac equation with potentials of Woods–Saxon shape [50,74].

The two-body interaction V_α contains the exchange contributions of different mesons $\alpha = \sigma, \delta, \omega, \rho, \eta, \pi$. The interaction vertices Γ_α for particles 1 and 2 contain the corresponding γ-matrices for scalar (σ, δ), vector (ω, ρ), and pseudovector (η, π) coupling and the isospin matrices $\vec\tau$ for the isovector mesons δ, ρ, and π. For the Bonn interaction [73], a form factor of monopole-type is attached to each vertex and $D_\alpha(\mathbf{r}_1, \mathbf{r}_2)$ 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].

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],

$$\bar G_{aba'b'}(W) = \bar V_{aba'b'} + \frac{1}{2}\sum_{cd}\frac{\bar V_{abcd}\bar G_{cda'b'}(W)}{W - \varepsilon_c - \varepsilon_d}, \tag{4}$$

where in the RBHF theory $|a\rangle, |b\rangle$ are solutions of the relativistic Hartree–Fock (RHF) equations, $\bar V_{aba'b'}$ 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):

$$(T + U + \frac{1}{2}M\omega^2 r^2)|a\rangle = e_a|a\rangle, \tag{5}$$

where $e_a = \varepsilon_a + M$ 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]:

$$\langle a|U|b\rangle = \sum_{c=1}^{N}\langle ac|\bar G|bc\rangle, \tag{6}$$

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 $R_{\rm box} = 8$ 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 AV8' [80] (without and with the 3N forces UIX 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

$$E = \frac{3^{4/3}}{4}\hbar\omega N^{4/3} \approx 1.082\,\hbar\omega N^{4/3}. \tag{7}$$

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.