Beyond Hartree-Fock in Nuclear Physics

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Abstract

To get a proper handle on correlations in nuclear systems and relate these to the underlying forces, forms an essential part in basic nuclear physics research and has wide ranging implications for our understanding of how subatomic matter organizes itself and what phenomena emerge. To identify the mechanisms which are responsible for the occurence or not of so-called magic numbers in various regions of the nuclear chart, requires systematic studies of correlations and nuclear forces. In this work we analyze the evolution of effective single-particle energies for the chain of oxygen, calcium, nickel and tin isotopes and study the role of two- and three-body forces in terms of their central, spin-orbit and tensor force components. The aim is to understand the role of these components towards the respective driplines of the above isotopic chains. Nuclear forces based on chiral effective field theory and systematically fit to nuclear data are employed in these studies.

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1. Introduction

The understanding of nuclear structure and reactions and thereby properties of nuclei in terms of the underlying strong force and the pertinent laws of motion, involves a number of approximations that pose a great challenge

to nuclear theory. Similarly, our interpretations of experimentally measurable quantities rely as well on several assumptions and approximations. As an example, concepts such as an independent particle motion and various mean-field approaches based thereupon, play an important role in the analysis and interpretation of experimental results. Eventual deviations from such a mean-field picture are interpreted as a possible measure of correlations, with the potential of providing a better understanding of the role of the underlying strong force in a nuclear many-body environment. A popular theoretical approach for studying correlations beyond a given mean field, is the nuclear shell model, see for example Refs. **???**. It rests on the assumption that the state functions used in nuclear structure studies can be approximated by various Slater determinants based on a particular orthonormal set of single-particle states. The shell model has been rather successful in describing many of the observed features of nuclei and experimental probes like nucleon transfer and knockout reactions have been essential in supporting a mean-field picture of nuclei. Single-particle properties have been extracted by measurements of nucleon-adding and nucleon-removing transfer reactions, establishing thereby a link between observables and theoretical interpretations, see for example Refs. **??** and discussions therein.

However, in nuclear physics, the analysis and theoretical interpretations of correlations beyond a mean field picture are complicated by the fact that the strong force is represented by various effective models and Hamiltonians in the energy regime of nuclear structure studies. These effective Hamiltonians are nowadays based on chiral effective field theory (EFT), see for example Refs. **?????????**. The EFT nuclear interactions that are currently employed in nuclear structure calculations employ normally pions and nucleons as effective degrees of freedom. Compared with former interaction models inspired by a one-boson-exchange approximation (see Refs. **??** for relevant reviews), interactions based on chiral EFT exhibit currents that are consistent with the underlying Lagrangian that defines the interactions. Furthermore, chiral EFT interactions allow for systematic improvements since they are based on power counting in terms of the probed momentum scale over a given cutoff scale Λ. The power counting introduces also a systematic recipe for constructing nucleon-nucleon (NN) forces, three-nucleon ($3N$) forces, and forces of higher rank.

To get a proper handle on correlations in nuclear systems and relate these to the abovementioned underlying forces, forms an essential part in basic nuclear physics research and has wide ranging implications for our un-

derstanding of how subatomic matter organizes itself and what phenomena emerge. For example, to identify the mechanisms which are responsible for the occurence or not of so-called magic numbers in various regions of the nuclear chart, will most likely require systematic studies of correlations beyond standard shell-model calculations, which often are limited to one or at most two major oscillator shells. For exotic isotopes close to the so-called drip lines, continuum degrees of freedom and more complicated many-body forces may become important, as demonstrated recently in Refs. **??** for the chains of oxygen and calcium isotopes.

The NN interaction has traditionally been studied in terms of its central, spin-orbit and tensor force. These terms accomodate to a large degree our phenomenological knowledge of the strong interaction, which, when applied in a nuclear many-body context, is subjected to various degrees of renormalization. In particular, the tensor force, a non-central component of the nuclear force, has been shown to play an important role for the development of magic numbers of nuclei with large N/Z ratios, see Refs. **?????**. Furthermore, the spin-orbit force which arises from the nuclear forces, is of the order of the average binding energy per nucleon and plays an important role in defining nuclear single-particle fields. Its importance is essential in order to account for magic numbers and large shell gaps in nuclei and lead, in the early days of nuclear physics, to the introduction of an empirical one-body spin-orbit force **??**. To relate such an empirical spin-orbit force to the underlying nuclear forces is an unresolved and outstanding problem in nuclear physics, see for example Refs. **??**. In Refs. **??**, the large splittings in energy between states that can be interpreted as representing single-particle spin-orbit partners in for $A = 15$ and $A = 39$, could be related both to the two-body spin-orbit force and a contribution to the spin-orbit force from three-body forces. In Ref. **?**, the authors showed that the two-nucleon spin-orbit force gave approximately half of the observed splitting, while the other half came from pion exchange interactions between three or more nucleons.

In order to shed light on these issues, we present in this work an analysis of effective single-particle energies and their evolution as function of neutron numbers for selected oxygen, calcium, nickel and tin isotopes. The interactions which define the single-particle energies contain two-body and three-body forces defined within the framework of chiral effective field theory. We optimize the chiral interaction up to next-to-next-to leading order (NNLO) using the recently developed model-based, derivative-free algorithm POUNDerS **?**. The cutoff dependence of the chiral forces and the various

optimizations allow us in turn to study the convergence properties of chiral forces in a nuclear many-body environment. Furthrmore, these interactions are in turn decomposed in terms of a central, spin-orbit and tensor force component **??????**. This decomposition allows thereby for a systematic analysis of the spin-orbit force and the tensor force as functions of varying neutron and proton numbers. The single-particle energies for the above isotopes are computed using Hartree-Fock theory, many-body perturbation theory and coupled-cluster theory **?**. The effective single-particle energies are defined as one particle (protons and neutrons) on top of nuclei with j-filled shells. Although this definition of an effective single-particle energy is questionable, see for example the discussion in Ref. **?**, it has been widely used in a nuclear structure, see for example Refs. **??????**.

After these introductory remarks, we present in the next section our theoretical framework, with the definition of effective single-particle energies and their relation to the decomposition of the nuclear forces in central, spin-orbit and tensor components. The nuclear interactions we include in our analysis are only briefly reviewed here. Where details are needed, we refer the reader to our recent parametrization of chiral forces in Ref. **?**. Section 3 presents our main findings while Sec. 4 outlines our conclusions and perspectives.

2. Theoretical framework

In this section we present first our basic definitions of Hamiltonians with and without three-body forces and link these expressions with the derivation the so-called monopole interaction and its connection with single-particle energies at a mean-field level. The interactions are in turn analyzed in terms of a multi-component expansion of the nuclear forces, with an emphasis of the central, spin-orbit and tensor components. These terms accomodate our basic phenomenological knowledge of the strong interaction. We end this section with a summary on how to parametrize chiral interactions. These interactions, which are constrained to reproduce several nuclear observables via an optimization procedure, form the input to our analysis.

2.1. Definitions

Our Hamiltonian contains one-body, two-body and three-body contributions and in the equations below, we label states below the Fermi level F as $i, j, \ldots$ while states above the Fermi level are defined by $a, b, \ldots$. General single-particle states are given by the letters $p, q \ldots$. The quantities $pq \ldots$

represent the quantum numbers of various single-particle states, namely $p = (n_p, l_p, j_p, m_{j_p}, t_{z_p})$. The commutation relations for creation and annihilations operators with respect to a given reference state are then given by

$$\left\{a_p^\dagger, a_q\right\} = \delta_{pq}, p, q \leq F \qquad \left\{a_p, a_q^\dagger\right\} = \delta_{pq}, p, q > F.$$

The action of the creation and annihilation operators with respect to a reference state Φ_0 are then given by $a_i|\Phi_0\rangle = |\Phi_i\rangle$ where a state labeled by $|\Phi_i\rangle$ means that a particle in a single-particle state i has been removed. Similarly, we have $a_a^\dagger|\Phi_0\rangle = |\Phi^a\rangle$, $a_i^\dagger|\Phi_0\rangle = 0$ and $a_a|\Phi_0\rangle = 0$. With the above definitions, we write our Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V} + \hat{W},$$

where the single-particle part is given by

$$\hat{H}_0 = \sum_{pq} \langle p|\hat{h}_0|q\rangle a_p^\dagger a_q.$$

This part of the Hamiltonian is commonly defined in terms of some external potential like the three-dimensional harmonic oscillator or a particular mean-field basis. Similarly, the two-body part of the Hamiltonian is given by

$$\hat{V} = \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle_{\rm AS} a_p^\dagger a_q^\dagger a_s a_r$$

where we have employed antisymmetric matrix elements defined as

$$\langle pq|\hat{v}|rs\rangle_{\rm AS} = \langle pq|\hat{v}|rs\rangle - \langle pq|\hat{v}|sr\rangle.$$

We will assume throughout this work that the two-body operator $\hat{v}$ is given by a nucleon-nucleon interaction. The models for the two-nucleon interaction will be defined in Sec. **??**. Finally, the three-body part of our Hamiltonian operator is defined by

$$\hat{W} = \frac{1}{36}\sum_{pqrstu} \langle pqr|\hat{w}|stu\rangle_{\rm AS} a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s,$$

where we have defined the antisymmetric matrix elements

$$\langle pqr|\hat{w}|stu\rangle_{\rm AS} = \langle pqr|\hat{w}|stu\rangle + \langle pqr|\hat{w}|tus\rangle + \langle pqr|\hat{w}|ust\rangle - \langle pqr|\hat{w}|sut\rangle - \langle pqr|\hat{w}|tsu\rangle - \langle pqr|\hat{w}|uts\rangle.$$

We will in the discussions to come drop the AS subscript, assuming thereby that all matrix elements are antisymmetrized. Introducing a reference state $|\Phi_0\rangle$ as our new vacuum state leads to a redefinition of the Hamiltonian in terms of a constant reference energy E_0 defined as

$$E_0 = \sum_{i\leq F}\langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij\leq F}\langle ij|\hat{v}|ij\rangle + \frac{1}{6}\sum_{ijk\leq F}\langle ijk|\hat{w}|ijk\rangle,$$

and a normal-ordered Hamiltonian

$$\hat{H}_N = \sum_{pq}\langle p|\tilde{f}|q\rangle a_p^\dagger a_q + \frac{1}{4}\sum_{pqrs}\langle pq|\tilde{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r + \frac{1}{36}\sum_{\substack{pqr\\stu}}\langle pqr|\hat{w}|stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

where

$$\langle p|\tilde{f}|q\rangle = \langle p|\hat{h}_0|q\rangle + \sum_{i\leq F}\langle pi|\hat{v}|qi\rangle + \frac{1}{2}\sum_{ij\leq \alpha_F}\langle pij|\hat{w}|qij\rangle,$$

represents a correction to the single-particle operator $\hat{h}_0$ due to contributions from the nucleons below the Fermi level. The two-body matrix elements are now modified in order to account for medium-modified contributions from the three-body interaction, resulting in

$$\langle pq|\tilde{v}|rs\rangle = \langle pq|\hat{v}|rs\rangle + \sum_{i\leq F}\langle pqi|\hat{w}|rsi\rangle. \tag{1}$$

In Eq. (1), the effective two-body interaction $\tilde{v}$ can contain both a standard two-nucleon interaction and a density dependent contribution stemming from a three-body interaction $\hat{w}$.

An important ingredient in studies of effective interactions and their applications to nuclear structure, is the so-called monopole interaction, normally defined in terms of a nucleon-nucleon interaction $\hat{v}$ **??????????**

$$\bar{V}_{\alpha_p\alpha_q} = \frac{\sum_J (2J+1)\langle(\alpha_p\alpha_q)J|\hat{v}|(\alpha_p\alpha_q)J\rangle}{\sum_J(2J+1)}, \tag{2}$$

where the total angular momentum of a two-body state J runs over all possible values. In the above equation we have defined a nucleon-nucleon interaction in a so-called angular-momentum coupled representation with the symbol $\alpha_{p,q}$ representing all possible quantum numbers except the magnetic substates $m_{j_{p,q}}$ The monopole Hamiltonian can be interpreted as an

angle-averaged matrix element. We have assumed that the single-particle angular momenta j_p and j_q couple to a total two-particle angular momentum J. The summation over J with the value $2J+1$ can be replaced by $\sum_J(2J+1) = (2j_p+1)(2j_q+1)$ if $\alpha_p \neq \alpha_q$. If $\alpha_p = \alpha_q$ we can generalize this equation to, assuming that our states can represent either protons or neutrons,

$$\sum_J (2J+1) = (2j_p+1)(2j_q+1-\delta_{\alpha_p\alpha_q}). \tag{3}$$

The spherical single-particle states, provide an important ingredient for the formation of shells and interplay between spherical configurations and deformation in nuclei. Large shell gaps obtained from a monopole Hamiltonian are a prerequisite to obtain certain magic numbers. Equation (2) can also be expressed in terms of the medium-modified two-body interaction defined in Eq. (1), that is we can have

$$\tilde{V}_{\alpha_p\alpha_q} = \frac{\sum_J (2J+1)\langle(\alpha_p\alpha_q)J|\tilde{v}|(\alpha_p\alpha_q)J\rangle}{\sum_J(2J+1)}. \tag{4}$$

As stated in the introduction, one of the aims of this work is to study the role of three-body interactions in nuclear structure, with an emphasis on the evolution of single-particle energies.

The single-particle energy ϵ_p resulting from for example a self-consistent Hartree-Fock field, or from first order in many-body perturbation theory, is given by (in an uncoupled basis)

$$\epsilon_p = \langle p|\tilde{f}|p\rangle = \langle p|\hat{h}_0|p\rangle + \sum_{i\leq F}\langle pi|\hat{v}|pi\rangle + \frac{1}{2}\sum_{ij\leq\alpha_F}\langle pij|\hat{w}|pij\rangle,$$

where we have included the three-body interaction as well. We can rewrite this equation in an angular coupled basis (jj-coupled basis) as

$$\epsilon_{\alpha_p} = \langle\alpha_p|\hat{h}_0|\alpha_p\rangle + \frac{1}{2j_p+1}\sum_{\alpha_i\leq\alpha_F}\sum_J (2J+1)\langle(\alpha_p\alpha_i)J|\hat{v}|(\alpha_p\alpha_i)J\rangle, \tag{5}$$

or

$$\epsilon_{\alpha_p} = \langle\alpha_p|\hat{h}_0|\alpha_p\rangle + \frac{1}{2j_p+1}\sum_{\alpha_i\leq\alpha_F}\sum_J (2J+1)\langle(\alpha_p\alpha_i)J|\tilde{v}|(\alpha_p\alpha_i)J\rangle, \tag{6}$$

where the first equation contains a two-body force only while Eq. (6) includes the medium-modified contribution from the three-body interaction as well.

In Eqs. (5) and (6), we have used a compact notation for the single-particle states, with the symbol α_p etc representing all possible quantum numbers except the magnetic substates m_{j_p}, that is $\alpha_p = (n_p, l_p, j_p, t_{z_p})$. The symbol α_F stands now for all single-particle states up to the Fermi level, excluding again the magnetic substates. In the above two-body interaction matrix elements $\langle(\alpha_p\alpha_i)J|\hat{v}(\tilde{v})|(\alpha_p\alpha_i)J\rangle$ we have dropped additional quantum numbers like the isospin projection. Our interactions are diagonal in the projection of the total isospin but breaks both isospin symmetry and charge symmetry.

Depending on the choice of single-particle Hamiltonian, the quantity $\langle\alpha_p|\hat{h}_0|\alpha_p\rangle$ could represent the expectation value of the single-particle kinetic energy or the eigenstate of a single-particle Hamiltonian $\hat{h}_0$. The latter could for example be the solution of Schrödinger's equation for a particle moving in a Woods-Saxon like single-particle potential, or the widely employed harmonic oscillator in three dimensions.

Using the definition of the single-particle energy in Eq. (5), the definition of the monopole matrix element in Eqs. (2) or (4) and Eq. (3), we can rewrite Eq. (5) as

$$\epsilon_{\alpha_p} = \langle\alpha_p|\hat{h}_0|\alpha_p\rangle + \sum_{\alpha_i\leq\alpha_F} N_{\alpha_i}\bar{V}_{\alpha_p\alpha_i}, \tag{7}$$

with $N_{\alpha_i} = 2\alpha_i + 1$, and Eq. (6) as

$$\epsilon_{\alpha_p} = \langle\alpha_p|\hat{h}_0|\alpha_p\rangle + \sum_{\alpha_i\leq\alpha_F} N_{\alpha_i}\tilde{V}_{\alpha_p\alpha_i}. \tag{8}$$

2.2. Spin-tensor decomposition

The effective interaction discussed in the previous subsection is a scalar two-body operator. A general scalar two-body operator $\hat{v}$ can be written as

$$\hat{v} = \sum_k \hat{v}_k = \sum_k \boldsymbol{C^{(k)}} \cdot \boldsymbol{Q^{(k)}}, \tag{9}$$

where the operators $\boldsymbol{C^{(k)}}$ and $\boldsymbol{Q^{(k)}}$ are irreducible spherical tensor operators of rank k, acting in spin and coordinate space, respectively. The value of k is limited to $k \leq 2$ since the total eigenspin of the two-nucleon system is either 0 or 1. The term with $k = 0$ refers to the central component of the two-body operator. The values of $k = 1$ and $k = 2$ are called the vector and the tensor components, respectively. The vector term is also called the two-body spin-orbit term, although it also contains the anti-symmetric spin-orbit term, see

for example Ref. **?** for further details. Using standard angular momentum algebra it is rather straightforward to relate the matrix elements $\hat{v}_k$ to those of say $\hat{v}$ or $\tilde{v}$.

One possible decomposition of the effective interaction is to express the k-th component of the interaction $\langle(\alpha_p\alpha_q)J|\hat{v}_k|(\alpha_r\alpha_s)J\rangle$ in a jj-coupled basis, where $\hat{v}_k$ is related to the matrix elements $\langle(\alpha_p\alpha_q)J|\hat{v}|(\alpha_r\alpha_s)J\rangle$ (or $\langle(\alpha_p\alpha_q)J|\tilde{v}|(\alpha_r\alpha_s)J\rangle$ through the relation

$$\begin{aligned}\langle(\alpha_p\alpha_q)J|\hat{v}_k|(\alpha_r\alpha_s)J\rangle &= (-1)^J(2k+1)\sum_{LL'SS'}\langle\alpha_p\alpha_q|LSJ\rangle\langle\alpha_r\alpha_s|L'S'J\rangle\left\{\begin{array}{ccc} L & S & J \\ S' & L' & k\end{array}\right\} \\ &\times\sum_{J'}(-1)^{J'}(2J'+1)\left\{\begin{array}{ccc} L & S & J' \\ S' & L' & k\end{array}\right\}\sum_{\alpha'_p\alpha'_q\alpha'_r\alpha'_s}\langle\alpha'_p\alpha'_q|LSJ'\rangle \\ &\times\langle\alpha'_r\alpha'_s|L'S'J'\rangle\langle(\alpha'_p\alpha'_q)J'|\hat{v}|(\alpha'_r\alpha'_s)J'\rangle. \qquad (10)\end{aligned}$$

The two-particle matrix elements are normalized and antisymmetrized. A similar expression applies to the medium-modified two-body interaction $\tilde{v}$ of Eq. (1) as well. The symbol $\langle\alpha_p\alpha_q|LSJ\rangle$ is a shorthand for the $LS-jj$ transformation coefficient,

$$\langle\alpha_p\alpha_q|\lambda SJ\rangle = \sqrt{(2j_p+1)(2j_q+1)(2\lambda+1)(2S+1)}\left\{\begin{array}{ccc} l_p & \frac{1}{2} & j_p \\ l_q & \frac{1}{2} & j_q \\ \lambda & S & J\end{array}\right\},$$

see for example Ref. **?**. The transformation from an LS basis to a jj-coupled scheme is then given by the relation

$$|(\alpha_p\alpha_q)J\rangle = \sum_{LS}\langle\alpha_p\alpha_q|LSJ\rangle|(\tilde{\alpha}_p\tilde{\alpha}_q)LSJ\rangle,$$

where the symbol like $\tilde{\alpha}_p$ refers to the quantum numbers in an LS basis, that is $\tilde{\alpha}_p = (n_p, l_p, s_p, t_{z_p})$.

To derive Eq. (10), we have used the fact that the two-body matrix elements of $\hat{v}_k$ can also be interpreted in the representation of the LS-coupling scheme as in Refs. **??????**. This representation allows for a more direct comparison with the nucleon-nucleon interaction, a quantity normally defined in terms of the partial waves of the center-of-mass and relative motion system, see for example Ref. **?**. Similar to the decomposition in the jj-scheme, the LS-coupled matrix element of a given component k $\langle(\tilde{\alpha}_p\tilde{\alpha}_q)LSJ'T|\,\hat{v}_k\,|(\tilde{\alpha}_r\tilde{\alpha}_s)LSJ'T\rangle$

are related to the corresponding matrix elements of the total interaction in the jj-scheme by

$$\begin{aligned}\langle(\tilde{\alpha}_p\tilde{\alpha}_q)LSJ'T|\,\hat{v}_k\,|(\tilde{\alpha}_r\tilde{\alpha}_s)L'S'J'T\rangle &= \frac{1}{\sqrt{(1+\delta_{\tilde{\alpha}_p\tilde{\alpha}_q})(1+\delta_{\tilde{\alpha}_r\tilde{\alpha}_s})}}(-1)^{J'}\hat{k}\begin{Bmatrix} L & S & J' \\ S' & L' & k \end{Bmatrix} \\ &\times\sum_J(-1)^J\hat{J}\begin{Bmatrix} L & S & J \\ S' & L' & k \end{Bmatrix}\sum_{\alpha_p\alpha_q\alpha_r\alpha_s}\langle\alpha_p\alpha_q|LSJ\rangle\langle\alpha_r\alpha_s|L'S'J\rangle \\ &\times\sqrt{(1+\delta_{\alpha_p\alpha_q})(1+\delta_{\alpha_r\alpha_s})}\,\langle(\alpha_p\alpha_q)JT|\,\hat{v}\,|(\alpha_r\alpha_s)JT\rangle\,.\end{aligned}$$

In this work we will use Eq. (10) in our analysis of the various matrix elements in Eqs. (2) and (4) and the single-particle energies of Eqs. (7) and (8).

3. Results

4. Conclusions and perspectives

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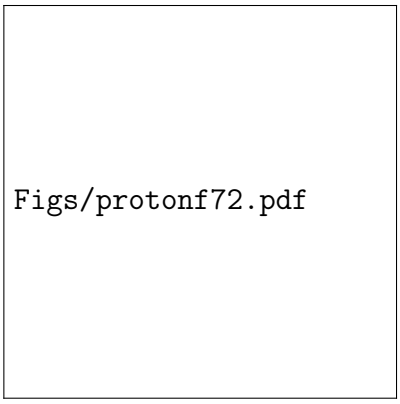
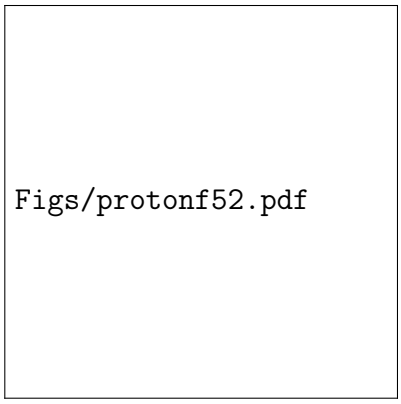
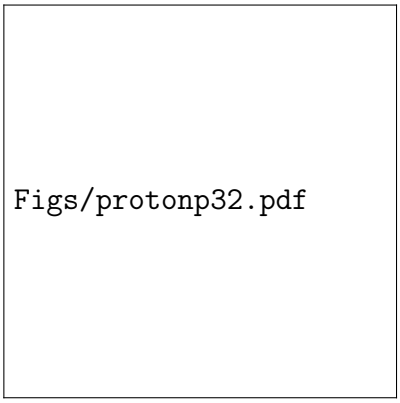


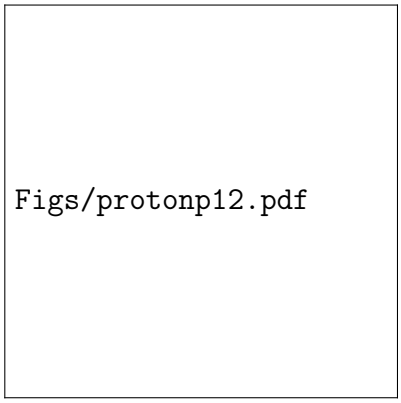
(a) Results for the $0f_{7/2}$ single-particle state



(b) Results for the $0f_{5/2}$ single-particle state



(c) Results for the $1p_{3/2}$ single-particle state



(d) Results for the $1p_{1/2}$ single-particle state

Figure 1: Contributions from the central, spin-orbit and tensor components to the proton single-particle energies of $1p0f$ single-particle states. The closed-shell cores are ^{40}Ca, ^{48}Ca, ^{52}Ca, ^{54}Ca and ^{60}Ca. The results have been obtained with a harmonic oscillator basis and an oscillator energy $\hbar\omega = 10.5$ MeV using the N^{3}LO interaction model of Ref. **?**.