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# No-core shell model for $^{48}\text{Ca}$ , $^{48}\text{Sc}$ and $^{48}\text{Ti}$

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## Abstract

We report the first no-core shell model results for  $^{48}\text{Ca}$ ,  $^{48}\text{Sc}$  and  $^{48}\text{Ti}$  with derived and modified two-body Hamiltonians. We use an oscillator basis with a limited  $\hbar\Omega$  range around  $40/A^{1/3} = 11\text{MeV}$  and a limited model space up to  $1 \hbar\Omega$ . No single-particle energies are used. We find that the charge dependence of the bulk binding energy of eight  $A = 48$  nuclei is reasonably described with an effective Hamiltonian derived from the CD-Bonn interaction while there is an overall underbinding by about  $0.4 \text{ MeV/nucleon}$ . However, resulting spectra exhibit deficiencies that are anticipated due to: (1) basis space limitations and/or the absence of effective many-body interactions; and, (2) the absence of genuine three-nucleon interactions. We introduce phenomenological modifications to obtain fits to total binding and low-lying spectra. The resulting no-core shell model opens a path for applications to experiments such as the double-beta ( $\beta\beta$ ) decay process.

## 1 Introduction

Motivated by the intense interest in nuclear double-beta ( $\beta\beta$ ) decay and the associated need for precision treatments of nuclear many body systems, we investigate

the ab-initio no core shell model (NCSM) for the lightest case for which  $\beta\beta$  decay has been measured. This ( $\beta\beta$ ) decay case involves  $^{48}\text{Ca}$ ,  $^{48}\text{Sc}$  and  $^{48}\text{Ti}$ .

Previous efforts have addressed  $A = 48$  nuclei with similar goals by solving the shell model of eight nucleons in the pf shell with an inert  $^{40}\text{Ca}$  core. Chief among these efforts is the work of Caurier et al. [1] who made predictions for the  $2\nu\beta\beta$  decay mode of  $^{48}\text{Ca}$ . They carried out a full  $0\hbar\Omega$  calculation for the nuclei involved in this decay, using a KB3 effective interaction [2]. Single-particle energies extracted from experiment were used to model the valence-core interactions. They obtained a satisfactory description of the spectroscopy (energy levels of positive parity, E2 and M1 transitions) when they used a factor of 0.77 to renormalize the nuclear matrix elements (NME) of the Gamow-Teller (GT) operator  $\sigma\tau_{\pm}$ . This quenching factor accounts for possible missing nucleon correlations and/or non-nucleonic contributions. It is noteworthy that their calculated half-life  $T_{1/2}^{2\nu} = 3.6 \times 10^{19}$  years is in good agreement with the experimental result  $T_{1/2}^{2\nu} = 4.3 \times 10^{19}$  years, measured later [3].

Similar calculations have been performed using either slightly different parameters in the Hamiltonian [4] or more severely truncated model spaces (allowing at most 4 nucleons lifted from the  $f_{7/2}$  sub-shell in  $^{48}\text{Ca}$  and  $^{48}\text{Ti}$  and at most 5 in  $^{48}\text{Sc}$ ) [5]. Such calculations have also been extended to the  $0\nu\beta\beta$  decay mode of  $^{48}\text{Ca}$  [6].

Caurier et al. [7] also performed a systematic calculation of the spectroscopic properties (positive parity energy levels, B(E2), M1, quadrupole moments, GT strengths) of several  $A = 48$  isotopes:  $^{48}\text{Ca}$ ,  $^{48}\text{Sc}$ ,  $^{48}\text{Ti}$ ,  $^{48}\text{V}$ ,  $^{48}\text{Cr}$  and  $^{48}\text{Mn}$ . The model space consisted again of 8-nucleons in the full pf shell and they used a minimally monopole modified realistic KB3 interaction along with experimental single particle energies. Their results reproduced well the existing data with few parameters.

In ref. [8] the authors also performed a full pf shell model calculation of the  $2\nu\beta\beta$  decay rate of  $^{48}\text{Ca}$  using a Hamiltonian given as a set of 195 two-body NME. Since the model parameters could not be accurately determined starting from a realistic NN force, they showed how modifications in the Hamiltonian (retaining, however, the acceptable agreement with experiment) have significant influence on the value of the decay rate. The significance of nuclear shell structure in the  $2\nu\beta\beta$  NME was also analyzed in ref. [9].

Capilla et al. [10] performed a shell model calculation of the  $2\nu\beta\beta$  decay rate

emphasizing the role of the spin-orbit term compared with the other terms of a schematic potential that also included central and tensor terms.

Beyond these applications to  $A = 48$ , the role of additional correlations has been extensively investigated. For example, the proton-neutron quasi-random phase approximation (pnQRPA) methods have been employed (see for example [11] and the refs. therein). However, within these methods only a few classes of nucleon-nucleon (NN) correlations are taken into account and there is still debate whether missing correlations may be important [12]-[13]. Moreover, the calculated NME's for the two neutrino double beta decay ( $2\nu\beta\beta$ ) mode are very sensitive to variations of the particle-particle interaction strength parameter, exactly in the region of physical interest. As a result, one cannot fix adequately this parameter for the more interesting  $0\nu\beta\beta$  decay calculations.

Most recently, Honma et al. have developed a new semi-realistic valence Hamiltonian for pf-shell nuclei which provides impressive fits to a wide range of nuclear properties in the region [14]. Further research will be needed to elucidate the distinctions between our no-core Hamiltonian and the successful valence space Hamiltonian.

We also call the interested reader's attention to a recent review article by Brown that presents an extensive overview of important shell model literature addressing the  $A = 48$  nuclei as well as other regions [15].

As an alternative approach, we investigate the NCSM for these  $A = 48$  nuclei. This is the first time such calculations are reported for nuclei with  $A \geq 17$ . Our initial goal is to demonstrate the utility of such NCSM calculations in this region. We will display the current status of the NCSM and, with phenomenological adjustments, also demonstrate how far we still must go before making ab-initio predictions of fundamental processes such as  $0\nu\beta\beta$  decay rates. Due to the significant gap between present ab-initio NCSM theory and the best fit results, we defer evaluations of decay rates to later efforts.

To distinguish the ab-initio NCSM from the model with additive phenomenological terms, we refer to the latter as simply the "no-core shell model" or "NCSM" without the "ab-initio" adjective.

The main ingredients of our approach are the following:

- 1) We adopt the NCSM approach and approximate the full  $H_{eff}$  with a two-body cluster truncation. In solving the  $A = 48$  systems, all nucleons are treated with the same two-body Hamiltonian derived from a realistic NN interaction including Coulomb interaction between proton pairs. There are no single particle energies

involved and the eigenenergies are the total binding energies. We explore a very limited range of  $\hbar\Omega$ , around  $40/A^{1/3} = 11\text{MeV}$  and we limit the model space to  $1\hbar\Omega$  excitations.

2) We work in a neutron-proton basis so full isospin mixing is allowed including isospin mixing arising from the bare NN interaction and those induced within Heff itself.

3) For 48-Ca we evaluate both the positive ( $0\hbar\Omega$ ) and negative parity ( $1\hbar\Omega$ ) spectra.

4) Our spectra are free of spurious center of mass motion effects.

5) We provide a baseline for further improvements to Heff such as the inclusion of real and effective three-body forces.

Of course the present work has a significant drawback. Due to the limited model space and/or the neglect of effective many-body interactions, as well as the neglect of genuine three-body interactions, we must resort to additive phenomenological terms to obtain a good description of selected experimental data. The dependence on the parameters introduced, including the basis space parameters  $N_{max}$  and  $\hbar\Omega$ , as well as dependence on the forms and strengths of the additive potential terms, severely limit the predictive power of our present approach. On the other hand, the good descriptions achieved with our initial choice of additive terms provides insight into the shortcomings of our current Heff in the  $0\hbar\Omega$  and  $1\hbar\Omega$  model spaces.

The paper is organized as follows. In section 2 we give a brief description of the NCSM formalism. In section 3 we present our results and analysis and section 4 is devoted to conclusions and perspectives.

## 2 No core shell model (NCSM) formalism

In order to take a step towards increased predictive power, we adapt the recently derived ab-initio NCSM as we will briefly outline here. However, due to computational limitations translating into model space limitations, we expect and find that the spectroscopic results differ significantly from experiment. Since previous investigations summarized above have indicated the importance of obtaining good spectroscopic descriptions in order to minimize uncertainties in predictions of key experimental observables, we will introduce additive phenomenological corrections sufficient to fit experimental spectra.

## 2.1 Basic NCSM and Effective Hamiltonian

The NCSM [16]-[21] is based on an effective Hamiltonian derived from realistic “bare” interactions and acting within a finite Hilbert space. All  $A$ -nucleons are treated on an equal footing. The approach is demonstrably convergent to the exact result of the full (infinite) Hilbert space.

Initial investigations used two-body interactions [16] based on a G-matrix approach. Later, we implemented the Lee-Suzuki-Okamoto procedure [22, 23] to derive two-body and three-body effective interactions based on realistic NN and NNN interactions.

For pedagogical purposes, we outline the NCSM approach with NN interactions alone and point the reader to the literature for the extensions to include NNN interactions. We begin with the purely intrinsic Hamiltonian for the  $A$ -nucleon system, i.e.,

$$H_A = T_{\text{rel}} + \mathcal{V} = \frac{1}{A} \sum_{i < j}^A \frac{(\vec{p}_i - \vec{p}_j)^2}{2m} + \sum_{i < j=1}^A V_N(\vec{r}_i - \vec{r}_j), \quad (1)$$

where  $m$  is the nucleon mass and  $V_N(\vec{r}_i - \vec{r}_j)$ , the NN interaction, with both strong and electromagnetic components. Note the absence of a phenomenological single-particle potential. We may use either coordinate-space NN potentials, such as the Argonne potentials [24] or momentum-space dependent NN potentials, such as the CD-Bonn [25] which we select for the present investigation.

Next, we add the center-of-mass HO Hamiltonian to the Hamiltonian (1)  $H_{\text{CM}} = T_{\text{CM}} + U_{\text{CM}}$ , where  $U_{\text{CM}} = \frac{1}{2} Am\Omega^2 \vec{R}^2$ ,  $\vec{R} = \frac{1}{A} \sum_{i=1}^A \vec{r}_i$ . In the full Hilbert space the added  $H_{\text{CM}}$  term has no influence on the intrinsic properties. However, when we introduce our cluster approximation below, the added  $H_{\text{CM}}$  term facilitates convergence to exact results with increasing basis size. The modified Hamiltonian, with a pseudo-dependence on the HO frequency  $\Omega$ , can be cast into the form

$$H_A^\Omega = H_A + H_{\text{CM}} = \sum_{i=1}^A \left[ \frac{\vec{p}_i^2}{2m} + \frac{1}{2} m\Omega^2 \vec{r}_i^2 \right] + \sum_{i < j=1}^A \left[ V_N(\vec{r}_i - \vec{r}_j) - \frac{m\Omega^2}{2A} (\vec{r}_i - \vec{r}_j)^2 \right]. \quad (2)$$

In the spirit of Da Providencia and Shakin [26] and Lee, Suzuki and Okamoto [22, 23], we introduce a unitary transformation, which is able to accommodate the short-range two-body correlations in a nucleus, by choosing an antihermitian operator  $S$ , acting only on intrinsic coordinates, such that

$$\mathcal{H} = e^{-S} H_A^\Omega e^S. \quad (3)$$

In our approach,  $S$  is determined by the requirements that  $\mathcal{H}$  and  $H_A^\Omega$  have the same symmetries and eigenspectra over the subspace  $\mathcal{K}$  of the full Hilbert space. In general, both  $S$  and the transformed Hamiltonian are  $A$ -body operators. Our simplest, non-trivial approximation to  $\mathcal{H}$  is to develop a two-body ( $a = 2$ ) effective Hamiltonian, where the upper bound of the summations “ $A$ ” is replaced by “ $a$ ”, but the coefficients remain unchanged. The next improvement is to develop a three-body effective Hamiltonian, ( $a = 3$ ). This approach consists then of an approximation to a particular level of clustering with  $a \leq A$ .

$$\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(a)} = \sum_{i=1}^A h_i + \frac{\binom{A}{2}}{\binom{A}{a} \binom{a}{2}} \sum_{i_1 < i_2 < \dots < i_a}^A \tilde{V}_{i_1 i_2 \dots i_a}, \quad (4)$$

with

$$\tilde{V}_{12\dots a} = e^{-S^{(a)}} H_a^\Omega e^{S^{(a)}} - \sum_{i=1}^a h_i, \quad (5)$$

and  $S^{(a)}$  is an  $a$ -body operator;  $H_a^\Omega = h_1 + h_2 + h_3 + \dots + h_a + V_a$ , and  $V_a = \sum_{i < j}^a V_{ij}$ . Note that there is no sum over “ $a$ ” in Eq. (4) so there is no coupling between clusters in this approach. Also, we adopt the HO basis states that are eigenstates of the one-body Hamiltonian  $\sum_{i=1}^A h_i$ .

If the full Hilbert space is divided into a finite model space (“P-space”) and a complementary infinite space (“Q-space”), using the projectors  $P$  and  $Q$  with  $P + Q = 1$ , it is possible to determine the transformation operator  $S_a$  from the decoupling condition

$$Q_a e^{-S^{(a)}} H_a^\Omega e^{S^{(a)}} P_a = 0, \quad (6)$$

and the simultaneous restrictions  $P_a S^{(a)} P_a = Q_a S^{(a)} Q_a = 0$ . Note that  $a$ -nucleon-state projectors ( $P_a, Q_a$ ) appear in Eq. (6). Their definitions follow from the definitions of the  $A$ -nucleon projectors  $P, Q$ . The unitary transformation and decoupling condition, introduced by Suzuki and Okamoto and referred to as the unitary-model-operator approach (UMOA) [27], has a solution that can be expressed in the following form

$$S^{(a)} = \operatorname{arctanh}(\omega - \omega^\dagger), \quad (7)$$

with the operator  $\omega$  satisfying  $\omega = Q_a \omega P_a$ , and solving its own decoupling equation,

$$Q_a e^{-\omega} H_a^\Omega e^{\omega} P_a = 0. \quad (8)$$

Let us also note that  $\bar{H}_{a\text{-eff}} = P_a e^{-S^{(a)}} H_a^\Omega e^{S^{(a)}} P_a$  leads to the relation

$$\bar{H}_{a\text{-eff}} = (P_a + \omega^\dagger \omega)^{-1/2} (P_a + P_a \omega^\dagger Q_a) H_a^\Omega (Q_a \omega P_a + P_a) (P_a + \omega^\dagger \omega)^{-1/2}. \quad (9)$$

Given the eigensolutions,  $H_a^\Omega|k\rangle = E_k|k\rangle$ , in the infinite Hilbert space for the cluster, then the operator  $\omega$  can be determined from

$$\langle\alpha_Q|\omega|\alpha_P\rangle = \sum_{k\in\mathcal{K}}\langle\alpha_Q|k\rangle\langle\tilde{k}|\alpha_P\rangle, \quad (10)$$

where we denote by tilde the inverted matrix of  $\langle\alpha_P|k\rangle$ , i.e.,  $\sum_{\alpha_P}\langle\tilde{k}|\alpha_P\rangle\langle\alpha_P|k'\rangle = \delta_{k,k'}$  and  $\sum_k\langle\alpha'_P|\tilde{k}\rangle\langle k|\alpha_P\rangle = \delta_{\alpha'_P,\alpha_P}$ , for  $k, k' \in \mathcal{K}$ . In the relation (10),  $|\alpha_P\rangle$  and  $|\alpha_Q\rangle$  are the model-space and the Q-space basis states, respectively, and  $\mathcal{K}$  denotes a set of  $d_P$  eigenstates, whose properties are reproduced in the model space, with  $d_P$  equal to the dimension of the model space.

In practice, the exact (to numerical precision) solutions for the  $a=2$  cluster are obtained in basis spaces of several hundred  $\hbar\Omega$  in each relative motion NN channel.

We note that in the limit  $a \rightarrow A$ , we obtain the exact solutions for  $d_P$  states of the full problem for any finite basis space, with flexibility for the choice of physical states subject to certain conditions [28].

We define our P-space to consist of all A-particle configurations in the oscillator basis with oscillator energy less than or equal some cutoff value,  $N_m = N_{min} + N_{max}$ , where  $N$  is the sum of  $2n + l$  values of the occupied single particle states in the configuration.  $N_{min}$  is the minimum value required by the Pauli principle and equals 84 for these  $A = 48$  nuclei. Our P-spaces are equally described by the excitations allowed through  $N_{max}$  which begins with 0. The cluster space,  $P_2$ , is defined by the range of 2-body states encountered in the P-space.

Due to our cluster approximation a dependence of our results on  $N_{max}$  and on  $\hbar\Omega$  arises. For a fixed cluster size, the smaller the basis space, the larger the dependence on  $\hbar\Omega$ . The residual  $N_{max}$  and  $\hbar\Omega$  dependences can be used to infer the uncertainty in our results arising from the neglect of effective many-body interactions.

In light nuclei, the strategy has been to evaluate  $H_{eff}$  for each model space leading to a separate  $H_{eff}$  for positive and negative parity states. As one proceeds to heavier systems we reason that a better strategy is to use the same  $H_{eff}$  for both positive and negative parities e.g. use the  $1\hbar\Omega$   $H_{eff}$  in both the  $0\hbar\Omega$  and  $1\hbar\Omega$  model spaces. The logic for the revised strategy stems from two considerations: (1) either strategy will converge to the exact result in sufficiently large basis spaces; and (2) for adjoining spaces in heavier systems, the predominant sets of pairwise interactions are in the same configurations with just one pair at a time shifting to the larger space. Hence, the bulk of the binding should not be altered in proceeding from a

$0\hbar\Omega$  to a  $1\hbar\Omega$  model space in  $A=48$ , suggesting the same  $H_{eff}$  is preferred. For small model spaces, such as those investigated here, the revised strategy improves the splitting between positive and negative parity states for the physical reason just mentioned.

One simplification of this revised strategy is that  $H_{eff}$  is required only for every other increment in the basis space, such as  $1\hbar\Omega$ ,  $3\hbar\Omega$ ,  $5\hbar\Omega$ , etc., to evaluate the converging sequence.

In order to construct the operator  $\omega$  (10) we need to select the set of eigenvectors  $\mathcal{K}$ . We select the lowest states obtained in each two-body channel. It turns out that these states also have the largest overlap with the model space for the range of  $\hbar\Omega$  we have investigated and the P-spaces we select.

We input the effective Hamiltonian, now consisting of a relative two-body operator and the pure  $H_{CM}$  term introduced earlier, into an m-scheme Lanczos diagonalization process to obtain the P-space eigenvalues and eigenvectors [29]. At this stage we also add the term  $H_{CM}$  again with a large positive coefficient to separate the physically interesting states with  $0s$  CM motion from those with excited CM motion. We retain only the eigenstates with pure  $0s$  CM motion when evaluating observables. All observables that are expressible as functions of relative coordinates, such as the rms radius and radial densities, are then evaluated free of CM motion effects.

In the case of the  $0\hbar\Omega$  model space for  $^{48}Ca$ , the neutrons occupy part of the pf shell while the protons fill the sd shell. Now, for the  $1\hbar\Omega$  model space that we adopt for  $^{48}Ca$ , we take proton pairs in the Q-space as those with relative harmonic oscillator states having  $(2n + l) \geq 6$ . Similarly, we take neutron pairs in the  $1\hbar\Omega$  Q-space having  $(2n + l) \geq 8$ . For the neutron-proton pairs we take the Heff with pairs in the Q-space of  $(2n + l) \geq 7$ . This defines the effective Hamiltonian for both positive and negative parity states.

It is important to note that we retain this same Hamiltonian for all the  $A = 48$  results presented here even though some have protons in the pf shell. In so doing, we recognize that these are additional approximations that we expect to become less severe in future efforts with enlarged P-spaces.

Since we have chosen separate P-spaces for the neutrons and the protons, we felt the need to confirm that our treatment of the spurious CM motion remains valid. We tested this with the  $^{48}Ca$  positive parity spectrum in the following way. We lowered the Lagrange multiplier of the  $H_{CM}$  term from our conventional value

of 10.0 to a value of 2.0. In the past this was more than sufficient to reveal any deficiencies in our treatment of CM motion. In the present case this means that, since  $\hbar\Omega = 10\text{MeV}$ , our lowest spurious states are around 20 MeV of excitation in  $^{48}\text{Ca}$  (assuming the CM motion is treated correctly). This is about as low as we can safely go for a test since we still have significant separation of the spurious from the non-spurious states.

The test showed that six of the lowest 15 eigenvalues changed by 1 keV, a change in the 6th significant figure, while the other 9 were unchanged at this precision, indicating at most a change in the 7th significant figure. This numerically demonstrates that the CM motion in the NCSM is accurately treated by the constraint method even when neutrons and protons occupy different shells, as long as the model space is defined with a many-body cutoff as we have implemented.

The m-scheme basis dimensionalities are (12022, 139046, and 634744) for ( $^{48}\text{Ca}$ ,  $^{48}\text{Sc}$ , and  $^{48}\text{Ti}$ ) respectively in the  $0\hbar\Omega$  model spaces, and 2921360 for  $^{48}\text{Ca}$  in the  $1\hbar\Omega$  model space. By way of reference,  $^{48}\text{Ca}$  in the  $2\hbar\Omega$  model space produces an m-scheme matrix dimension of 214664244.

We close our outline on the theoretical framework with the observation that all observables require the same transformation as implemented on the Hamiltonian. To date, we have found rather small effects on the rms radius operator when we transformed it to a P-space effective rms operator at the  $a=2$  cluster level [20]. On the other hand, substantial renormalization was observed for the kinetic energy operator when using the  $a = 2$  transformation to evaluate its expectation value [30].

## 2.2 Phenomenological adjustments

To obtain NCSM spectroscopies fit to the data for these  $A = 48$  nuclei by means of additive phenomenological potentials is a major undertaking. Hence, we investigate here minimal approaches to modifying the theoretical Heff to improve selected spectroscopic properties. We consider this as a baseline effort for future investigations in larger model spaces where we believe there will be a reduced need for phenomenological terms.

Our overall fitting strategy is to emphasize the total binding energy and the lowest lying excited states.

Inspired by successful modifications found in Ref. [7], we first investigate whether a phenomenological S-wave or monopole interaction supplies the main missing in-

gradient from our NCSM realistic effective two-body Hamiltonians. We chose to add simple  $T = 0$  and  $T = 1$  delta functions and we found that they can produce greatly improved properties. However, we find it necessary to adjust the  $T = 0$  and  $T = 1$  strengths for each nucleus to obtain the good agreement with experimental properties. Thus, we conclude that, with this approach, six parameters are needed to obtain reasonable results for the binding energies and the positive parity spectra of the three nuclei we address. However, the spectrum of  $^{48}Sc$  is still rather poor.

In the hopes of obtaining a single NCSM Hamiltonian for the binding energies and spectra of these three nuclei, we then explored the utility of two-body central plus tensor forces added to the ab-initio  $H_{eff}$ . We achieve a reasonable description of a small set of the targeted properties in these three nuclei by fitting the strengths and ranges of these three terms.

The specific forms of the finite range central and tensor potentials we found acceptable are as follows:

$$V(r) = V_0 \exp(-(r/R)^2)/r^2 + V_1 \exp(-(r/R)^2)/r^2 + V_t S_{12}/r^3 \quad (11)$$

where the central strengths,  $V_0 = -14.40 \text{ MeV} - fm^2$  and  $V_1 = -22.61 \text{ MeV} - fm^2$  with  $R = 1.5 fm$ , the tensor strength  $V_t = -52.22 \text{ MeV} - fm^3$ , and  $S_{12}$  is the conventional tensor operator.

### 3 Results and Discussion

We begin with a survey of the ground state eigenenergies of  $A = 48$  nuclei presented in Fig. 1. The experimental values and extrapolations based on systematics [31] are presented as square points and portray the valley of stability with  $^{48}Ti$  being the most stable  $A = 48$  system. The upper set of results (round dots) are those obtained with the ab-initio NCSM as outlined above with  $\hbar\Omega = 10 \text{ MeV}$ , a typical choice for this region. Note that the trend of the even-even and odd-odd nuclear binding energies matches reasonably well with experiment except that theory consistently underbinds by about 20 MeV (0.4 MeV/nucleon). In other words, except for this underbinding, the ab-initio NCSM already predicts some subtle features of the valley of stability.

While all even-even nuclei obtained here in the ab-initio NCSM have the correct  $J^\pi = 0^+$  ground state spin and parity, the odd-odd nuclei generally have the incorrect ground state spin.

The point proton (neutron) rms radii are 3.51, 3.55, and 3.59 fm (3.75, 3.73, and 3.71 fm) for  $^{48}\text{Ca}$ ,  $^{48}\text{Sc}$  and  $^{48}\text{Ti}$  respectively, when evaluated with the bare operator in the intrinsic coordinate system. Of course, due to the limited model space, these results are insensitive to configuration mixing and are controlled by the choice of  $\hbar\Omega$ .

Increasing  $\hbar\Omega$  leads to increased binding (and decreased rms radii) in this application of the ab-initio NCSM ( $\hbar\Omega = 10.5\text{MeV}$  would produce a good fit to the binding alone) but fails to improve the errors in ground state spins and other deficiencies in the spectral properties described below in more detail.

The overall binding energy picture is considerably improved with the phenomenological additions described above. These additive terms were fit by hand to the ground state energies of  $^{48}\text{Ca}$ ,  $^{48}\text{Sc}$  and  $^{48}\text{Ti}$  as well as the first excited positive and negative parity states in  $^{48}\text{Ca}$ . This limited amount of data under-constrains the fit and alternative parameterizations of the additive terms would yield equivalent fits to these limited data. Our approach here was to cease fitting when the first successful fit was obtained. Hence, all other properties of these  $A = 48$  nuclei, including the ground state energies of the remaining 5 nuclei presented in Fig. 1, constitute predictions of this model. With the additive terms, the ground state spins and parities for the eight nuclei evaluated now agree with experiment, where available.

We again stress that the ab-initio NCSM Hamiltonian and the fit Hamiltonians are pure 2-body Hamiltonians describing the interactions of all  $A = 48$  nucleons. There is no division into valence and core subsystems, no explicit mean field and no single-particle energies. In addition, all results that we present are free of effects from spurious CM motion. As mentioned above, we distinguish the ab-initio NCSM from the model with additive phenomenological terms by referring to the latter as simply the "no-core shell model" or "NCSM" without the "ab-initio" adjective. For convenience in labelling figures and tables, we employ  $H_{eff}$  or "CD-Bonn" for the former and "CD-Bonn + 3 terms" for the latter.

Fig. 2 presents the  $0\hbar\Omega$  model space results for  $^{48}\text{Ca}$  with the CD-Bonn effective Hamiltonian,  $[H_{eff}]$ , at three values of the basis space parameter,  $\hbar\Omega = 10(\text{twocases}), 11, \text{ and } 12$  MeV. The first column presents the experimental ground state and first two excited states. For  $\hbar\Omega = 10$  MeV, we present results for the 1995 version of CD-Bonn (second column in the figure labelled "CDB") and for the 2000 version (third column labelled "CDB2K") [25] in order to display the minor differences in the spectra from these two potentials.

The main impression from Fig. 2 is that the spectra in  $^{48}\text{Ca}$  are severely compressed relative to the experimental spreading. Inspecting the corresponding ground state wavefunctions reveals an absence of the expected dominance by the  $[0f_{7/2}]^8$  neutron configuration. Instead, the  $1p_{3/2}$  neutron state is significantly populated. We conclude that the expected energy spacing between the  $0f_{7/2}$  and the  $1p_{3/2}$  state is not supported by the ab-initio NCSM in such a small model space. This means there is insufficient spin-orbit splitting.

Here, we can remark that a recent mean-field study with similarly derived  $H_{eff}$  showed some deficiency in the spin-orbit splitting for  $^{16}\text{O}$  in smaller model spaces when compared with experiment [32]. Similarly, a detailed study of  $^{12}\text{C}$  neutrino scattering and magnetic transition observables revealed that the  $a = 2$  cluster approximation underpredicts the spin-orbit splitting needed to explain these data [33]. This deficiency appears to be solved by the addition of true three-nucleon forces which is beyond the scope of our present efforts. Detailed investigations of the binding energies and spectroscopy of p-shell nuclei have provided strong evidence of the need for true three-nucleon forces when local realistic NN interactions, such as CD-Bonn, are employed [34]. This need is manifest significantly in the spin-orbit properties.

We do not display the theoretical negative parity states in this case but we comment that they are similarly compressed relative to the experimental spreading. Furthermore, the lowest negative parity state appears at a rather high excitation energy. This feature is reminiscent of the results obtained for  $^{12}\text{C}$  where the negative parity spectra appeared high relative to the positive parity spectra for model spaces up through  $3\hbar\Omega$  [20].

Note, however, that when we adopt the new strategy discussed above, using the  $H_{eff}$  of the  $1\hbar\Omega$  model space for both the positive and negative parity states at  $\hbar\Omega = 10\text{MeV}$ , the relative spacings of the states within a given parity are essentially unchanged while the lowest negative parity excitation above the ground state is now at 6.9 MeV of excitation, a major improvement. This will be discussed shortly along with other results in Fig. 3.

Figs. 3 - 5 display, in column 2 labelled "CDB + 3 terms", the spectra for these  $A = 48$  nuclei resulting from our best fit Hamiltonian as described in the previous section. The resulting BE/A were presented in Fig. 1 for eight  $A = 48$  nuclei with this same Hamiltonian.

In each of the Figs. 3 - 5, we display the experimental spectrum in column 1

and the results of Ref. [7] in column 3.

As seen in Fig. 3, our fit yields a good description of the low-lying positive and negative parity states of  $^{48}\text{Ca}$ . In particular, we observe that the calculated first excited  $0^+$ , which was not involved in the fit, appears to be rather close to the experimental first excited  $0^+$ . On the other hand, we are missing another low-lying excited  $0^+$ . This may indicate that the intruder state inferred from the results presented in Ref. [7] is significantly mixed between the two low-lying excited  $0^+$  states in  $^{48}\text{Ca}$ .

The reasonable agreement of our  $^{48}\text{Ca}$  negative parity spectrum with experiment is significant considering that only the position of the first  $3^-$  state was involved in our fit. It is also significant since the negative parity spectrum is sensitive to a set of 2-body matrix elements that is considerably larger than the set controlling the positive parity spectrum. In particular, we are sensitive to matrix elements involving excitations from the sd states to the pf states as well as from the pf states to the sdg states.

Turning now to  $^{48}\text{Sc}$  shown in Fig. 4 we obtain one of the more important signatures of the success of the 3 term fit to these nuclei. Column 2 of Fig. 4 shows that we now obtain the correct ground state spin and a reasonable low-lying positive parity spectrum. Our spectrum is slightly more spread than the results of Caurier, et al., [7].

Our plan to apply these results for  $\beta\beta$  processes, leads us to comment on the  $1^+$  states in  $^{48}\text{Sc}$ . There are eight established  $1^+$  states below 5.1 MeV of excitation and our 3 term fit spectrum provides only five  $1^+$  states over the same span. Given our limited model space and the possibility of intruder states, we may expect additional states to appear when the model space is eventually enlarged. In the meantime, our beta transition strength function will be distributed over a more limited set of states in a way that will approximate the distribution among the more dense experimental spectrum of  $1^+$  states. Of course, we will include an even larger set of  $1^+$  states up to higher excitation energies when evaluating the double beta decay rate in a later effort.

Finally, we consider the case of  $^{46}\text{Ti}$  shown in Fig. 5. Here again, the low-lying positive parity spectrum from CDB + 3 terms is in reasonable agreement with experiment except that it is more spread. We note one particular deficiency - the  $0^+ - 2^+ - 4^+$  theoretical splitting is nearly that of a vibrator while the experimental spacings indicate a tendency toward rotational character. The fit of

Caurier, et al., [7] succeeds better in this collective property. It will be interesting to discover whether the rotational character emerges from our model as we proceed further into the open shell situation.

## 4 Conclusions and outlook

Our main goals have been to present the first NCSM results for  $^{48}\text{Ca}$ ,  $^{48}\text{Sc}$  and  $^{48}\text{Ti}$  with effective Hamiltonians derived directly from a realistic NN interaction and to investigate phenomenological improvements. The ab-initio results display the shortcomings of the limited model spaces presently available as well as possible shortcomings from neglecting three-body forces. We answer the question of whether the NCSM can be adjusted to obtain reasonable fits with additive phenomenological two-body potentials in the affirmative. In particular, we show that additive isospin-dependent central terms plus a tensor force can achieve accurate BE/A and reasonable spectra for these three systems. In addition, accurate BE/A are obtained for eight  $A = 48$  nuclei reproducing the experimental valley of stability. The net change of interaction energies is of the order of a few percent with the added phenomenological terms. More extensive searching could undoubtedly improve the fits to the low-lying spectra.

Future efforts motivated by the present results are many-fold. We intend to improve the ab-initio  $H_{eff}$  by extensions to the three-body cluster approximation and to include three-nucleon interactions. We foresee initial applications to  $\beta\beta$  decay, both the  $\nu\nu$  and  $0\nu$  decay channels, by first extending our calculations to the Gamow-Teller (+/-) strengths. In the near future, we will be able to address significantly larger basis states as well.

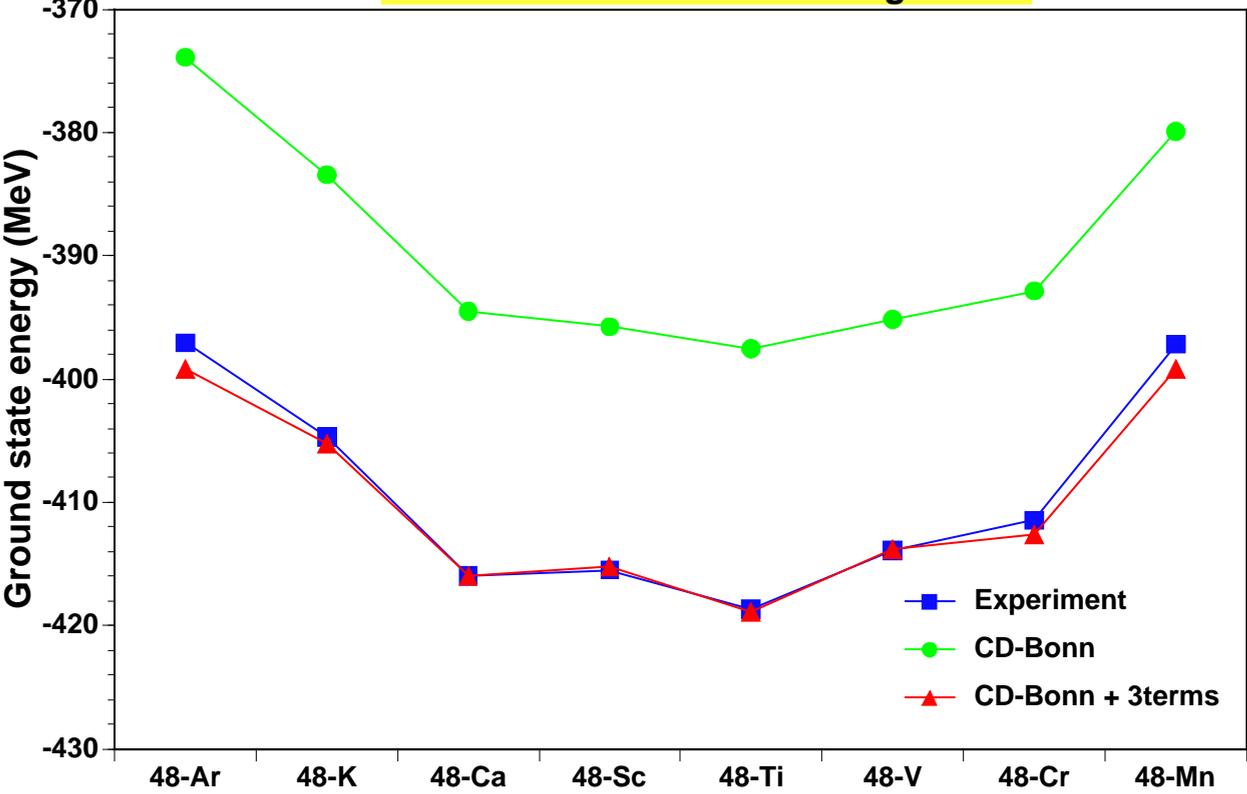
These future efforts represent major undertakings which we believe are warranted in light of the importance of retaining as much predictive power as possible when addressing  $\beta\beta$  decay.

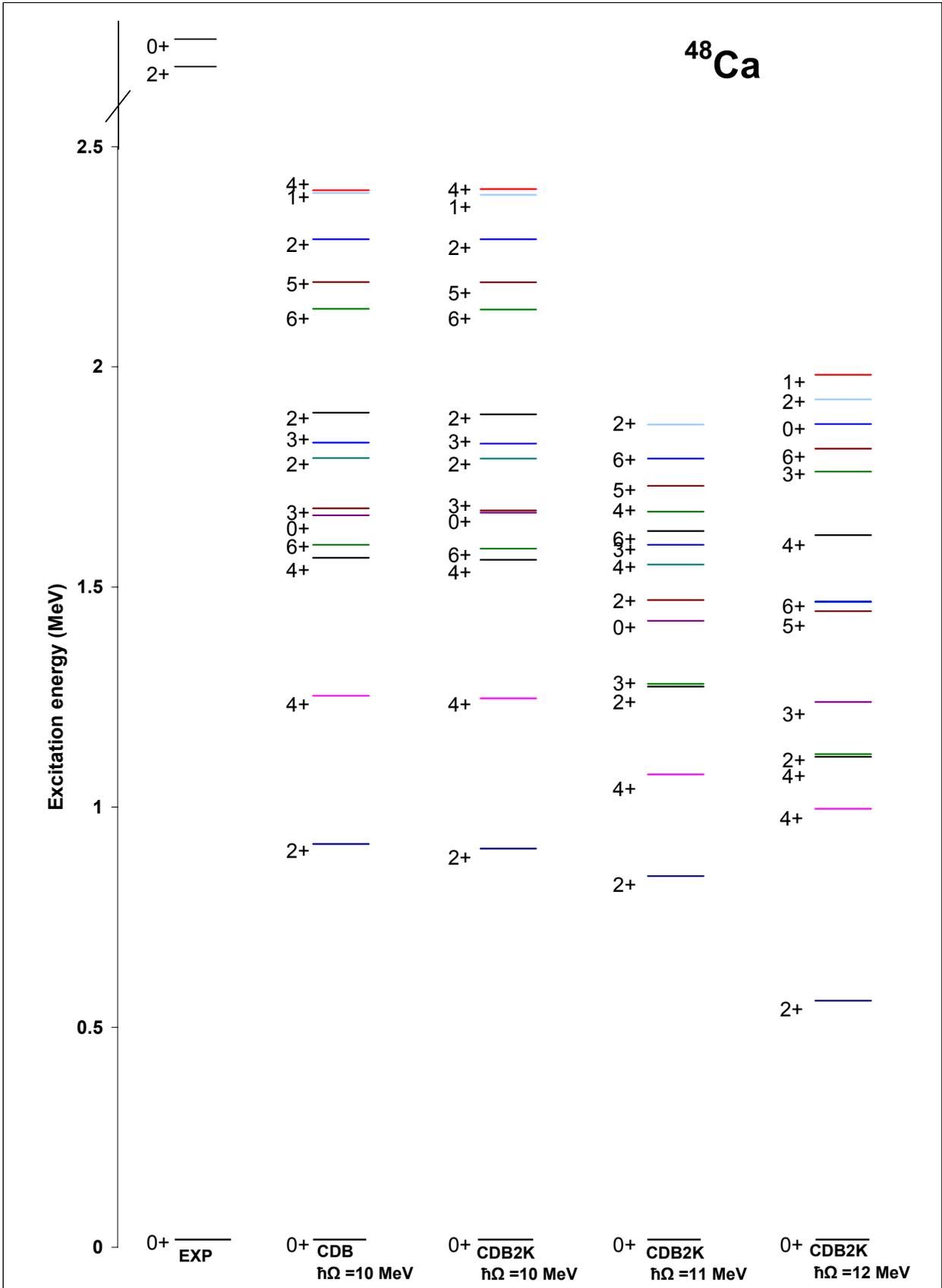
## 5 Acknowledgements

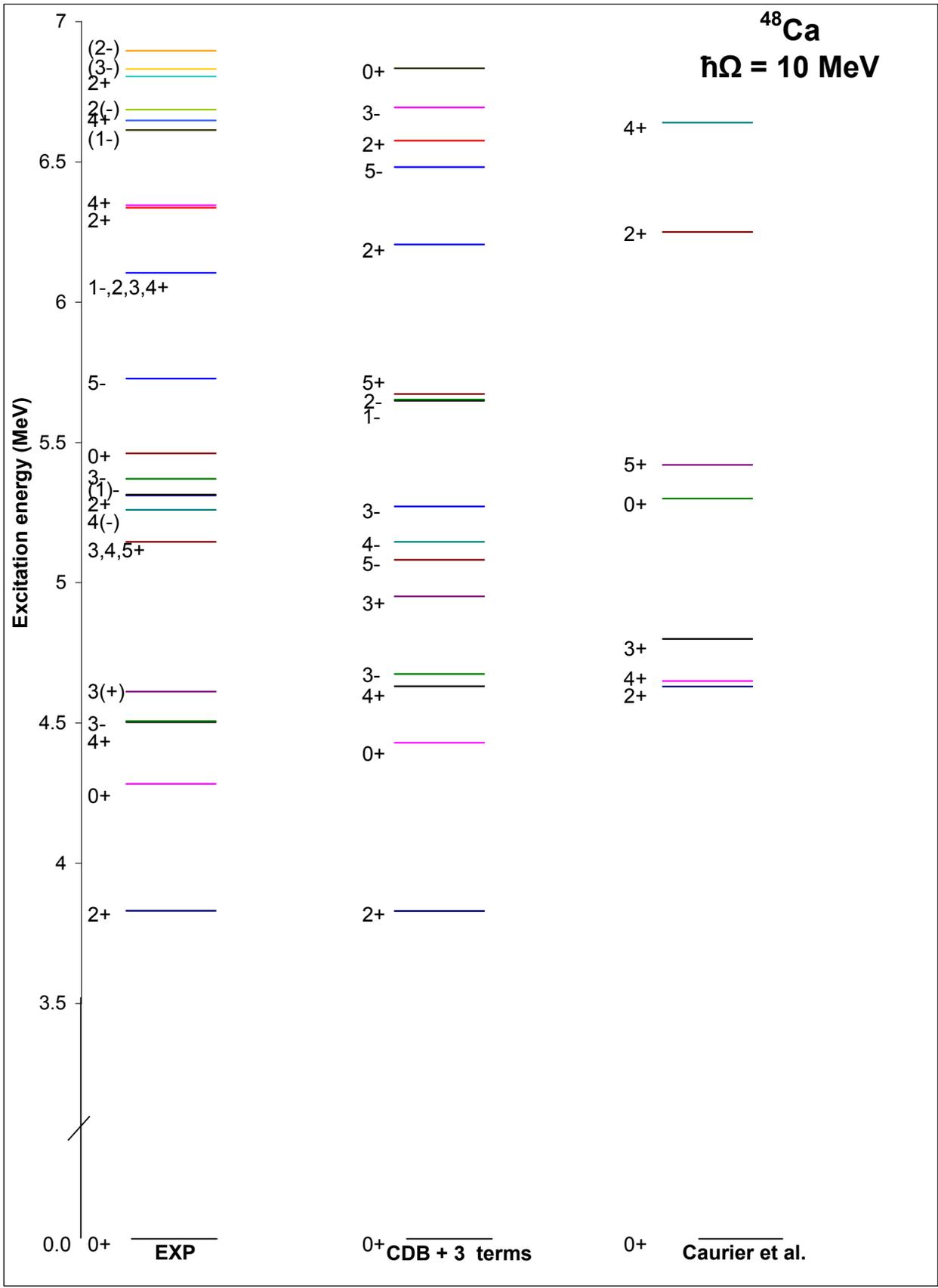
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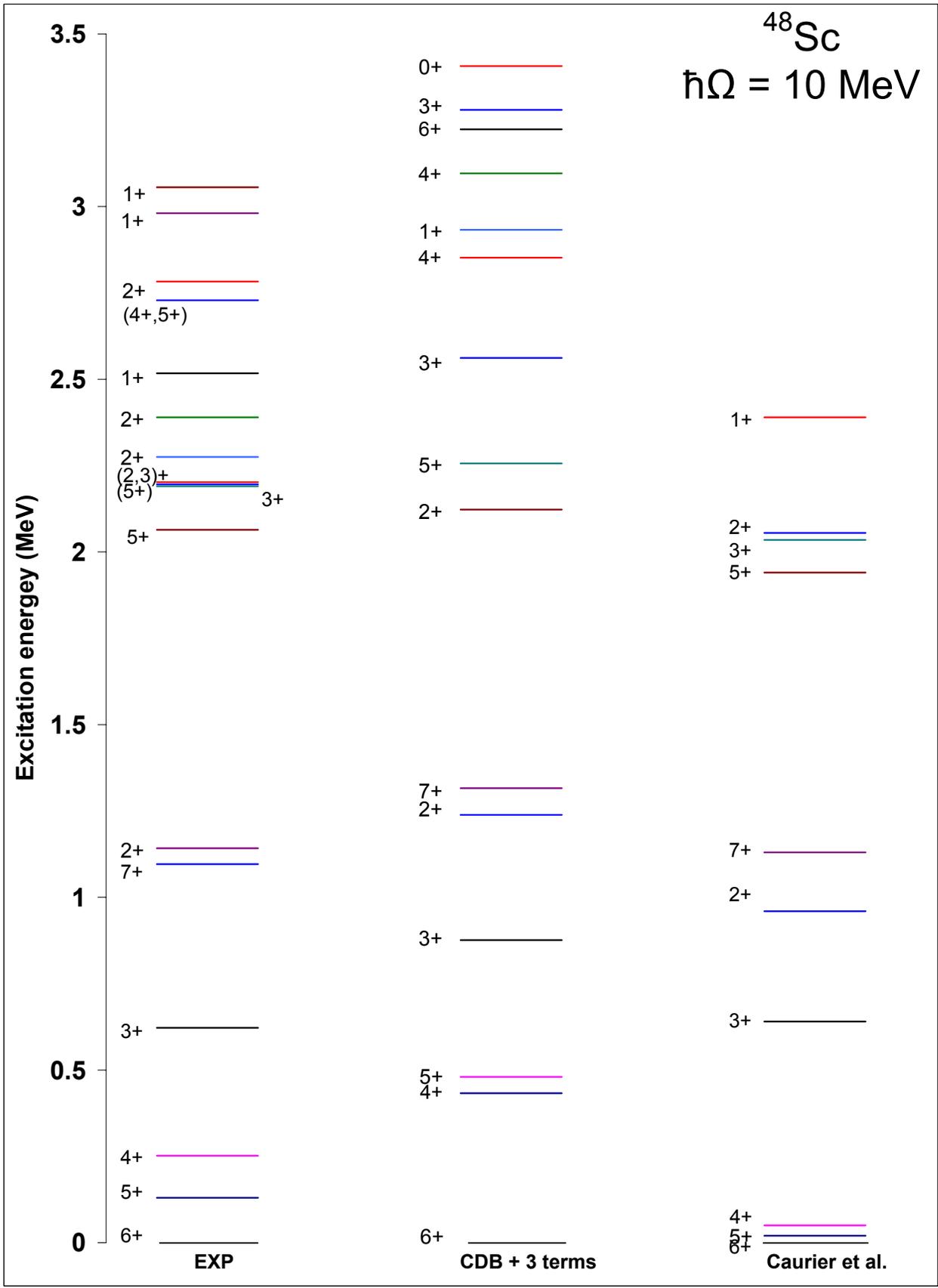
also supported in part by NSF grant INT0070789.

A=48 Ground State Energies

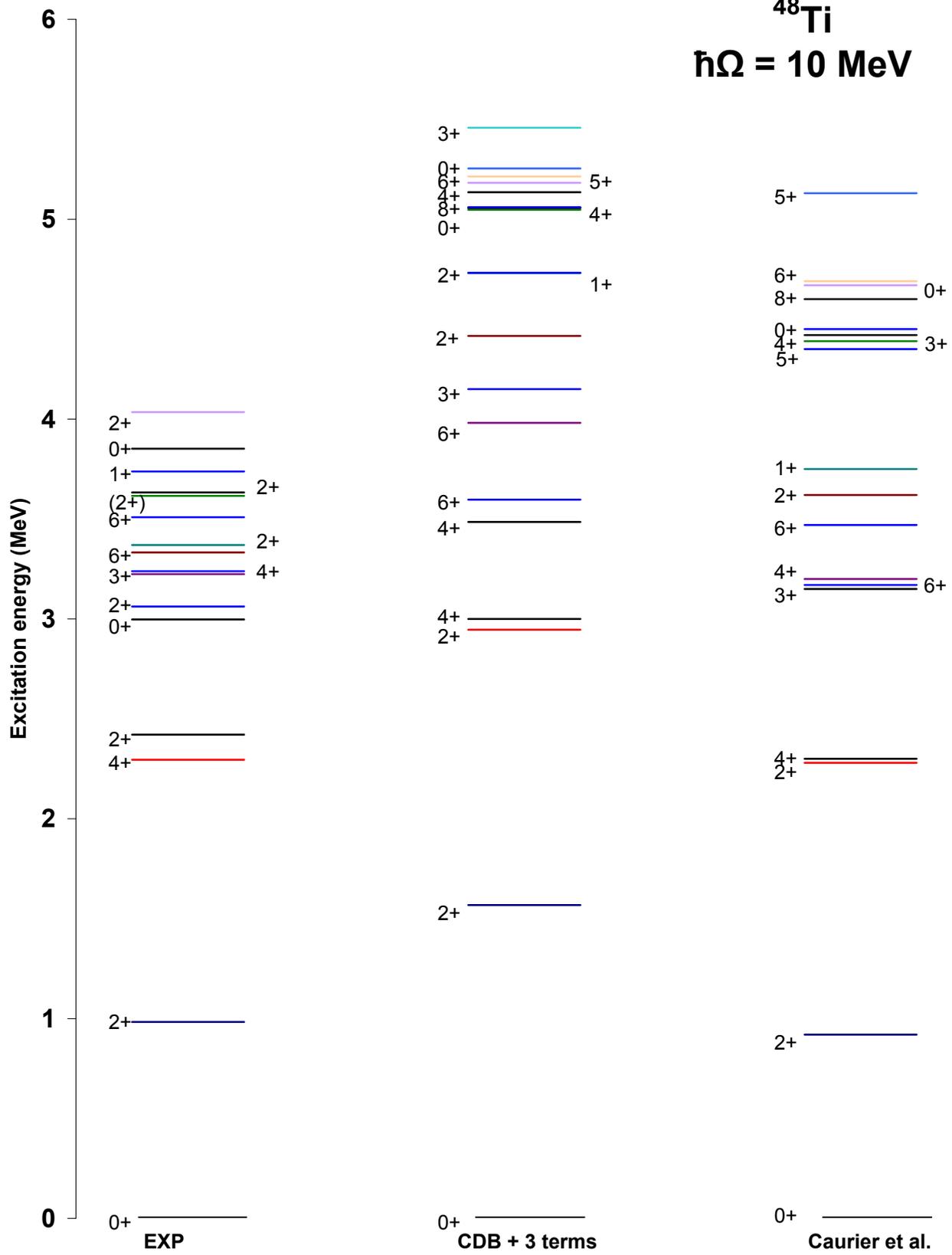








**$^{48}\text{Ti}$**   
 **$\hbar\Omega = 10 \text{ MeV}$**



## Figure and Table Captions

**Fig. 1:** (Color online) Ground state energies in MeV of  $A = 48$  nuclei. At the extremes of the valley of stability, these energies are determined by systematics and the label "experiment" is to be understood in that context. The ab-initio NCSM results labelled "CD-Bonn" are obtained with  $H_{eff}$  in the  $1\hbar\Omega$  model space,  $\hbar\Omega = 10$  MeV and isospin breaking in the P-space, as described in the text. The same  $H_{eff}$  with added gaussian central terms and a tensor force is used for the results labelled "CD-Bonn + 3 terms".

**Fig. 2:** (Color online)  $^{48}\text{Ca}$  positive parity excitation spectra (in MeV) for the CD Bonn (1995) (column 2) effective Hamiltonian (labelled "CDB") and the CD Bonn (2000) (columns 3-5) effective Hamiltonian (labelled "CDB2K") in the  $0\hbar\Omega$  harmonic oscillator basis space with  $\hbar\Omega = 10, 11,$  and  $12$  MeV compared with experiment (column 1). The CD-Bonn interactions are taken from Ref. [25].

**Fig. 3:** (Color online)  $^{48}\text{Ca}$  excitation spectra (in MeV) in the  $\hbar\Omega = 10$  MeV harmonic oscillator basis for the NCSM effective Hamiltonian plus additive corrections (CDB + 3 terms) compared with experiment and with the results of [7] (Caurier, et al.). Positive and negative parity spectra are shown in the first two columns and the strength parameters are given in the text.

**Fig. 4:** (Color online)  $^{48}\text{Sc}$  excitation spectra (in MeV) in the  $\hbar\Omega = 10$  MeV harmonic oscillator basis for the NCSM effective Hamiltonian plus additive corrections (CDB + 3 terms) compared with experiment and with the results of [7] (Caurier, et al.).

**Fig. 3:** (Color online)  $^{48}\text{Ti}$  excitation spectra (in MeV) in the  $\hbar\Omega = 10$  MeV harmonic oscillator basis for the NCSM effective Hamiltonian plus additive corrections (CDB + 3 terms) compared with experiment and with the results of [7] (Caurier, et al.).

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