Microscopic Calculations for Waiting-Point Nuclei*

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Abstract. Shell-model calculations for upper fp-shell nuclei using realistic interactions are reported. Valence nucleons beyond the N=28=Z core are considered to fill levels of the normal parity upper fp-shell and the unique parity configurations that consists either of the g9/2 level or the whole gds-shell. These two cases are handled within a standard M-scheme approach and an SU(3) picture, respectively. Results for low-lying energy spectra, single-particle occupancies and symmetry properties of the eigenstates are reported. Various truncations are considered that key on the number of nucleon pairs allowed to occupy the unique-parity space. The calculations demonstrate the importance of the unique-parity space to the structure of upper fp-shell nuclei.

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INTRODUCTION

The nuclear shell model has been applied successfully in a description of various aspects of nuclear structure, in large part because it is based on a minimum number of assumptions. Although direct diagonalization of the Hamiltonian matrix in the full Hilbert space would be desirable, the dimensionality of such a space is often too large to allow calculations of this type to be done. In the upper fp-shell, for example, we are unable to do this for some waiting-point nuclei like 68Se and 72Kr, which are important for the rp-process in nucleosynthesis [1]. Recently, in order to relax this restriction dramatically, various stochastic approaches, for instance, the Shell-Model Monte Carlo method [2], have been investigated. Alternatively, algebraic models using the symmetry properties of the systems under investigation have been developed [3].

The role of the intruder levels that penetrate down into lower-lying shells in atomic nuclei has been the focus of many studies and debates. These levels are found in heavy nuclei where the strong spin-orbit interaction destroys the underlying harmonic oscillator symmetry of the nuclear mean-field potential. They are important and have to be included in the model space if experimentally observed states of higher spin or opposite parity are to be described. In this contribution we report on calculations that consider the occupancy of these levels, their contribution to the nuclear deformation, and the role they play in the overall dynamics of the system.

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RESULTS FROM A REALISTIC INTERACTION

First, we carried out M-scheme shell-model calculations for the $^{64}$Ge and $^{68}$Se nuclei in the pf$_{5/2}$g$_{9/2}$ model space, assuming that the occupancy of the f$_{7/2}$ orbital was frozen [4]. This was done with different cuts of the full model space. The Hamiltonian we used was a G-matrix with a phenomenologically adjusted monopole part [5]. Also, a renormalized version of this interaction in the pf$_{5/2}$ space was introduced for describing beta decay [6]. Energy spectra for these two nuclei with both interactions are shown in Figure 1 where a comparison is made between those using the G-matrix and its renormalized version. Both describe the experimental data well.

![Figure 1](image_url) Figure 1. Energy spectra for $^{64}$Ge and $^{68}$Se. The basis that is used in the G-matrix calculation for $^{68}$Se is labeled by a sequence of three numbers, TPN, where T denotes the maximum total number of particles allowed in the intruder level and P and N denote the same for the protons and neutrons, respectively.

In Figure 2, results for the single-particle occupancies of states from the ground-state (g.s.) band of $^{64}$Ge are shown. The lower (solid) bars represent the occupation numbers in the pf$_{5/2}$g$_{9/2}$-space calculation from the many-particle basis states which have no particles in the intruder level while the upper (gray) bars refer to those that count the occupancy when the intruder level is active. It is obvious that including configurations with at most two particles (protons or neutrons) in the intruder is enough to describe them with the same success as when we use the full space. Similar behavior is observed in the beta and gamma bands of the nucleus.

Next, results for the pseudo-SU(3) symmetry in the states of different bands in $^{64}$Ge are shown in Figure 3 using the renormalized version of the interaction in the pf$_{5/2}$ space. The distribution of the second order Casimir operator $C_2$ of SU(3) in the g.s. and gamma bands indicates contribution of 50-60% for the leading SU(3) representation, which is an indication that the SU(3) symmetry is quite good. These observations suggest that the use of a symmetry-adapted, truncated set of basis states will give us better results for nuclei like $^{68}$Se but in such cases the intruder level will play an even more significant role.
RESULTS IN THE SU(3) MODEL WITH ACTIVE INTRUDER LEVELS

Until recently, SU(3) shell-model calculations – real SU(3) for light nuclei and pseudo-SU(3) for heavy – have been performed in either one (protons and neutrons filling the same shell, e.g. the ds-shell) or two (protons and neutrons filling different shells, e.g. for rare earth and actinide nuclei) spaces only. Results for low-energy spectra of even-even and odd-mass heavy deformed nuclei have been published over the years [7]. Their B(E2) transition strengths, including both scissors and twist modes and their fragmentation have been successfully but only qualitatively described [8].

This simplified picture has now been extended by explicitly taking intruder levels into account [9]. The model space consists of two parts for each type of particles – protons and neutrons – a normal parity pseudo-shell and a unique parity shell, composed of the higher orbitals with opposite parity. The many-particle basis states

\[ \{a_{\pi N}, a_{\pi U}\} \rho_\sigma (\lambda_\pi \mu_\pi), S_\pi; \{a_{\pi N}, a_{\pi U}\} \rho_\tau (\lambda_\pi \mu_\pi), S_\tau \rho(\lambda \mu)kL, S; JM \] (1)

are built as SU(3)-coupled states with a well-defined particle number and total angular momentum where \( a_{\pi \sigma} = \{N_{\pi \sigma}, f_{\pi \sigma}, \alpha_{\pi \sigma}(\lambda_{\pi \sigma} \mu_{\pi \sigma}), S_{\pi \sigma}\} \) are the basis-state labels for the four spaces in the model (\( \sigma \) stands for N or U and \( \tau \) - for \( \pi \) or \( \nu \)).

The Hamiltonian

\[ H = \sum_{\sigma, \tau} (H_{\pi \sigma} - GS_{\pi \sigma} S_{\pi \sigma}) - \frac{\chi}{2} Q Q - \sum_{\sigma \times \sigma'} GS_{\pi \sigma} S_{\pi \sigma'} \] (2)

contains spherical Nilsson single-particle energies.
Figure 3. Pseudo-SU(3) content of the low-lying states in different bands of $^{64}\text{Ge}$ using the renormalized version of the G-matrix interaction.

$$H_{sp}^{g_{\omega}} = \sum \hbar\omega\{\eta_i + 3/2\} - k\hbar\omega\{2l^\dagger_i s_i + \mu l^\dagger_i s_i\}$$

(3)

for protons and neutrons as well as the quadrupole-quadrupole and pairing interactions. The single-particle terms together with the proton and neutron pairing interaction mix the SU(3) basis states allowing for a realistic description of the energy spectra. Most of the parameters we use for $^{64}\text{Ge}(^{68}\text{Se})$ in the Hamiltonian were fixed from the systematics [10]:

$$\hbar\omega = 41/A^{1/3} = 10.25(10.04)$$

$$k_{\alpha\nu} = k_{\nu\alpha} = 0.0367(0.0367) \quad \mu_{\alpha\nu} = 0.0568(0.0568)$$

$$\chi = 22/A^{5/3} = 0.0214(0.0194) \quad G = 15/A = 0.234(0.221)$$

Those used for the single-particle terms in the pseudo spaces were taken to be consistent with single-particle energies in the G-matrix interaction used above:

$$k_{eN} = k_{\nu N} = 0.011(0.011) \quad \mu_{eN} = \mu_{\nu N} = 1.056(1.056)$$

The calculations were carried out using a set of basis states with (pseudo-)spin zero and one proton and neutron configurations. Since the most important configurations are those with highest spatial symmetry [11], we ignored all configurations that involve an odd number of particles in any of the four spaces and only consider the interplay between those having zero or two protons and/or two neutrons in the unique space. Then, from all the possible couplings we chose those irreducible representations with the highest value for the second order Casimir operator of (pseudo-)SU(3).

For our choice of coefficients in the Hamiltonian, the configurations with no particles in the unique space lie lowest and determine the structure of the lowest energy eigenstates. For $^{64}\text{Ge}$, the other two groups of basis states (with two and four
particles in the unique space) start to play a role above excitation energies of about 5 MeV. Also, since the spin-orbit interaction does not mix states from these groups it does not have any effect on the low-lying states. The mixing between configurations with different number of particles, although small, tracks back to pair scattering between the normal and unique parity spaces.

In Figure 4a one can see good agreement of the calculated results with experiment for the first states from the g.s and gamma bands of \(^{64}\text{Ge}\). For all the states calculated energies lie lower than the theoretical predictions with the G-matrix interaction. For \(^{68}\text{Se}\) (Figure 4b) the SU(3) results suggest a shifting in order between the second J=2 and first J=4 states. This agrees with the order found in experiment.

**REFERENCES**

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