N=Z and proton-rich nuclei in the Hartree-Fock mean field model with a separable nucleon-nucleon interaction

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Abstract

A new model for the effective two-body nucleon-nucleon interaction has been recently successful in calculation of ground state properties of spherical, doubly closed shell nuclei from ^{16}O to ^{208}Pb [1] and nuclear matter and neutron star properties [2]. The application of the density dependent finite range separable monopole (SMO) interaction has been now extended to axially symmetrical deformed nuclei. In this work we report on calculation of ground-state properties of even-even spherical and deformed $N = Z$ nuclei and proton-rich nuclei between the $N = Z$ and the proton-drip lines below ^{100}Sn. The results include total energy surfaces and deduced shapes, charge radii and two-proton separation energies.

1 Introduction

Nuclear ground state properties are still not fully understood despite enormous effort devoted to this problem over the last fifty years. Numerous models were developed to calculate observables, directly obtained from experiment, like ground state binding energies, nucleon density distributions, mean radii and electromagnetic multipole moments. Similarly, quantities without a unique experimental fingerprint, like shapes of nuclear ground states, derived from experimental data in a model dependent way, have been calculated in a variety of frameworks. There are two general points to mention. First, all these models have usually about 10 parameters which have to be fitted to experimental data. Correspondingly, calculated nuclear properties agree with experiment very well in regions not far from nuclei used to fit the models parameters. However, further away, in particular approaching the limits of nuclear existence as bound systems, where experimental data are scarce, we usually have as many different predictions of a value for a particular observable as is the number of different models we happen to choose. The second problem is that, closer to the region of nuclear stability, models based on very different physics, like for example relativistic, non-relativistic mean field models and the Finite-Range-Droplet-Model (FRDM), give the same or very close predictions for nuclear binding energies, radii and shapes. It follows that pursuing observables so insensitive to the physical basis of nuclear models will not improve our knowlegde of nuclear structure.

It is clear that it is desirable to develop novel approaches to nuclear modelling. One of the main problems is a poor understanding of nucleon correlations beyond the mean field. The SMO two-body interaction has been designed as suitable not only for adequate description of the mean-field but also for building of a converging perturbation series reflecting correlations in finite nuclei. Thus, for the first time in mean-field theories, SMO offers a way of calculating a fully correlated nuclear ground state beyond the mean field.

We have applied the SMO model to even-even N=Z and selected neutron-deficient nuclei with just the mean-field part. Differences found between theory and experiment will be used to test the perturbation approach in future work. In particular, N=Z nuclei may contain not only correlations between like nucleons but also between protons and neutrons as they occupy the same orbitals with expecting large overlap of the corresponding wave function. Development of stable shapes can be caused by small changes in the Fermi surface. Theoretical calculations (see e.g. [3, 4, 5, 6, 7, 8]) predict oblate and prolate shapes with large deformation in Ge, Se, Kr, Sr, Zr and Mo N=Z nuclei. In the recent calculation of ^{64}Ge, ^{68}Se, ^{72}Kr, ^{76}Sr, ^{80}Zr and ^{84}Mo by Yamagami et al. [9] the restriction to axial and reflection symmetrical shapes has been removed. As a consequence, some more exotic shapes (Y_{33}, Y_{32}) has been predicted. All these calculations assume that these nuclei have rigid shape with a sharp surface. However, the question arises whether the assumption of a rigid static deformation model is adequate in this region. Experimental data on excited states are scarce and hard to obtain. The existing evidence [10, 11, 12] seem to be going against this assumption. The experimental value of the ratio R=$E_{4_1^+}/E_{2_1^+}$ for ^{64}Ge, ^{72}Kr, ^{76}Sr and ^{80}Zr is far less than the 3.3 (see Table. 1), the value expected for a rigid rotor and indicates either gamma-soft or vibrational shapes.

The results reported in this work are based on the assumption of a rigid shape on N=Z nuclei. However, as stated above, this work is seen as a necessary basic test of the SMO model and the interaction used, with the prospect of further development.

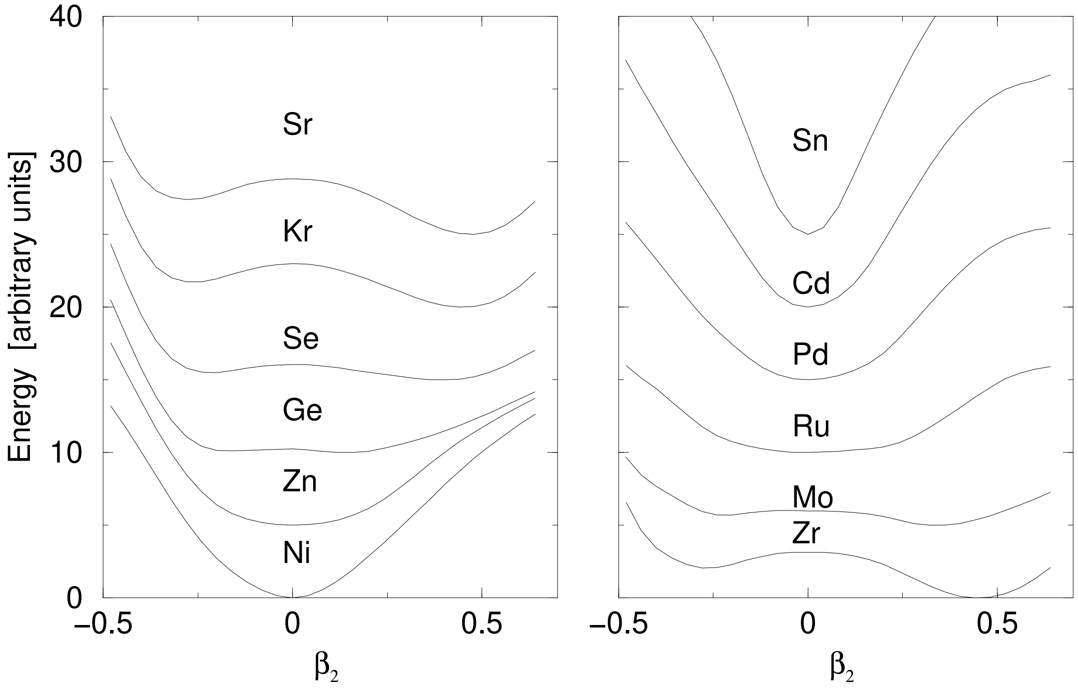

Figure 1: Calculated ground state total energy as a function of mass quadrupole deformation for $28 \leq Z \leq 50$ N=Z nuclei.

2 Hartree-Fock calculation using the monopole separable two-body interaction for axially deformed nuclei

2.1 The separable monopole interaction

This two-body interaction consists of two main parts (attractive and repulsive) which have the same mathematical form for the density and isospin dependence and differ only in the values of adjustable parameters. Having attractive and repulsive terms with different ranges is a common feature of density-dependent effective interactions and it is these terms which are responsible for most of the binding energy in finite nuclei and for the volume energy in nuclear matter.

Each term in the expression for the interaction is separable in the space coordinates of individual nucleons (and in isospin where applicable). This is the essential new property of this effective nucleon-nucleon interaction which makes it suitable for building a perturbation series in powers of the strength of the SMO interaction in order to include correlations in finite nuclei, beyond the mean field, with convergent results.

In coordinate space, the SMO is written as [1]

$$\begin{aligned} V(\vec{r}_1,\vec{r}_2) &= W_a f_a \rho^{\beta_a}(\vec{r}_1)\rho^{\beta_a}(\vec{r}_2)(1+a_a(t_1^+t_2^- + t_1^-t_2^+) + 4b_a t_{1z}t_{2z}) \\ &+ W_r f_r \rho^{\beta_r}(\vec{r}_1)\rho^{\beta_r}(\vec{r}_2)(1+a_r(t_1^+t_2^- + t_1^-t_2^+) + 4b_r t_{1z}t_{2z}) \\ &+ k\nabla_1^2\rho(\vec{r}_1)\nabla_2^2\rho(\vec{r}_2), \end{aligned} \tag{1}$$

where the function f_ξ is defined as

$$f_\xi = \left[\int \mathrm{d}^3\vec{r}\,\rho^{\alpha_\xi}(\vec{r})\right]^{-1}, \tag{2}$$

for subscripts $\xi = a, r$. Throughout this work, the three terms in (1) are referred to, in the order they appear in the above expression, as the attractive (a), repulsive (r) and derivative terms.

In addition, we use the standard form of the spin-orbit interaction from the Skyrme interaction;

$$W_{ls} = c(\nabla\rho\cdot\sigma)(\sigma\cdot\nabla) \tag{3}$$

which provides an energy

$$E_{ls} = -c\int d^3r\,\rho\nabla\mathcal{J} \tag{4}$$

and a contribution to the mean field of

$$U_{ls} = c\nabla\mathcal{J}. \tag{5}$$

$\mathcal{J}$ is the spin-orbit current -

$$\nabla\mathcal{J} = -i\sum_\alpha \psi_\alpha\nabla\times\sigma\psi_\alpha. \tag{6}$$

Note that in the case of spherical symmetry, the mean-field contribution is identical to the spin-orbit term in our calculation of spherical nuclei. In that calculation, a small contribution to the mean-field, which did not alter spin-orbit splittings was included due to rearrangement terms. Our constant c in the above equations corresponds to $t_4/2$ in the notation of Skyrme interactions. The Coulomb interaction is treated in the standard way and both direct and the exchange terms (in the Slater approximation) contribute to the total energy.

The computer code developed for calculation of properties of axially deformed nuclei in Hartree-Fock + BCS model with a Skyrme effective interaction, used recently for calculation of shape-coexistence effects in light and medium neutron rich nuclei [13], has been adapted for the separable monopole interaction (Eq. 1). Pairing had to be added to the model for correct treatment of open-shell nuclei. We use the BCS volume pairing with a cut-off [13]. This method is interesting because it treats pairing as a valence-particle effect and emphasizes the role of the nuclear surface in describing bulk properties of the nucleus, although it does not affect the overall quality of the effective nucleon-nucleon interaction. The set of parameters SMO2 [2] was used in the present work.

Table 1: Ground state quadrupole deformation parameter β_2 as calculated in different nuclear models.

A	Element	SMO2	RMF[6]	MSk7[8]	FRDM[4]	$E_{2_1^+}$[14]) [MeV]	R[a]	δ E_{tot} [MeV]
56	Ni	0.0	0.0	-0.12	0.0	2.7	1.45	
60	Zn	0.0	0.17	0.12	0.18	1.0	2.18	
64	Ge	0.12	0.22	-0.19	0.22	0.90	2.28	
		-0.16						0.150
68	Se	0.40	-0.28	-0.25	0.29	0.85	2.27	
		-0.20						0.518
72	Kr	0.47	-0.36	-0.29	-0.34	0.71	1.86	
		-0.24						1.70
76	Sr	0.48	0.41	0.42	0.42	0.26	2.84	
80	Zr	0.44	0.44	0.40	0.43	0.29	2.86	
84	Mo	0.36	-0.25	0.0	0.053	0.44	2.52	
		-0.24						0.71
88	Ru	0.0	0.11	0.0	0.05	0.62	2.30	
92	Pd	0.0	0.11	0.0	0.03	–	–	
96	Cd	0.0	0.00	0.0	0.05	–	–	
100	Sn	0.0	0.00	0.0	0.00	–	–	

[a] Ratio $E_{4_1^+}/E_{2_1^+}$. Data taken from [10, 11, 12].

2.2 Calculated properties

After adding a quadrupole constraint $\hat{Q} \propto r^2 Y_{20}/(1+f(r))$ to the HF field, where the function $f(r)$ suppresses $\hat{Q}$ at large distances [13], a systematic survey has been performed of ground state properties of N=Z even-even nuclei in the region 28≤Z≤50 and neutron-deficient nuclei between the N=Z line and the two-proton drip line towards the limits of nuclear existence. The calculated deformed shapes are characterized by a dimensionless quadrupole mass deformation parameter

$$\beta_2 = \sqrt{\frac{\pi}{5}} \frac{< r^2 Y_{20} >}{A < r^2 >} \tag{7}$$

where $< r^2 >$ is the mean square radius of the mass distribution. Deformation parameters β_2^π (β_2^ν) of the proton (neutron) distributions were defined in an analoguous way. We do not consider β_4 deformation parameters in the present work (although their values have been calculated) as they are much less clearly connected to experimental data.

Mean square radii are calculated in the usual way for the total, proton and neutron distributions [13]. The correction for the finite size of the proton is

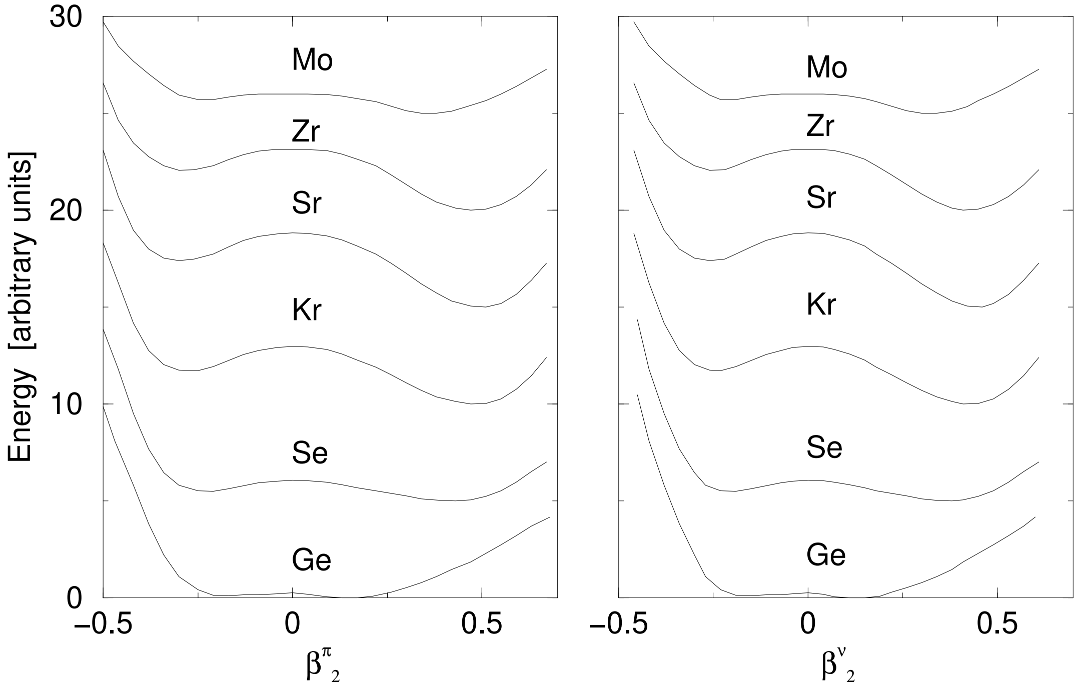

Figure 2: Calculated ground state total energy as a function of proton (left panel) and neutron (right panel) quadrupole deformation for 32≤Z≤42 N=Z nuclei.

included in the radius of the charge distribution as

$$r_{\rm ch}^2 = r_{\rm p}^2 + \underbrace{r_{\rm ch,p}^2}_{0.743\,{\rm fm}^2} - \frac{N}{Z}\underbrace{r_{\rm ch,n}^2}_{0.119\,{\rm fm}^2} , \tag{8}$$

where $r_{\rm ch,p/n}$ are the nucleon radii.

3 Results and comparison with experiment and other calculations

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The total energy surfaces as a function of quadrupole deformation for ^{56}Ni, ^{60}Zn, ^{64}Ge, ^{68}Se, ^{72}Kr, ^{76}Sr, ^{80}Zr, ^{84}Mo, ^{88}Ru, ^{92}Pd, ^{96}Pd and ^{100}Sn are shown in Fig. 1. We see a gradual departure from sphericity with increasing Z which starts at Z=32, reaches maximum for Z=38, 40 and returns to sphericity at Z=44. As expected, this deformation dependence on Z follows the same pattern for the proton and neutron matter separately (see Fig. 2). The values of deformation parameter β_2 corresponding to the minimum total energy are summarized in Table. 1 in comparison with results of some other model calculations. It is

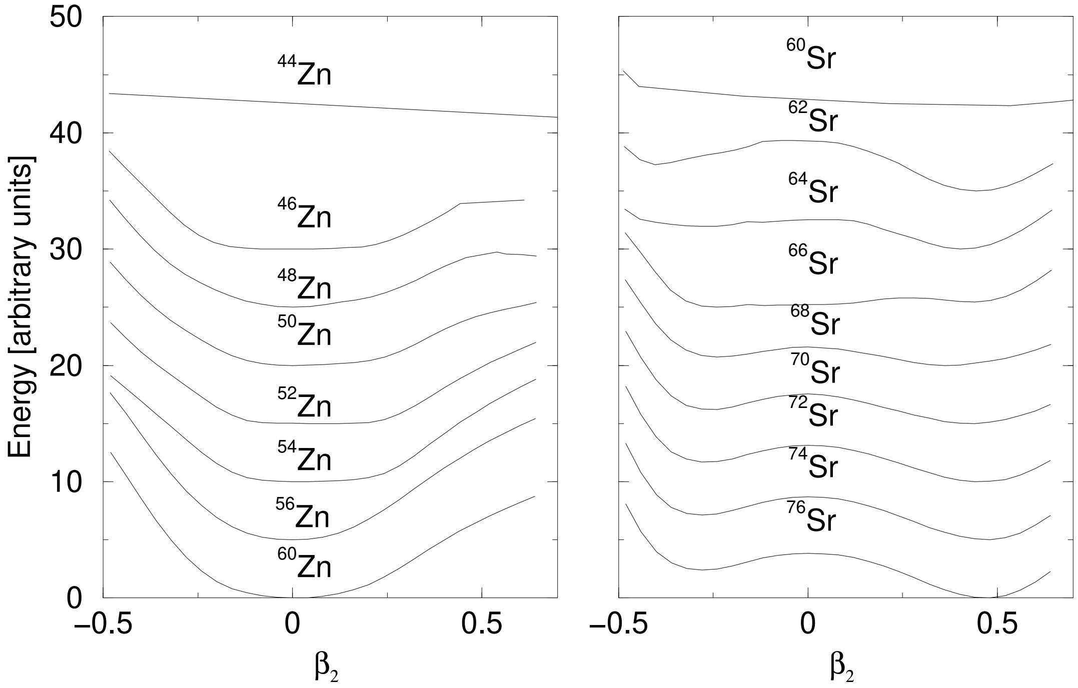

Figure 3: Calculated ground state total energy as a function of quadrupole deformation for Zn and Sr even-even nuclei beyond the 2p drip-line.

interesting to notice that if there is a discrepancy between this work and some of the previous calculations, usually the SMO predicts two coexisting minima and one of them will be in agreement with the other predictions. This may indicate that there is delicate balance between calculated coexisting minima in all models. It would be useful if the deformation corresponding to the two lowest energy minima was always given. The extracted mass deformation parameter β_2 is very close to deformation parameters β_2^π and β_2^ν for the neutron and proton systems, as expected (see Fig. 2) for all N=Z nuclei studied in this work. The present model is not adapted for a proper calculation of odd-A nuclei as yet, but allows predictions of two-proton drip line. The results are shown in Fig. 4 and are in a good agreement with predictions of the other current models.

It is interesting to investigate the development of nuclear shapes beyond the 2p drip-line. The SMO2 model indicates that even-even nuclei with a growing neutron deficiency have still a definite shape, determined by a well defined minimum in the total energy surface. We can seek a 'line of existence' for a particular element given by N and Z for which this minimum disappers. Illustration of this study is shown in Fig.4. It is clear that both shell effects and deformation keep playing an important role beyond the 2p drip-line. The last even-even isotope of each element which retains a particular shape is given in Table. 2.

An important observable closely connected to nuclear shapes is the mean-

Table 2: Lightest even-even isotopes of 28≤Z≤50 nuclei with a defined shape as predicted by the SMO2 model.

Element	Z	N	Element	Z	N
Ni	28	16	Zr	40	28
Zn	30	18	Mo	42	28
Ge	32	20	Ru	44	28
Se	34	22	Pd	46	30
Kr	36	26	Cd	48	34
Sr	38	24	Sn	50	36

Table 3: Calculated rms radii (in fm) of charge and neutron distributions in 28≤Z≤50 N=Z nuclei.

	SMO2		RMF[6]		HFMF[8]
Element	r_{ch}	r_n	r_{ch}	r_n	r_{ch}
^{56}Ni	3.767	3.594	3.709	3.573	3.79
^{60}Zn	3.844	3.664	3.883	3.742	3.87
^{64}Ge	3.946	3.757	3.985	3.843	3.97
^{68}Se	4.117	3.918	4.089	3.943	4.07
^{72}Kr	4.209	4.005	4.180	4.036	4.16
^{76}Sr	4.303	4.097	4.283	4.139	4.29
^{80}Zr	4.352	4.141	4.350	4.207	4.35
^{84}Mo	4.377	4.165	4.165	4.187	4.30
^{88}Ru	4.350	4.142	4.370	4.221	4.35
^{92}Pd	4.404	4.195	4.410	4.261	4.40
^{96}Cd	4.456	4.245	4.436	4.289	4.45
^{100}Sn	4.505	4.293	4.460	4.312	4.49

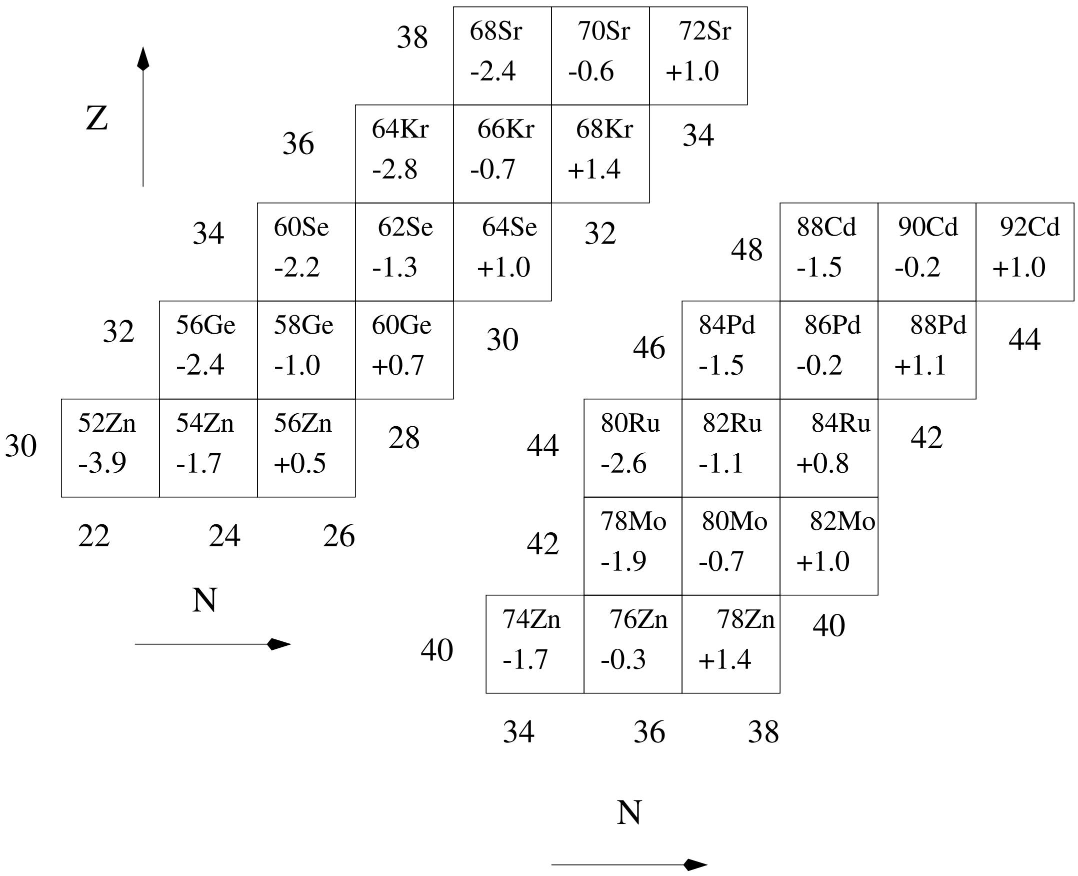

Figure 4: S_{2p}=B(A,Z)-B(A+2,Z+2) for 30≤Z≤48 N=Z even-even nuclei. Values (in MeV) are given for three isotopes of each element. These span the stability limit allowing for some uncertainty in calculated total binding energies B.

square radius of nucleon distributions in atomic nuclei. This subject will be discussed in more detail elsewhere. Here we only compare (see Table. 3) results of the SMO2 model with values obtained using RMF [6] and non-relativistic Skyrme HF models [8]. Results of all the three calculations agree with each other remarkably well. No experimental data exist in this region to date.

4 Summary

We have shown that the newly developed separable monopole interaction describes adequately N=Z and proton rich nuclei in a Hartree-Fock+BCS model. This serves as the first step towards a more realistic model which will include correlations in the mean field through convergent perturbation theory.

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