Available online at www.sciencedirect.com
SCIENCE DIRECT
International Journal of Mass Spectrometry 251 (2006) 243–251
International Journal of Mass Spectrometry
www.elsevier.com/locate/ijms

Large-scale self-consistent nuclear mass calculations

M.V. Stoitsov [a,b,c,d], J. Dobaczewski [a,b,e], W. Nazarewicz [a,b,e,*], P. Borycki [a,b,f]

[a] *Department of Physics & Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
[b] *Physics Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831, USA*
[c] *Joint Institute for Heavy-Ion Research, Oak Ridge, Tennessee 37831, USA*
[d] *Institute of Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, Sofia-1784, Bulgaria*
[e] *Institute of Theoretical Physics, Warsaw University, ul. Hoża 69, 00-681 Warsaw, Poland*
[f] *Institute of Physics, Warsaw University of Technology, ul. Koszykowa 75, 00-662 Warsaw, Poland*

Received 10 January 2006; received in revised form 26 January 2006; accepted 31 January 2006
Available online 3 March 2006

Abstract

The program of systematic large-scale self-consistent nuclear mass calculations that is based on the nuclear density functional theory represents a rich scientific agenda that is closely aligned with the main research directions in modern nuclear structure and astrophysics, especially the radioactive nuclear beam physics. The quest for the microscopic understanding of the phenomenon of nuclear binding represents, in fact, a number of fundamental and crucial questions of the quantum many-body problem, including the proper treatment of correlations and dynamics in the presence of symmetry breaking. Recent advances and open problems in the field of nuclear mass calculations are presented and discussed.

PACS: 21.10.Dr; 21.60.Jz; 31.15.Ew

Keywords: Nuclear mass; Many-body problem; Density functional theory; Large scale calculation; Spontaneous symmetry breaking

1. Introduction

The study of nuclei far from stability is an increasingly important part of a nuclear physics portfolio [1–3]. As radioactive beams gradually expand the borders of the nuclear landscape, theoretical modeling of the nucleus is changing in significant ways. The crucial question for the field [2], namely "What binds protons and neutrons into stable nuclei and rare isotopes?", nicely underlines this point: indeed, the data on rare isotopes with the large neutron-to-proton imbalance indicate that there are many gaps in our present understanding.

Short-lived exotic nuclei offer unique tests of those aspects of the nuclear theory that depend on neutron excess [4,5]. The major challenge is to predict or describe in detail exotic new properties of nuclei far from the stability valley, and to explain the origins of these properties. New ideas and progress in computer technology have allowed nuclear theorists to understand bits and pieces of nuclear structure quantitatively.

The new experimental developments inevitably require safe and reliable theoretical predictions of nuclear properties throughout the whole nuclear chart in two main directions: (i) along the isospin axis, i.e., going outwards from the beta stability line to the neutron and proton drip lines, and (ii) towards the uncharted territory of super-heavy elements at the limit of mass and charge. The tool of choice is the nuclear density functional theory (DFT) based on the self-consistent Hartree–Fock–Bogoliubov (HFB) method. The key component is the universal energy density functional, which will be able to describe properties of finite nuclei as well as extended asymmetric nucleonic matter. The development of such a universal functional, including dynamical effects and symmetry restoration, is one of the main goals of the field.

By employing various criteria (agreement with measured masses, radii, low-lying excited states, giant vibrations, rotational properties, and other global nuclear characteristics), one aims at adjusting the coupling constants of the functional. By finding correlations between parameters, one hopes to reduce their number and to understand physical reasons why different parametrizations yield similar results. One may also want to expand the parametrizations to cover aspects dictated by

* Corresponding author.
E-mail address: witek@utk.edu (W. Nazarewicz).

1387-3806/$ – see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.ijms.2006.01.040

physics arguments and/or motivations coming from the effective field theory and QCD. The main challenges in this quest have been nicely summarized through five questions [6]:

- What is the form of the nuclear energy density functional?
- What are the constraints on the nuclear energy density functional?
- What is the form of the pairing functional?
- How to account for quantum correlations and symmetry-breaking effects?
- How to optimize computational techniques and error analysis?

The aim of this paper is to briefly review the present state of the large-scale microscopic nuclear mass calculations and to discuss improvements needed. Section 2 introduces the DFT and Skyrme-HFB method. Some details concerning global mass calculations are given in Section 3. The long-term program is outlined in Section 4. Finally, the summary is given in Section 5.

2. Nuclear energy density functional

A theoretical framework aiming at the microscopic description of nuclear masses and capable of extrapolating into an unknown territory must fulfill several strict requirements. First, it must be general enough to be confidently applied to a region of the nuclear landscape whose properties are largely unknown. Second, it should be capable of handling symmetry-breaking effects resulting in a large variety of intrinsic nuclear deformations. Thirdly, it should describe finite nuclei and the bulk nuclear matter. Finally, in addition to observables, the method should provide associated error bars.

These requirements are met by the DFT in the formulation of Kohn and Sham [7]. The main ingredient of the non-relativistic nuclear DFT [8] (for relativistic nuclear DFT, see Ref. [9]) is the energy density functional that depends on densities and currents representing distributions of nucleonic matter, spins, momentum, and kinetic energy, as well as their derivatives (gradient terms). Standard Skyrme functionals employed in self-consistent mean-field calculations are parametrized by means of about ten coupling constants that are adjusted to basic properties of nuclear matter (e.g., saturation density, binding energy per nucleon) and to selected data on magic nuclei. The functionals are augmented by the pairing term which describes nuclear superfluidity [10]. When not corrected by additional phenomenological terms, standard functionals reproduce total binding energies with an rms error of the order of 2–4 MeV [11–13]. However, they have been successfully tested over the whole nuclear chart to a broad range of phenomena, and usually perform quite well when applied to energy differences, radii, and nuclear moments and deformations [8].

Historically, the first nuclear energy density functionals appeared in the context of Hartree–Fock (HF) or HFB methods and zero-range interactions such as the Skyrme force. However, it was realized afterwards that – in the spirit of the DFT – an effective interaction could be secondary to the functional, i.e., it is the density functional that defines the force. This is the strategy that we are going to follow.

2.1. The densities

The main ingredients of the nuclear DFT are the local nucleonic densities. Following the standard definitions [14,10], one considers local particle–hole (p–h) densities: particle $\rho(\boldsymbol{r})$, kinetic $\tau(\boldsymbol{r})$, spin $\boldsymbol{s}_k(\boldsymbol{r})$, spin-kinetic $\boldsymbol{T}_k(\boldsymbol{r})$, current $\boldsymbol{j}_k(\boldsymbol{r})$, tensor-kinetic $\boldsymbol{F}_k(\boldsymbol{r})$, spin-current $\mathsf{J}_{kl}(\boldsymbol{r})$, as well as the corresponding local particle–particle (p–p; or pairing) densities: $\tilde{\rho}(\boldsymbol{r})$, $\tilde{\tau}(\boldsymbol{r})$, $\tilde{\boldsymbol{s}}_k(\boldsymbol{r})$, $\tilde{\boldsymbol{T}}_k(\boldsymbol{r})$, $\tilde{\boldsymbol{j}}_k(\boldsymbol{r})$, $\tilde{\boldsymbol{F}}_k(\boldsymbol{r})$, and $\tilde{\mathsf{J}}_{kl}(\boldsymbol{r})$.

The local p–h and p–p densities are defined by the spin-dependent one-body density matrices:

$$\begin{aligned}\rho(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') &= \tfrac{1}{2}\rho(\boldsymbol{r},\boldsymbol{r}')\delta_{\sigma\sigma'} + \frac{1}{2}\sum_i(\sigma|\sigma_i|\sigma')\rho_i(\boldsymbol{r},\boldsymbol{r}'),\\ \tilde{\rho}(\boldsymbol{r}\sigma,\boldsymbol{r}'\sigma') &= \tfrac{1}{2}\tilde{\rho}(\boldsymbol{r},\boldsymbol{r}')\delta_{\sigma\sigma'} + \frac{1}{2}\sum_i(\sigma|\sigma_i|\sigma')\tilde{\rho}_i(\boldsymbol{r},\boldsymbol{r}').\end{aligned} \tag{1}$$

For instance,

$$\rho(\boldsymbol{r}) = \rho(\boldsymbol{r},\boldsymbol{r}),\quad \tau(\boldsymbol{r}) = \nabla_{\boldsymbol{r}}\nabla_{\boldsymbol{r}'}\rho(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}'=\boldsymbol{r}},\quad \tilde{\rho}(\boldsymbol{r}) = \tilde{\rho}(\boldsymbol{r},\boldsymbol{r}),$$
$$\mathsf{J}_{ij}(\boldsymbol{r}) = \frac{1}{2i}(\nabla_i - \nabla_i')\rho_j(\boldsymbol{r},\boldsymbol{r}')|_{\boldsymbol{r}'=\boldsymbol{r}}. \tag{2}$$

Since the nuclear DFT deals with two kinds of nucleons, the isospin degree of freedom has to be introduced and the isoscalar and isovector densities have to be considered[10].

2.2. The energy density functional

The energy density functional has the form

$$E[\rho,\tilde{\rho}] = \int \mathrm{d}^3\boldsymbol{r}\mathcal{H}(\boldsymbol{r}), \tag{3}$$

where energy density $\mathcal{H}(\boldsymbol{r})$ is usually written as a sum of the p–h energy density $H(\boldsymbol{r})$ and the p–p energy density $\tilde{H}(\boldsymbol{r})$. According to the DFT, there exists a nuclear universal energy functional that yields the exact binding energy of the nuclear system. This functional includes, in principle, all many-nucleon correlations.

The actual form of the nuclear energy functional is unknown. The strategy adopted by many practitioners is to build a functional around that generated by the Skyrme interaction. The most general form of the energy density functional that is quadratic in local densities and preserves the basic symmetries of the strong interaction, such as time-reversal symmetry, charge invariance, and proton–neutron symmetry, has been proposed in [10]. In practical applications, however, simplified forms of this functional have been used. For instance, one particular representation of the energy functional for the ground states of even–even

nuclei can be written as:

$$
\begin{aligned}
H(\boldsymbol{r}) = {} & \frac{\hbar^2}{2M}\tau + \frac{1}{2}t_0\left[\left(1+\frac{1}{2}x_0\right)\rho^2 - \left(\frac{1}{2}+x_0\right)\sum_q \rho_q^2\right] \\
& + \frac{1}{4}t_1\left[\left(1+\frac{1}{2}x_1\right)\rho\left(\tau - \frac{3}{4}\Delta\rho\right) - \left(\frac{1}{2}+x_1\right)\right. \\
& \left.\times \sum_q \rho_q\left(\tau_q - \frac{3}{4}\Delta\rho_q\right)\right] + \frac{1}{4}t_2\left[\left(1+\frac{1}{2}x_2\right)\right. \\
& \left.\times \rho\left(\tau + \frac{1}{4}\Delta\rho\right) + \left(\frac{1}{2}+x_2\right)\sum_q \rho_q\left(\tau_q + \frac{1}{4}\Delta\rho_q\right)\right] \\
& + \frac{1}{12}t_3\rho^\alpha\left[\left(1+\frac{1}{2}x_3\right)\rho^2 - \left(x_3+\frac{1}{2}\right)\sum_q \rho_q^2\right] \\
& - \frac{1}{8}\left(t_1x_1 + t_2x_2\right)\sum_{ij}\mathsf{J}_{ij}^2 + \frac{1}{8}\left(t_1 - t_2\right)\sum_{q,ij}\mathsf{J}_{q,ij}^2 \\
& - \frac{1}{2}W_0\sum_{ijk}\varepsilon_{ijk}\left[\rho\nabla_k\mathsf{J}_{ij} + \sum_q \rho_q\nabla_k\mathsf{J}_{q,ij}\right] + H^C(\boldsymbol{r})
\end{aligned}
\tag{4}
$$

and

$$
\tilde{H}(\boldsymbol{r}) = \frac{1}{2}V_0\left[1 - V_1\left(\frac{\rho}{\rho_0}\right)^\gamma\right]\sum_q \tilde{\rho}_q^2, \tag{5}
$$

where q labels the neutron ($q = n$) or proton ($q = p$) densities and the quantities which do not carry index q are the isoscalar densities (sums of proton and neutron densities; e.g., $\rho \equiv \rho(\boldsymbol{r}) = \rho_n(\boldsymbol{r}) + \rho_p(\boldsymbol{r})$).

The p–p energy functional (5) corresponds to a density-dependent delta interaction. Usually, $\gamma = 1$, $\rho_0 = 0.16\,\mathrm{fm}^{-3}$, and $V_1 = 0$, 1, or 1/2 for volume-, surface-, or mixed-type pairing. In Eq. (4), $H^C(\boldsymbol{r})$ stands for the Coulomb energy density with the exchange term treated in the Slater approximation.

As seen from Eqs. (4) and (5), typical Skyrme density functionals include about 14 unknown parameters. Some of them are usually adjusted to reproduce the basic properties of the infinite nuclear matter while the remaining coupling constants are fitted to known nuclear masses, radii, and other measured properties.

2.3. Variational equations

By varying the energy functional (3) with respect to the density matrices ρ and $\tilde{\rho}$ one arrives at the HFB equations:

$$
\begin{pmatrix} h - \lambda & \tilde{h} \\ \tilde{h} & -h + \lambda \end{pmatrix}\begin{pmatrix} U \\ V \end{pmatrix} = E\begin{pmatrix} U \\ V \end{pmatrix}, \tag{6}
$$

where $U = U(E, \boldsymbol{r}\sigma)$, $V = V(E, \boldsymbol{r}\sigma)$ are the HFB wave functions, and h and $\tilde{h}$ are the local particle and pairing mean-field Hamiltonians.

The HFB equations (6), also called the Bogoliubov-de Gennes equations by condensed matter physicists, are the generalized Kohn-Sham equations of the DFT. It is worth noting that – in its original formulation [15] – the DFT formalism implicitly includes the full correlation functional. In most nuclear applications, however, the correlation corrections are added afterwards. Those corrections usually include the following terms: the center-of-mass correction, rotational correction associated with the spontaneous breaking of rotational symmetry, vibrational correction (quantum zero-point vibrational fluctuations), particle-number correction due to the broken gauge invariance, as well as other terms.

The spectrum of quasi-particle energies E is continuous for $|E| > -\lambda$ and discrete for $|E| < -\lambda$. However, when solving the HFB equations on a coordinate-space lattice of points or by expanding quasi-particle wave functions in a finite basis, the quasi-particle spectrum is discretized and one can use the notation $V_k(\boldsymbol{r}\sigma) = V(E_k, \boldsymbol{r}\sigma)$ and $U_k(\boldsymbol{r}\sigma) = U(E_k, \boldsymbol{r}\sigma)$. Since for $E_k > 0$ and $\lambda < 0$ the lower components $V_k(\boldsymbol{r}\sigma)$ are localized functions of $\boldsymbol{r}$, the density matrices,

$$
\begin{aligned}
\rho(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') &= \sum_k V_k(\boldsymbol{r}\sigma)V_k^*(\boldsymbol{r}'\sigma'), \\
\tilde{\rho}(\boldsymbol{r}\sigma, \boldsymbol{r}'\sigma') &= -\sum_k V_k(\boldsymbol{r}\sigma)U_k^*(\boldsymbol{r}'\sigma'),
\end{aligned}
\tag{7}
$$

are always localized. The norms N_k of the lower components define the total number of particles

$$
N_k = \sum_\sigma \int \mathrm{d}^3\boldsymbol{r}|V_k(\boldsymbol{r}\sigma)|^2, \quad N = \sum_k N_k = \int \mathrm{d}^3\boldsymbol{r}\rho(\boldsymbol{r}). \tag{8}
$$

For spherical nuclei, the self-consistent HFB equations are best solved in the coordinate space where they form a set of 1D radial differential equations [16,17]. In the case of deformed nuclei, however, the solution of deformed HFB equations in coordinate space is a difficult and time-consuming task. For axial nuclei, the corresponding 2D differential equations can be solved by using the basis-spline methods (see, e.g., Ref. [18]). For triaxial nuclei, 3D solutions in a restricted space are possible by using the so-called two-basis method [19].

3. Large-scale microscopic nuclear mass calculations

The large-scale microscopic nuclear mass calculations, such as those of Refs. [13,20–22], typically require that the variational equations are repeatedly solved for thousands of nuclei. For example, when adjusting the parameters of the energy density functional to measured masses, one has to calculate ground-state configurations of around two-thousand nuclei many times during the fitting process. Actually, the situation is even more complicated, as several independent calculations have to be carried out for a given nucleus to find the ground-state energy of the system among several coexisting local minima. Furthermore, if odd-A and odd–odd nuclei are considered during the fitting process, many one-quasiparticle and two-quasiparticle states have to be considered to find the actual ground state. Finally, when the functional has been established, properties of around ten-thousand

particle-bound nuclei throughout the nuclear chart can be computed. All in all, fitting a functional and preparing a mass table is a challenging computational problem that requires highly optimized numerical codes and excellent utilization of modern multiprocessor computer resources.

Our group has been laying out theoretical foundations and constructing computational tools to tackle this ambitious task. We utilize a fast HFBRAD code for spherical HFB calculations [23], which takes no more than 10 CPU minutes per nucleus on an Intel Xeon 2.8 GHz processor, as well as the HFBTHO code for axially deformed HFB calculations [24,25] with acceptable processor speed - averaging to about 1 CPU hour per nucleus.

The large-scale mass calculations based on the HFBTHO code, extended with a minimal MPI (message passing interface) communication in order to run in a parallel regime across the nodes of the multiprocessor computer, are illustrated in Figs. 1 and 2, which display, respectively, calculated charts of nuclear deformations and two-neutron separation energies for particle-bound even–even nuclei. We used the SkP energy functional [16], which has a general form given by Eqs. (4) and (5). Our load-balancing routine, which scales the problem to 200 processors, allows us to perform these calculations in a single 24 wall-clock hour run on a 4 Tflop machine Cheetah at ORNL (1 Tflop $= 1 \times 10^{12}$ floating-point operations/sec) [22]. For the details of the Skyrme-HFB deformed nuclear mass table with SLy4 and SkP energy density functionals, see [26].

At present, calculations of nuclear masses performed by using the Skyrme density functionals fitted to experimental data give results precise up to the rms deviation of about 0.70 MeV. However, standard functionals that have been adjusted not only to masses but to several other nuclear characteristics reproduce nuclear masses with the rms deviations of only 3.14 MeV (SkP) or 5.10 MeV (SLy4) [24]. It is obvious that such a situation calls for improvement and a consistent search for better density functionals must be pursued. In the following, some particular aspects of our Skyrme-DFT calculations are briefly discussed.

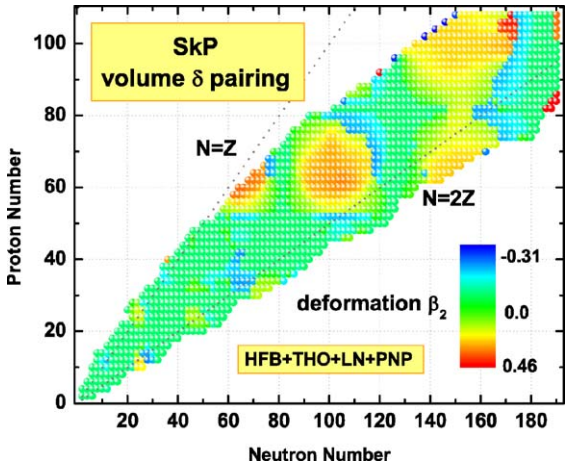

Fig. 1. Quadrupole deformations β_2 for all even–even particle-bound nuclei calculated with the SkP energy density functional [16] in the p–h channel and the volume delta pairing using the deformed HFBTHO code with 20 THO shells.

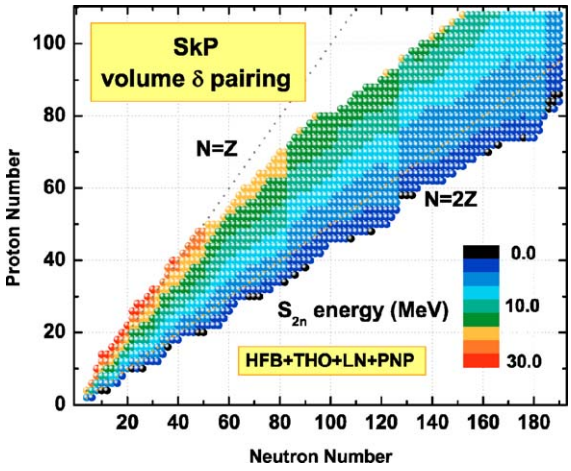

Fig. 2. Similar to Fig. 1 except for two-neutron separation energies.

3.1. Transformed harmonic oscillator basis

Going away from the beta stability valley towards particle drip lines, the Fermi energy becomes very small and the nucleonic densities and fields acquire large spatial extensions due to the coupling to the particle continuum. In this region of weakly bound nuclei, the asymptotic behavior of nuclear densities has an effect on nuclear properties. Consequently, when performing calculations for drip-line systems, it is important to have a firm grasp on physics at large distances. The recently developed HFBTHO technique based on the transformed harmonic oscillator (THO) method [27,28,22] is very helpful in this respect: it is fast, efficient, and easy to implement.

Fig. 3 shows the neutron density of the deformed nucleus ^{110}Zn obtained in two configurational calculations based on expansions in the harmonic oscillator (HO) and THO bases [27,28,22] compared to full-fledged 2D coordinate-space calculations [30,29] with the box boundary conditions. Every point in the figure corresponds to the value of the neutron density at a given Gauss-integration node in the z–ρ plane. Since the nucleus is deformed, and there are always several nodes near a sphere of the same radius $r = \sqrt{z^2 + \rho^2}$, there can be seen some scatter of points corresponding to different densities in different directions. While the significant deviation from the correct decaying behavior is seen in the HO results, the THO expansion agrees very well with the deformed coordinate-space method. Other promising techniques that can alternatively be used in this context are the Gaussian-expansion basis method [31] and the Berggren expansion method [32].

3.2. Regularization of the contact pairing interaction

When employing contact pairing interactions such as the density-dependent delta force resulting in the pairing functional (5), one has to apply a cut-off procedure and use a finite space of single-particle states [16]. When this space increases, the pairing energy diverges for any strength of the interaction; therefore, one has to readjust the pairing strength for each size of the single-particle space [17]. Such renormalization procedure

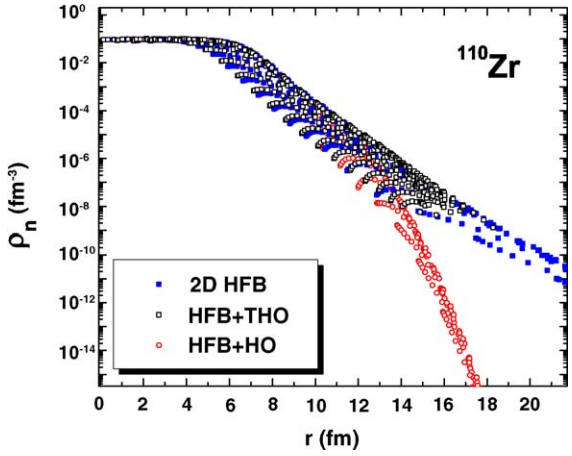

Fig. 3. Comparison of the neutron densities (in logarithmic scale) calculated with SLy4 Skyrme parametrization and volume delta pairing for the deformed nucleus ^{110}Zn using coordinate-space 2D calculations (solid squares) with the configurational calculations based on THO (open squares) and HO (open circles) basis [29]. Each point corresponds to one Gauss-integration node in the z–ρ plane, and the results are plotted as functions of the distance from the origin, $r = \sqrt{z^2 + \rho^2}$.

is performed in the spirit of the effective field theory, whereupon contact interactions are used to describe low-energy phenomena while the coupling constants are readjusted for any given energy cut-off to take into account neglected high-energy effects. It has been shown that by carrying out renormalization for each value of the cut-off energy, one practically eliminates the dependence of the HFB results on the size of the single-particle space.

Recently, the subject of the contact pairing force has been addressed in [33–37] suggesting the renormalization procedure can be replaced by a regularization scheme which removes the cut-off energy dependence of the pairing strength. Differences between the HFB results emerging from the pairing renormalization and pairing regularization procedures have been analyzed in [38] for both spherical and deformed nuclei. Fig. 4 shows differences between the HFB-SkP results for the deformed Er nuclei obtained using pairing renormalization and regularization. While the regularization method is better theoretically motivated, it is seen that both methods give indeed very similar results.

3.3. Particle number projection

The advantage of the mean-field approach to the pairing problem lies in its simplicity that allows a straightforward interpretation in terms of pairing fields and deformations (pairing gaps) associated with the spontaneous breaking of gauge symmetry. However, in the intrinsic-system description, the particle-number invariance is internally broken. Therefore, to relate to experiment, the particle number symmetry needs to be restored. This can be done on various levels, including the quasiparticle random phase approximation, Lipkin–Nogami (LN) method, the projected LN method (PLN) [39,22,21], and the particle-number projection before variation (PNP) [40–42].

Recently, particle-number restoration before variation has been incorporated for the first time into the Skyrme-DFT framework employing zero-range pairing [43]. It was demonstrated that the resulting projected HFB equations can be expressed in terms of local gauge-angle-dependent densities. In [43], results of PNP calculations have been compared with those obtained within LN and PLN methods. While the PLN gives results close

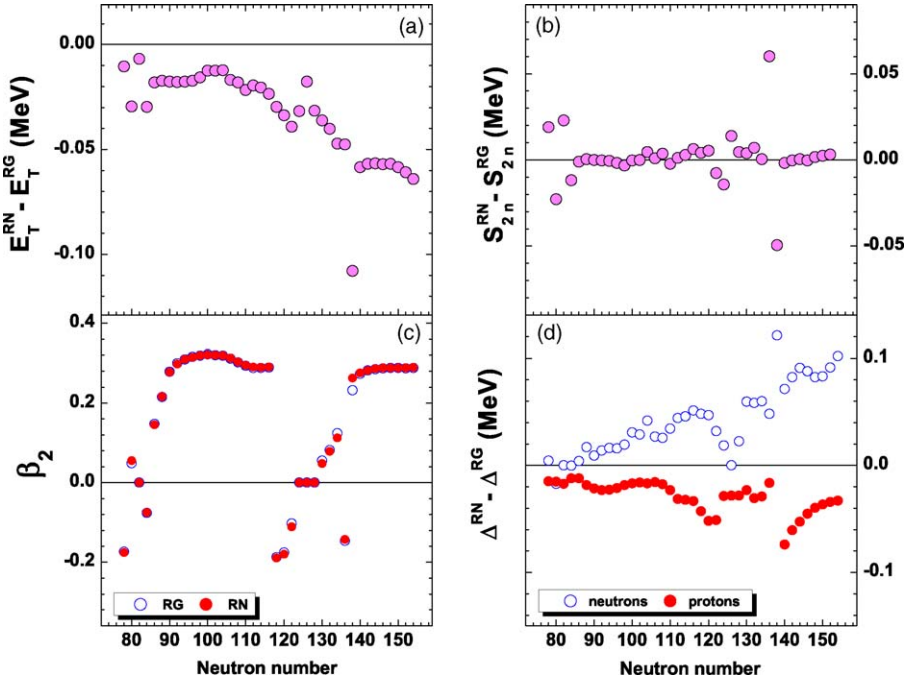

Fig. 4. Differences between pairing renormalization (RN) and regularization (RG) procedures for (a) total binding energies, (b) two neutron separation energies, and (d) the average neutron and proton gaps. Equilibrium quadrupole deformations are shown on panel (c). Calculations are performed for the chain of Er isotopes within the deformed HFBTHO method using SkP Skyrme parametrization and mixed delta pairing.

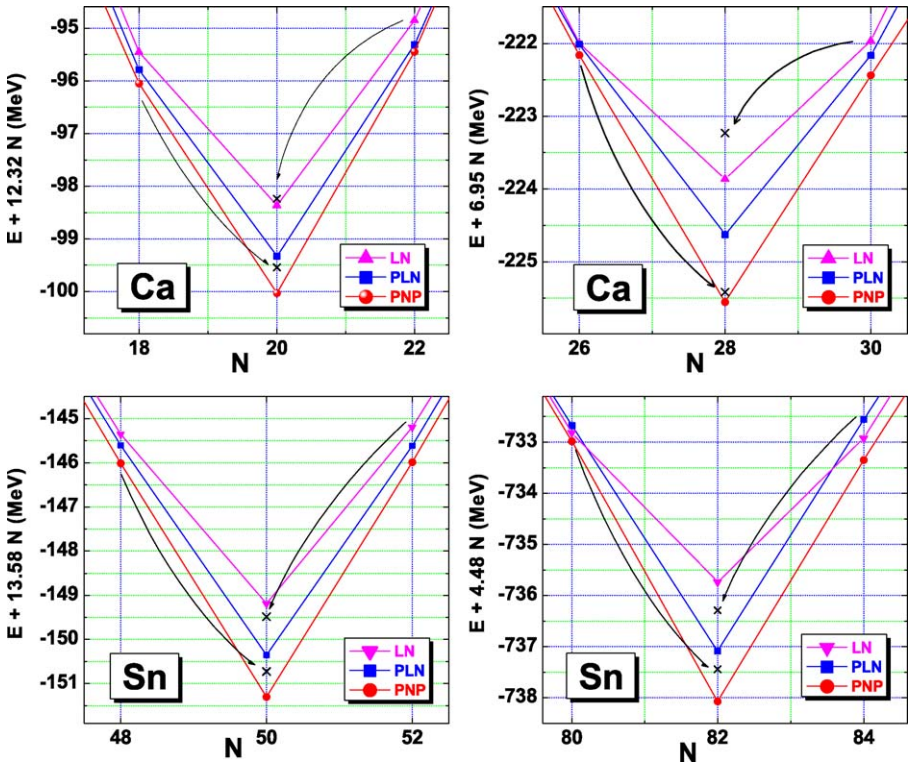

Fig. 5. The total binding energy (with respect to a linear reference) as a function of the neutron number N for even–even nuclei around doubly magic ^{40}Ca, ^{48}Ca, ^{100}Sn, ^{132}Sn calculated in LN, PLN, and PNP methods by using the SLy4 functional and mixed pairing. The crosses for magic nuclei indicate the PLN results obtained by projecting from neighboring nuclei, as indicated by arrows.

to PNP for open-shell nuclei, for closed-shell nuclei it breaks down with more than one MeV difference in the total binding energy; see Fig. 5. This pathological behavior of LN and PLN methods around closed-shell nuclei can be partly cured by performing particle-number projection from neighboring open-shell systems [44]. This result is important in the context of large-scale microscopic mass calculations such as those of Ref. [21]. To be on the safe side, however, it is always recommended to apply the complete PNP procedure around closed shells.

4. Towards the universal nuclear energy density functional

Developing a nuclear density functional requires a better understanding of the density and gradient dependence, spin and isospin effects, and pairing, as well as an improved treatment of symmetry-breaking effects and many-body correlations. Below are summarized the areas of current theoretical activities in this field.

4.1. Density and gradient dependence

An important avenue is to enrich the density dependence of the isoscalar and isovector coupling constants, both in the p–h [45,46] and p–p channels [47–49]. In particular, as the energy functional is supposed to describe those nuclear features that are related to collective dynamics, it seems important to enrich the density dependence of the effective mass in order to differentiate between its value in the bulk and at the Fermi surface [50,20].

One of the crucial challenges in microscopic theory of nuclear masses is to better understand salient features of the nuclear symmetry energy. The symmetry energy can be extracted directly from the calculated binding energy of finite nuclei, after subtracting shell effects [51]. The goal is to understand connections between the symmetry energy and isoscalar and isovector mean fields, and in particular the influence of effective mass and pair correlations on symmetry energy versus the isospin. Such understanding will allow us to better determine isospin corrections to nuclear mean fields and energy density functionals.

Recently, important indications on how to construct the nuclear energy functional have been obtained within the effective field theory (see, e.g., Refs. [52–54]). Even if one still has to readjust and fine-tune the parameters for a precise description of nuclear data, one can gain important insights into the structure of the functional, especially the dependence of the coupling constants on nuclear densities. In addition, the systematic, controlled momentum expansion on which the effective field theory is based offers a way to estimate theoretical errors (see Section 4.4).

4.2. Time-odd fields

In the self-consistent method, the average nucleonic field is obtained from the nucleonic density. Consequently, in a highly polarized high-spin state, the mean-field potential is expected to acquire appreciable time-odd components [55,56]. However, such terms should be present in all nuclear states with

non-zero angular momentum, including ground states of odd-mass and odd-odd nuclei [57]. It is rather clear that without getting a handle on the time-odd fields, it will be impossible to make precise predictions for binding energies of most of the nuclei.

The time-odd terms are very poorly known. An important task is to learn about them through an analysis of high-spin states and spin–isospin excitations. Some of the time-odd fields have been studied in [58] in the context of Gamow-Teller beta decays in radioactive nuclei by constraining the energy functional to the empirical spin–isospin Landau parameters. The coupling constants of the remaining terms can, in principle, be found by performing systematic studies of rotating nuclei. This strategy has recently been followed in the Skyrme-HF analysis of high-spin terminating states [59,60]. Those fully aligned states have fairly simple single-particle configurations, and they provide an excellent testing ground for the time-odd densities and fields.

4.3. Dynamical corrections

The correlation term, accounting for correlations going beyond the simple product state, is an integral part of the DFT. Since nuclei are self-bound systems, many-body correlations due to spontaneous symmetry-breaking effects are of particular importance. A large part of those correlations can indeed be included by considering symmetry-breaking product states. Within the mean-field approach, one can understand many physical observables by directly employing broken-symmetry states; however, for finite systems, a quantitative description often does require symmetry restoration. For this purpose, one can apply a variety of theoretical techniques, in particular projection methods, the generator coordinate method (GCM), the random phase approximation (RPA), and various approximations performed on top of self-consistent mean fields [61–63].

In this context, it is important to recall that the realistic energy density functional does not have to be related to any given effective Hamiltonian. This creates a problem if a symmetry is spontaneously broken. While the projection can be carried out in a straightforward manner for energy functionals that are related to a Hamiltonian, the restoration of spontaneously broken symmetries of a general density functional still poses a conceptional dilemma that needs to be properly addressed [64–66].

Since the correlation term is a part of the functional, it should be treated as such during the variational procedure and during the fitting process in which the functional's coupling constants are determined. So far, perhaps with the exception of the center-of-mass term (see Section 4.3.1 below), such an ambitious program has not been carried out. In the near future, one hopes to work out approximate expressions for the correlation term that would capture the essence of results of microscopic calculations performed on top of self-consistent mean fields. In this way, the hope is to develop the tractable parametrization of the correlation energy in terms of local densities that would allow an explicit inclusion of dynamical effects into the energy functional.

4.3.1. Center-of-mass correction

The center-of-mass (c.m.) correction, due to the violation of the translational invariance, is always included in calculations, but its practical implementations differ from functional to functional [57,8]. For some functionals, the treatment is fully variational; for some others the c.m. term is computed following the HFB procedure; for some functionals a simple one-body approximation is used. These apparently technical differences do matter as the actual form of the c.m. correction has a significant impact on the surface properties [57].

A good example nicely illustrating the above point has recently been discussed in [51]: for the two functionals, SLy4 and SLy6, which were fitted with precisely the same strategy but differ in their treatment of c.m. correction, the surface energy coefficient differs by as much as 0.7 MeV. While the two-body (albeit perturbative) treatment of the c.m. correction does not reduce the overall rms error of the fit to nuclear masses [20], it certainly has a significant impact on binding energies of highly deformed configurations (such as fission isomers), fission barriers, and fission trajectories.

4.3.2. Particle-number and isospin corrections

As already discussed in Section 3.3, efficient numerical codes that allow for large-scale, self-consistent variational calculations after projecting onto a good particle number have been developed [43]. The particle-number conserving HFB equations [40,41] with Skyrme functionals can be simply obtained from the standard Skyrme–HFB equations in coordinate space by replacing the intrinsic densities and currents by their gauge-angle dependent counterparts. Using the variation-after-projection method, one can properly describe transitions between normal and superconducting phases in finite systems, which are inherent in (semi)magic nuclei.

As mentioned above, the restoration of broken symmetries in the framework of DFT causes a number of questions, mainly related to the density dependence of the underlying interaction and to different treatment of particle–hole and particle–particle channels [42,67]. These questions are a matter of ongoing intensive research [65,66].

Related to the particle-number symmetry, but different in origin and treatment, is the question of the spontaneous isospin breaking. The isospin-breaking correction is of particular importance around the $N \sim Z$ line. The isoscalar pairing is believed to contribute to the additional binding of $N = Z$ nuclei, the so-called Wigner energy [68]. However, basic questions regarding the collectivity of such a phase still remain unanswered, and should be part of the future scientific agenda.

Apart from the presence of charge-dependent terms in the functional, such as the Coulomb term, the isospin symmetry is broken by the quasiparticle mean field (the generalized product wave function is not an eigenstate of isospin). Several techniques have been developed to restore isospin (see the discussion in [10,69] and references quoted therein). It is fair to say, however, that in spite of many attempts to extend the quasiparticle approach to incorporate the effect of proton-neutron correlations, no symmetry-unrestricted mean-field calculations of proton–neutron pairing, based on realistic effective interaction

and the isospin-conserving formalism, have been carried out so far.

4.3.3. Rotational and vibrational zero-energy corrections

The rotational–vibrational correlations are important aspects of nuclear collective dynamics; they also contribute to nuclear binding through quantum zero-point corrections. To estimate the magnitude of the rotational–vibrational corrections, one usually applies RPA [70], GCM [63], or the Gaussian overlap approximation to GCM [71–74].

Regardless of the approach used, a key point is the choice of collective subspace. In the case of GCM and related methods, the collective manifold is determined by the set of external fields associated with the collective motion of the system. In most practical applications, one considers five quadrupole degrees of freedom that give rise to nuclear rotations and quadrupole vibrations, octupole deformations, and pairing vibrations [75,70]. An important step towards the microscopic description of correlation energies are the recent large-scale benchmark calculations of ground-state quadrupole correlations of binding energies for all even-even nuclei, from ^{16}O up to the superheavy systems [63].

4.4. Fitting strategy and error analysis

One of the still-unsolved questions is an appropriate selection of experimental data that would allow for a more-or-less unique determination of the coupling constants defining the energy functional. To this end, one usually uses certain constraints obtained by extrapolating nuclear data to an infinite system and selected data for finite nuclei. The sensitivity of the final fit to the choice of this data set leads to a plethora of parameterizations currently available in the literature.

Most of the currently used density functionals correctly reproduce generic trends in nuclear masses – as selected masses are usually considered in the data set – but their descriptions of other quantities vary. Moreover, they often significantly differ in parameters or coupling constants [8]. This suggests that yet-unresolved correlations may exist between these parameters, and only certain combinations thereof are important [76,51]. Such correlations would explain the fact that widely different parameterizations lead to fairly similar results.

The present stage of theory requires constructing new energy density functionals supplemented by a complete error and covariance analysis. It is not sufficient to "predict" properties of exotic nuclei by extrapolating properties of those measured in experiment. One must also quantitatively determine errors related to such an extrapolation. Moreover, for experimental work it is essential that an improvement gained by measuring one or two more isotopes be quantitatively known. From a theoretical perspective, one must also know the confidence level with which the parameters of the functional are determined. An analysis of this type constitutes a standard approach in other domains of physics, but they are seldom performed in theoretical nuclear structure research.

5. Summary

This paper discusses the status, advances, open problems, and perspectives in the area of large-scale microscopic nuclear mass calculations. This field of research is past phenomenological approaches that gave us a very good understanding of general features and trends, but lacked fundamental derivations and had limited predictive power. At present, the focus is on microscopic descriptions of nuclei whereupon they are treated as finite quantum objects built of (quasi)nucleons. Nuclear ground states and masses are in this approach determined by basic fields, which are the particle and spin densities along with their derivatives and gradients up to the second order in relative momenta. These fields interact in such a way that the total energy of a given system is a functional of densities, defined and understood in the general framework of the Kohn–Sham theory. The determination of such a universal functional, along with all the dynamic corrections required by data, is the main purpose of current investigations. In this endeavor, we strive not only to have a reliable theoretical tool to calculate properties of very exotic systems that will not be soon accessible in experiment, but also wish to have a spectroscopic quality description of well-known systems, in which very precise data do exist now, and can be used as a rich source for determination of theoretical parameters. Such a program of research should not only be rooted in the fundamentals of low-energy QCD methods and ideas, but also, by definition, must rely on experiment for elements that cannot be derived from first principles. It is a vast and ambitious program presently under way.

Acknowledgments

This work was supported in part by the U.S. Department of Energy under Contract Nos. DE-FG02-96ER40963 (University of Tennessee), DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory), by the National Nuclear Security Administration under the Stewardship Science Academic Alliances program through DOE Research Grant DE-FG03-03NA00083; by the Polish Committee for Scientific Research (KBN) under contract No. 1 P03B 059 27 and by the Foundation for Polish Science (FNP).

References

[1] 2002 NSAC Long-Range Plan, http://www.sc.doe.gov/henp/np/nsac/docs/LRP_5547_FINAL.pdf.
[2] Guidance for Implementation of the 2002 NSAC Long-Range Plan, http://www.sc.doe.gov/np/nsac/docs/nsac-report-final1_Tribble.pdf.
[3] 2004 NUPECC Long-Range Plan, http://www.nupecc.org/lrp02/long_range_plan_2004.pdf.
[4] J. Dobaczewski, W. Nazarewicz, Phil. Trans. Roy. Soc. Lond. A 356 (1998) 2007.
[5] RIA Theory Bluebook: A Road Map, http://www.orau.org/ria/RIATG/Blue_Book_FINAL.pdf.
[6] INT-05–3 Program Nuclear Structure Near the Limits of Stability, http://www.physics.unc.edu/∼engelj/int05/dft.html.
[7] W. Kohn, L.J. Sham, Phys. Rev. A 140 (1965) 1133.
[8] M. Bender, P.-H. Heenen, P.-G. Reinhard, Rev. Mod. Phys. 75 (2003) 121.

[9] G.A. Lalazissis, P. Ring, D. Vretenar (Eds.), Extended Density Functionals in Nuclear Structure Physics, Springer-Verlag, 2004.
[10] E. Perlińska, S.G. Rohoziński, J. Dobaczewski, W. Nazarewicz, Phys. Rev. C 69 (2004) 014316.
[11] Z. Patyk, A. Baran, J.F. Berger, J. Dechargé, J. Dobaczewski, P. Ring, A. Sobiczewski, Phys. Rev. C 59 (1999) 704.
[12] D. Lunney, J.M. Pearson, C. Thibault, Rev. Mod. Phys. 75 (2003) 1021.
[13] S. Goriely, M. Samyn, J.M. Pearson, E. Khan, E. Phys. J. A 25 (Suppl. 1) (2005) 71.
[14] Y.M. Engel, D.M. Brink, K. Goeke, S.J. Krieger, D. Vautherin, Nucl. Phys. A 249 (1975) 215.
[15] L.N. Oliveira, E.K.U. Gross, W. Kohn, Phys. Rev. Lett. 60 (1988) 2430.
[16] J. Dobaczewski, H. Flocard, J. Treiner, Nucl. Phys. 422 (1984) 103.
[17] J. Dobaczewski, W. Nazarewicz, T.R. Werner, J.-F. Berger, C.R. Chinn, J. Dechargé, Phys. Rev. C 53 (1996) 2809.
[18] E. Terán, V.E. Oberacker, A.S. Umar, Phys. Rev. C 67 (2003) 064314.
[19] B. Gall, P. Bonche, J. Dobaczewski, H. Flocard, P.-H. Heenen, Z. Phys. A348 (1994) 183.
[20] S. Goriely, M. Samyn, M. Bender, J.M. Pearson, Phys. Rev. C 68 (2003) 054325.
[21] M. Samyn, S. Goriely, M. Bender, J.M. Pearson, Phys. Rev. C 70 (2004) 044309.
[22] M.V. Stoitsov, J. Dobaczewski, W. Nazarewicz, S. Pittel, D.J. Dean, Phys. Rev. C 68 (2003) 054312.
[23] K. Bennaceur, J. Dobaczewski, Comput. Phys. Commun. 168 (2005) 96.
[24] J. Dobaczewski, M. Stoitsov, W. Nazarewicz, Proc. Int. Conf. on Nuclear Physics, Large and Small, Cocoyoc, Mexico, April 19–22, 2004; AIP Conf. Proc. 726, (2004) 51; nucl-th/0404077.
[25] M.V. Stoitsov, J. Dobaczewski, W. Nazarewicz, P. Ring, Comput. Phys. Commun. 167 (2005) 43.
[26] Skyrme–HFB deformed nuclear mass table http://www.fuw.edu.pl/~dobaczew/thodri/thodri.html.
[27] M.V. Stoitsov, W. Nazarewicz, S. Pittel, Phys. Rev. C 58 (1998) 2092.
[28] M.V. Stoitsov, J. Dobaczewski, P. Ring, S. Pittel, Phys. Rev. C 61 (2000) 034311.
[29] A. Blazkiewicz, V.E. Oberacker, A.S. Umar, M. Stoitsov, Phys. Rev. C 71 (2005) 054321.
[30] V.E. Oberacker, A.S. Umar, E. Terán, A. Blazkiewicz, Phys. Rev. C 68 (2003) 064302.
[31] E. Hiyama, Y. Kino, M. Kamimura, Prog. Part. Nucl. Phys. 51 (2003) 223.
[32] N. Michel, W. Nazarewicz, M. Ploszajczak, K. Bennaceur, Phys. Rev. Lett. 89 (2002) 042502.
[33] A. Bulgac, Y. Yu, Phys. Rev. Lett. 88 (2002) 042504.
[34] A. Bulgac, Phys. Rev. C 65 (2002) 051305(R).
[35] Y. Yu, A. Bulgac, Phys. Rev. Lett. 90 (2003) 222501.
[36] A. Bulgac, Y. Yu, Int. J. Mod. Phys. E 13 (2004) 147.
[37] T. Nikšić, P. Ring, D. Vretenar, Phys. Rev. C 71 (2005) 044320.
[38] P.J. Borycki, J. Dobaczewski, W. Nazarewicz, M.V. Stoitsov, Phys. Rev. C., submitted for publication.
[39] J. Dobaczewski, W. Nazarewicz, Phys. Rev. C 47 (1993) 2418.
[40] J.A. Sheikh, P. Ring, Nucl. Phys. A 665 (2000) 71.
[41] J.A. Sheikh, P. Ring, E. Lopes, R. Rossignoli, Phys. Rev. C 66 (2002) 044318.
[42] M. Anguiano, J.L. Egido, L.M. Robledo, Nucl. Phys. A 696 (2001) 467.
[43] M.V. Stoitsov, J. Dobaczewski, W. Nazarewicz, J. Terasaki, Eur. Phys. J. A 25 (Suppl. 1) (2005) 567, in preparation.
[44] P. Magierski, S. Ćwiok, J. Dobaczewski, W. Nazarewicz, Phys. Rev. C 48 (1993) 1686.
[45] T. Duguet, P. Bonche, Phys. Rev. C 67 (2003) 054308.
[46] B. Cochet, K. Bennaceur, J. Meyer, P. Bonche, T. Duguet, Int. J. Mod. Phys. E 13 (2004) 187.
[47] J. Dobaczewski, W. Nazarewicz, P.-G. Reinhard, Nucl. Phys. A 693 (2001) 361.
[48] J. Dobaczewski, W. Nazarewicz, M.V. Stoitsov, Eur. Phys. J. A 15 (2002) 21.
[49] T. Duguet, Phys. Rev. C 69 (2004) 054317.
[50] M. Farine, J.M. Pearson, F. Tondeur, Nucl. Phys. A 696 (2001) 396.
[51] P.-G. Reinhard, M. Bender, W. Nazarewicz, T. Vertse, Phys. Rev. C 73 (2006) 014303.
[52] S.J. Puglia, A. Bhattacharyya, R.J. Furnstahl, Nucl. Phys. A 723 (2003) 145.
[53] A. Bhattacharyya, R.J. Furnstahl, Nucl. Phys. A 747 (2005) 268.
[54] R.J. Furnstahl, J. Phys. G 31 (2005) S1357.
[55] J. Dobaczewski, J. Dudek, Phys. Rev. C 52 (1995) 1827.
[56] A.V. Afanasjev, P. Ring, Phys. Rev. C 62 (2000) 031302.
[57] M. Bender, K. Rutz, P.-G. Reinhard, J.A. Maruhn, Eur. Phys. J. A 7 (2000) 467.
[58] M. Bender, J. Dobaczewski, J. Engel, W. Nazarewicz, Phys. Rev. C 65 (2002) 054322.
[59] H. Zduńczuk, W. Satuła, R. Wyss, Phys. Rev. C 71 (2005) 024305
H. Zduńczuk, W. Satuła, R. Wyss, Int. J. Mod. Phys. E 14 (2005) 451.
[60] W. Satuła, R. Wyss, H. Zduńczuk, Eur. Phys. J. A 25 (Suppl. 1) (2005) 551.
[61] P. Ring, P. Schuck, The Nuclear Many-Body Problem, Springer-Verlag, Berlin, 1980.
[62] P.-G. Reinhard, K. Goeke, Rep. Prog. Phys. 50 (1987) 1.
[63] M. Bender, G. Bertsch, and P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102503; arxiv. org/abs/nucl-th/0508052, Phys. Rev. C, in press.
[64] J.P. Perdew, A. Savin, K. Burke, Phys. Rev A 51 (1995) 4531.
[65] M. Stoitsov et al., in preparation; talk at the INT Workshop on Towards a Universal Density Functional for Nuclei, September 2005. http://www.int.washington.edu/talks/WorkShops/int_05_3/People/Stoitsov_M/mstoitsov.pdf.
[66] M. Bender, T. Duguet, Talks at the INT Workshop on Pairing Degrees of Freedom in Nuclei and the Nuclear Medium, November 2005. http://www.int.washington.edu/talks/WorkShops/int_05_3/People/Duguet_T/duguet.pdf http://www.int.washington.edu/talks/WorkShops/int_05_3/People/Bender_M/Bender.pdf.
[67] M. Stoitsov, J. Dobaczewski, W. Nazarewicz, P.G. Reinhard, J. Terasaki, in: Aldo Covello (Ed.), Proceedings of the 8th International Spring Seminar on Nuclear Physics, Key Topics in Nuclear Structure, Paestum, Italy 2004,World Scientific, Singapore, p. 167.
[68] W. Satuła, R. Wyss, M. Rafalski, Eur. Phys. J. A 25 (Suppl. 1) (2005) 559.
[69] S. Głowacz, W. Satuła, R.A. Wyss, Eur. Phys.J. A 19 (2004) 33.
[70] S. Baroni, M. Armati, F. Barranco, R.A. Broglia, G. Colo, G. Gori, E. Vigezzi, J. Phys. G 30 (2004) 1353.
[71] M. Bender, G. Bertsch, P.-H. Heenen, Phys. Rev. C 69 (2004) 034340.
[72] P. Fleischer, P. Klüpfel, P.-G. Reinhard, J.A. Maruhn, Phys. Rev. C 70 (2004) 054321.
[73] L. Próchniak, P. Quentin, D. Samsoen, J. Libert, Nucl. Phys. A 730 (2004) 59.
[74] H. Goutte, J.F. Berger, P. Casoli, D. Gogny, Phys. Rev. C 71 (2005) 024316.
[75] K. Sieja, A. Baran, K. Pomorski, Eur. Phys. J. A 20 (2004) 413.
[76] G.F. Bertsch, B. Sabbey, M. Uusnäkki, Phys. Rev. C 71 (2005) 054311.