Isospin Invariant Skyrme Density Functional Approach

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One of the great challenges in the twenty-first century is to provide a unified and microscopic understanding of nuclear species across the whole nuclear landscape. The *ab-initio* and configuration interaction methods when applied to heavier systems with many active particles present insurmountable computational challenges as the configuration space explodes rapidly. In nuclear physics, the method of choice to study heavier systems is the mean-field approach based on effective forces. The mean-field theory in the form of Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) approximations transform the many-body problem into a solvable one-body problem. This kind of approach to many-body quantum physics can be found in many other fields such as condensed matter physics, atomic and molecular physics and quantum chemistry. The most popular among the mean-field based approach is the density functional theory (DFT). In nuclear physics, energy density functional depends on densities and currents that represent distributions of nucleonic matter, spins, momentum, and kinetic energies. DFT approach first appeared in nuclear physics in 1956 when it was demonstrated that zero-range density dependent nucleon-nucleon interaction can be completely expressed in terms of the local densities [1, 2]. However, the modern DFT approaches that reproduce the nuclear masses with quite a remarkable rms deviation of the order of 600 keV with respect to the mass measurements, are not rooted in the nuclear Hamiltonian. These energy density functionals are validated by mathematical theorems demonstrating the existence of a universal energy density functional for a many-body system that, in principle, can lead to exact results as that using the many-body Schrödinger approach [3, 4].

The DFT approach in nuclear physics replaces phenomenological methods with a well founded microscopic theory that delivers maximum predictive power with quantified uncertainties. Presently, there is a world-wide effort to develop a universal nuclear energy density functional that is capable of describing nuclear structure and reactions in a self-consistent manner. In the United States, under the aegis of SciDAC, UNEDF project [5] has been initiated and the mission of this project is to develop an optimal energy density functional using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties. This project has given a major impetus in our quest to understand the nuclear many-body problem. Already, several important contributions have been reported in the UNEDF initiative and a substantial progress is expected in the coming years.

In the quest of developing a universal nuclear density functional, the existing density formulations ought to be enriched by incorporating the neglected degrees of freedom, for instance, in spin and isospin channels. A large scale effort is presently being undertaken to improve the spin sector of the Skyrme density functionals by re-fitting the coupling constants with the explicit inclusion of the tensor densities [6]. In the isospin sector, most of the functionals include densities in the isoscalar channel and only t_z component in the isovector channel; t_x and t_y or neutron-proton mixed components of isovector densities are completely neglected. In the heavier nuclei where neutrons and protons, on avg., different configuration spaces

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the neglect of the neutron-proton mixed densities could be rationalized. However, in the lighter- and medium- mass regions, neutrons and protons occupy same configuration space and the exclusion of the isovector densities cannot be justified. There are several observations that indicate deficiencies inherent in the existing density functional and other approaches to describe nuclei in the vicinity of the $N = Z$ line. For instance, it is quite well established that binding energies of the nuclei close to the $N = Z$ line are unpredicted by most of the models [7]. In the phenomenological models, the mass formula needs to be complemented by the so called Wigner term to account for the extra correlations present near the $N = Z$ line [8].

In some earlier studies, neutron-proton mixing has been investigated in the particle-particle channel only [9, 10]. In the particle-hole sector, this mixing was completely neglected and is obviously flawed in a fully self-consistent HFB treatment. Recently, a new density functional approach has been proposed [11] with the inclusion of neutron-proton mixed densities in the particle-particle and as well as in the particle-hole channel. The density functional has been constructed following general rules, in particular, by respecting spin and isospin symmetries. It has been shown that the generalized functional gives rise to new spin-isospin combinations for the densities that are absent in the traditional approaches. We expect that these new densities and the corresponding terms in the density functional may lead to new modes in excitation spectra, hitherto, unexplored in nuclear structure physics.

In the present work we have formulated the isospin invariant Skyrme energy density functional approach with the inclusion of all possible neutron-proton mixed densities in the cylindrical coordinate system. The validation for employing such a coordinate system is borne out from the well known empirical observation that most of the nuclei in the periodic table are axially symmetric and cylindrical coordinate frame is then the appropriate system of choice. Further, the numerical calculations become extremely simplified in the axial limit and it is possible to undertake systematic studies of the properties of nuclei over the entire nuclear landscape. Several systematic studies, for instance, binding energies of around six-thousand nuclei that are known to exist has been performed in the axial limit using the popular computer code, HFBTHO [12]. In the present work, we have generalized this code to the isospin-invariant Skyrme density functional in the HF level and shall present detailed expressions for various densities and potentials involved in the development of the code. The computer code has been rewritten in the isospin representation and the details of the new code shall be presented. In a parallel effort [13], neutron-proton mixed densities have also been implemented in the computer code, HFODD [14]. This code solves the Skyrme energy density functional in three-dimensional Cartesian basis. In order to investigate the accuracy of the present study, we shall compare our results with those obtained using HFODD.

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