Energy-density-functional calculations including proton–neutron mixing†

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We performed calculations based on the Skyrme energy density functionals that include an arbitrary mixing between protons and neutrons. This is the first step towards the density functional calculation including proton–neutron (p-n) pairing. The p-n pairing is a long-standing open problem in nuclear physics, and its possible relations to various nuclear phenomena have been widely discussed.[2] However, in spite of several theoretical studies over the years since the late sixties, a consistent theoretical treatment of the p-n pairing is still missing. Our ultimate goal is to develop a consistent symmetry-unrestricted energy-density-functional (EDF) approach including the p-n mixing both in the pairing and particle–hole (p-h) channels. To treat the p-n pairing within the EDF framework, one needs to generalize the quasiparticle states as mixtures of protons and neutrons. In connection with this extension of quasiparticles, one also needs to extend density functionals to those with mixing between protons and neutrons. In this work, as a first step in achieving our goal, we consider an extension of EDFs including the p-n mixing in the p-h channel, with both the rotational and isospin symmetries conserved. We developed a code for the p-n mixing calculation by extending the code "HFODD,"[3] which solves the nuclear Skyrme–Hartree–Fock(–Bogolyubov) problem by using the Cartesian deformed harmonic-oscillator basis. In this p-n mixing calculation, we performed the so-called isocranking calculation by adding the isocranking term to the Hamiltonian: $\hat{h}' = \hat{h} - \vec{\lambda}\cdot\hat{\vec{t}}$. Here, $\hat{\vec{t}}$ is the isospin operator. The isocranking term is analogous to that used in the standard tilted-axis-cranking calculations for high-spin states. By adjusting the isocranking frequency $\vec{\lambda}$, we can control the size and direction of the isospin of the system. We first performed isocranking calculations for $A = 14$ and $A = 48$ systems with the Coulomb interaction switched off, and we confirmed that our code is correctly implemented. In this case, the total and single-particle energies are independent of the direction of the isospin of the system. Next, we performed calculations with the Coulomb interaction included. In this model, isobaric analog states (IASs) are calculated by adjusting the isocranking frequency. We developed an efficient method for determining the isocranking frequency, with which we successfully calculated the $T \simeq 4$ states in $A = 40 - 56$ isobars.

The isocranking calculation is a simple linear constraint method. We also implemented in our code an improved method for optimization with constraints, known as "the augmented Lagrange method," and employed it for the calculation of the high-isospin states in ^{48}Cr. Such calculations can be used to study the nuclear symmetry energy.

In Fig. 1, we plot the energies of the $I = 0^+, T = 1$ triplet of states in the $A = 14$ isobars calculated using the SkM* EDF. The $T_z = 0$ IAS representing the excited $I = 0^+, T = 1$ state in ^{14}N is calculated by using the isocranking model and is described by a single time-even Slater determinant built of single-particle p-n mixed orbitals. Fig. 1 illustrates that the model is indeed capable of quantitatively describing the excitation energies of the $0^+, T = 1$ IASs. One can see that there is asymmetry between the energy differences $|E(T_z = 0) - E(T_z = -1)|$ and $|E(T_z = 0) - E(T_z = 1)|$, which may be related to charge asymmetry and independence of the NN interaction. To investigate this point, we also started a systematic calculation of the $T = 1$ triplets in the A=10–58 region.

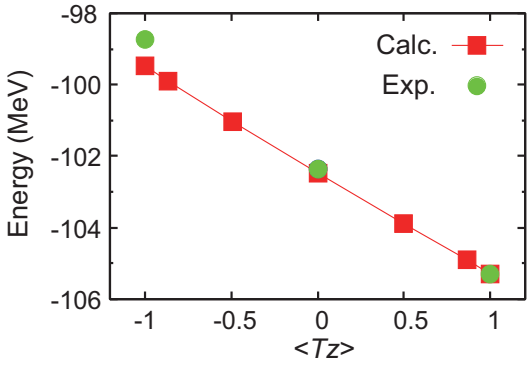

Fig. 1. Energies of $T \simeq 1$ states in $A = 14$ isobars in comparison with the experimental data[4]. To correct the deficiency of the SkM* EDF, the calculated curve is shifted up by 3.2 MeV.

References
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4) National Nuclear Data Center, Brookhaven National Laboratory, http://www.nndc.bnl.gov/.

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