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Nuclear dynamics with the Barcelona-Catania-Paris-Madrid functional

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We modify the open-source Sky3D code, which implements a time-dependent Hartree-Fock method with a Skyrme functional, so that it uses the Barcelona-Catania-Paris-Madrid (BCPM) energy density functional instead. We run static ground state simulations and dynamical giant quadrupole resonance simulations to demonstrate the capabilities of the approach. Static simulations of nuclei in their ground state are benchmarked against a reference code. The binding energies of static ground state nuclei show differences below 0.3% with respect to the reference. We also simulate quadrupole resonances employing the time-dependent code and find results that are stable and compatible with previous Sky3D simulations.

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1. Introduction

Atomic nuclei are systems of protons and neutrons (known as "nucleons") bound together by the strong interaction [1]. Effective models of the nuclear interaction are often employed to describe the static and dynamic properties of nuclei [1]. Our work is based on Time-Dependent Density Functional Theory (TDDFT), a microscopic model that allows for a consistent description of static and dynamical properties of nuclei [2, 3]. Several implementations of TDDFT exist in nuclear theory literature. We rely on the open-source, widely available Sky3D code [4].

TDDFT requires a nuclear energy density functional (EDF) as a starting point. The original release of Sky3D implements TDDFT employing the Skyrme EDF. The Barcelona-Catania-Paris-Madrid (BCPM) EDF has been successfully applied to describe nuclear radii, energies, multipolar deformations, nuclear fission, and nuclear matter [3]. A useful feature of BCPM is its functional simplicity, which leads to a low computational cost [5]. Motivated by the potential advantages of this functional, we modified Sky3D to incorporate the BCPM functional. This is a first step towards a full open-source computational implementation of TDDFT with the BCPM EDF.

2. The BCPM energy density functional

We employ the implementation of BCPM described in Ref. [3]. The EDF is decomposed into bulk, surface and pairing terms as well as additional corrections, $E_{\rm BCPM} = E_{\rm bulk}+E_{\rm surf}+E_{\rm pair}+E_{\rm com}$. The bulk term is polynomial in the local density, ρ, and isospin asymmetry, $I = \frac{\rho_n-\rho_p}{\rho}$ [3],

$$E_{\rm bulk} = \int d\vec{r} \left[(1-I^2) \sum_{n=1}^{5} c_n \left(\frac{\rho}{\rho_0}\right)^n + I^2 \sum_{n=1}^{5} d_n \left(\frac{\rho}{\rho_{0n}}\right)^n \right] \rho. \tag{1}$$

Here, $\rho_0 = 0.16$ fm^{-3} is the saturation density of symmetric nuclear matter and $\rho_{0n} = 0.155$ fm^{-3} is a reference density for neutron matter [3]. The polynomial proportional to the c_n (d_n) constants accounts for the equation of state (EoS) of symmetric nuclear (neutron) matter. This introduces 10 parameters ($c_1...c_5$, $d_1...d_5$), that are fit to microscopic simulations of the EoS [3]. This term is very similar to the zero-range and density-dependent terms of Skyrme EDFs.

The surface term in BCPM is parametrized through a finite-range Gaussian form factor [3],

$$E_{\rm surf} = \frac{1}{2} \sum_{q,q'=-1/2}^{1/2} V_{q,q'} \iint d\vec{r}_1 d\vec{r}_2 \, \rho_q(\vec{r}_1) e^{-\frac{(\vec{r}_1-\vec{r}_2)^2}{r_0^2}} \rho_{q'}(\vec{r}_2). \tag{2}$$

q and q' represent the isospin components, whereas r_0 and $V_{q,q'}$ are in principle free parameters. In practice, r_0 is fixed and the strengths are determined so that the bulk limit of Eq. (2) matches the ρ^2 term of Eq. (1) [3]. There is no equivalent to this term in Skyrme EDF, and we compute it in momentum space, employing a convolution and the fast Fourier transforms within Sky3D [4]. The pairing functional in BCPM is given by [3]

$$E_{\rm pair} = \iint d\vec{r}_1 d\vec{r}_2 \, V_{\rm pair} \left[1 - \eta \left(\frac{\rho(\vec{r})}{\rho_{0,\rm pair}} \right)^F \right] \delta(\vec{r}_1 - \vec{r}_2), \tag{3}$$

where V_{pair}, $\rho_{0,pair}$, F and η are additional free parameters. The center-of-mass correction $E_{\rm com}$ in BCPM reduces the bare nucleon mass by an $A-$dependent factor [3]. In total, BCPM requires 14 parameters: $c_1...c_5$, $d_1...d_5$, r_0, F, η and $V_{\rm pair}$, which we take from Ref. [3].

Nucleus	**E (MeV) Bench.**	**E (MeV) BCPM3D**	**% diff.**
^{4}He	-28.363	-28.329	0.1%
^{12}C	-89.351	-89.204	0.2%
^{16}O	-127.008	-126.595	0.3%
^{40}Ca	-342.330	-341.961	0.1%
^{48}Ca	-415.878	-415.305	0.1%
^{56}Ni	-478.991	-478.137	0.2%
^{78}Ni	-643.969	-642.246	0.3%
^{100}Sn	-823.749	-822.289	0.2%
^{208}Pb	-1637.938	-1634.809	0.2%

Table 1: Binding energies of doubly magic nuclei in static simulations with BCPM.

Particle	**E (MeV) Bench.**	**E (MeV) BCPM3D**	**% diff.**
$\nu\ 1s_{1/2}$	-37.766	-37.772	0.02%
$\nu\ 1p_{3/2}$	-28.660	-28.654	0.02%
$\nu\ 2s_{1/2}$	-15.774	-15.794	0.1%
$\nu\ 1d_{3/2}$	-14.623	-14.622	0.007%
$\nu\ 1d_{7/2}$	-9.195	-9.182	0.1%
$\pi\ 1s_{1/2}$	-36.671	-36.668	0.008%
$\pi\ 1p_{3/2}$	-28.851	-28.837	0.04%
$\pi\ 1d_{5/2}$	-19.931	-19.918	0.07%
$\pi\ 2s_{1/2}$	-15.339	-15.344	0.03%

Table 2: Some single-particle energies of ^{48}Ca in static simulations with BCPM.

3. Static ground state simulations

We benchmarked our new code, dubbed BCPM3D, with a reference static, spherical BCPM code [6]. Table 1 shows the binding energies of doubly magic nuclei. Columns 2 and 3 show binding energies predicted by the reference code and BCPM3D, respectively. The discrepancies listed in the last column indicate that the differences are extremely small ~0.1% – 0.3%. Table 2 shows some of the single-particle energy levels obtained for ^{48}Ca, the lightest nucleus studied with $Z \neq N$, which showcases the influence of isospin-dependent terms. The single-particle levels are indicated in the first column, whereas columns 2 and 3 again correspond to the reference code and BCPM3D. The percentile discrepancies between the two codes, in the last column, show an excellent level of agreement ($\leq$0.1%). Other closed shell isotopes show a similar level of agreement in single-particle energies [7].

4. Giant quadrupole resonances with the BCPM functional

After benchmarking static simulations with BCPM3D, we focus on dynamical simulations. We choose giant quadrupole resonances as they provide physics insight for properties like the nuclear compressibility and effective masses [8] with relatively low computational demands. Following Sky3D standards, we impart a quadrupolar boost to a nucleus at $t = 0$ fm/c and evolve it over time. The time-dependent quadrupole moment signals are filtered to avoid artifacts in the Fourier transforms to energy space. Figure 1 compares the quadrupole moment as a function of time for ^{16}O with the Skyrme (blue, results based on the SV-bas parametrization) and BCPM (red) EDFs. The BCPM functional predicts lower oscillation frequencies and amplitudes than the Skyrme functional, and thus a weaker resonance with lower average excitation energy. We have also computed quadrupole resonances for Cd and Sn isotopes, and have found good agreement in the centroid energies with respect to other numerical benchmarks [7]. We note that, even though the quadrupole boost imparted on the nucleus is isoscalar, TDDFT simulations for $N \neq Z$ nuclei may excite the corresponding isovector mode [9].

5. Conclusions and future outlook

We have modified the Sky3D code to perform TDDFT calculations with the BCPM EDF. BCPM3D simulations agree with a reference BCPM code. There is a $\lesssim 1\%$ difference relative to our benchmark in the single-particle energies and total binding energies of doubly closed-shell nuclei. We have also found stable numerical results for dynamical simulations of quadrupole resonances. There are several potential avenues for expanding our work, including BCPM3D benchmarks in calculations where pairing effects become relevant. BCPM3D also offers enormous potential to study dynamical processes [5].

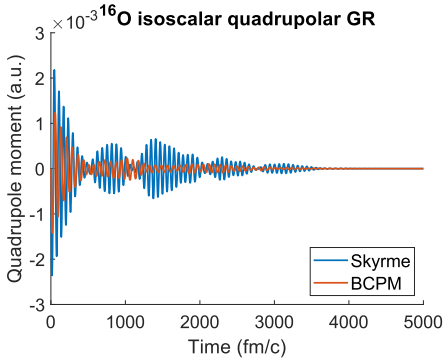

Figure 1: Quadrupole strength in arbitrary units as a function of time in ^{16}O after a quadrupole kick. Skyrme and BCPM TDDFT simulations are compared to one another.

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