Journal of Physics: Conference Series **533** (2014) 012055 doi:10.1088/1742-6596/533/1/012055

Hartree-Fock-Bogoliubov calculations of deformed weakly bound nuclei using continuous bases

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Abstract. The Hartree-Fock-Bogoliubov equations for deformed weakly bound nuclei are solved using a basis of Pöschl-Teller-Ginocchio and Bessel/Coulomb wave functions, which possess proper asymptotic behavior. Results compare well with standard Hartree-Fock-Bogoliubov calculations using box boundary condition or transformed harmonic oscillator basis.

1. Introduction

The precise description of weakly bound and unstable nuclei is a very challenging task in nuclear structure theory. The fundamental theoretical problem is to consistently describe both structure and reaction aspects of weakly bound nuclei, which requires a rigorous treatment of the many-body continuum. Many facilities have been or are built throughout the world in order to generate nuclei close to drip-lines, such as the projects FAIR in GSI, Germany and SPIRAL2 in GANIL, France, as well as the RIBF facility at RIKEN, Japan and the ISAC and ARIEL accelerators at TRIUMF, Canada.

In order to systematically study the whole nuclear chart, it is necessary to use density functional theory (DFT), used in conjunction with the Hartree-Fock-Bogoliubov (HFB) theory, as other methods, such as configuration interaction, become much too expensive numerically for nuclei bearing many nucleons. HFB equations can be solved on the one hand in coordinate space using box boundary condition (denoted in this paper as HFB/Box) [1, 2, 3] and on the other hand with diagonalization techniques by expanding HFB states in a harmonic oscillator (HO) or transformed harmonic oscillator (THO) basis [4]. These methods (denoted in this paper as HFB/HO or HFB/THO) are very fast and allow large-scale calculations [5, 6]. However, the HO and THO bases cannot reproduce simultaneously all asymptotic properties. Differences between calculations using the THO and the coordinate-space bases have been noticed for example in pairing properties of nuclei (see Sec. 3 and Ref. [7]).

The inclusion of continuum at basis level is definitely the most precise method in order to mitigate these problems. For this, the exactly solvable Pöschl-Teller-Ginocchio (PTG) potential [8] provides a numerically stable continuous basis. Phase shifts of real-energy scattering states vary indeed smoothly therein so that real-energy continua can be precisely discretized with Gauss-Legendre quadrature. This method to solve HFB equations with PTG basis is denoted as HFB/PTG in this paper.

Numerical calculations have been performed for a strongly deformed nucleus ^{110}Zr, and two HFB solutions for ^{40}Mg with different, prolate and oblate, deformations.

The paper is organized as it follows. The HFB/PTG algorithm is described in Sec. 2. Results of numerical calculation are presented in Sec. 3. Brief summary and conclusions are given in Sec. 4. All shown tables and figures were previously published in Ref. [9].

2. The HFB/PTG approach

Our aim is to develop an efficient method of solving the HFB equations

$$\begin{pmatrix} h-\lambda & \tilde{h} \\ \tilde{h} & -h+\lambda \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = E \begin{pmatrix} U \\ V \end{pmatrix} \tag{1}$$

for deformed weakly bound nuclei. h and $\tilde{h}$ denote the particle-hole and the particle-particle (hole-hole) components of the single-particle Hamiltonian, respectively, U and V the upper and the lower components of the single-quasiparticle wave function, of energy E, and λ is the chemical potential [3]. We now outline the calculational scheme of the HFB/PTG method:

(1) One starts with deformed HFB calculations in the HO basis (HFB/HO). This provides a good approximate solution for the HF potential and the effective mass. They are then averaged over angular and spin degrees of freedom.

(2) For each ℓj subspace, one fits the associated PTG potential to the averaged HF potential when it possesses bound or narrow resonant states in this ℓj subspace. If no such states appear in the HF ℓj spectrum, a set of Bessel/Coulomb wave functions [10] is selected for the ℓj partial wave basis. Bound and resonant states of the averaged HF potential are always bound in the PTG basis, and one takes into account only scattering states of real energy, so that the PTG basis does not make use of complex-valued states.

(3) One diagonalizes the HFB eigenvalue equations in the basis composed of the PTG and Bessel/Coulomb wave functions. This step continues until self-consistency is achieved.

3. Numerical examples

We have made a feasibility test of the HFB/PTG method for deformed neutron-rich nuclei ^{110}Zr and ^{40}Mg. All calculations were done using the SLy4 density functional. For the pairing interaction, we use the surface-type delta pairing with the strength $t_0' = -519.9$ MeV fm^3 for the the density-independent part and $t_3' = -37.5t_0'$ MeV fm^6 for the density-dependent part with a sharp energy cut-off at 60 MeV in the quasiparticle space. They have been fitted to reproduce the neutron pairing gap of ^{120}Sn. These values are consistent with those given in Ref. [11]; the slight difference is due to different cut-off procedures, sharp cut-off in our case and smooth cut-off in Ref. [11].

In the case of axially deformed nuclei, few HFB/Box calculations are available to check the HFB/PTG results. We consider the well-deformed nucleus ^{110}Zr (deformation $\beta \approx 0.4$), already studied in Ref. [7] and two states with different deformations for the drip line nucleus ^{40}Mg.

Table 1 compares the three approaches with respect to ground state properties of ^{110}Zr. In general they yield similar values. The differences seen in Table 1 are partially due to different structure of the model spaces adopted and the associated fitting of the pairing strength.

Proton and neutron densities for nuclei ^{110}Zr and ^{40}Mg are displayed in Fig. 1, with comparison with THO results (circles) for ^{110}Zr, in normal scale (left column panels) and logarithmic scale (right column panels).

While agreement between the PTG and THO densities for ^{110}Zr is good in normal scale, we can notice discrepancies in asymptotic properties, which are visible from the figure in logarithmic scale (see Fig. 1). It is obvious that all densities calculated with the THO basis eventually follow the common asymptote dictated by the scaling function, while they are well reproduced with

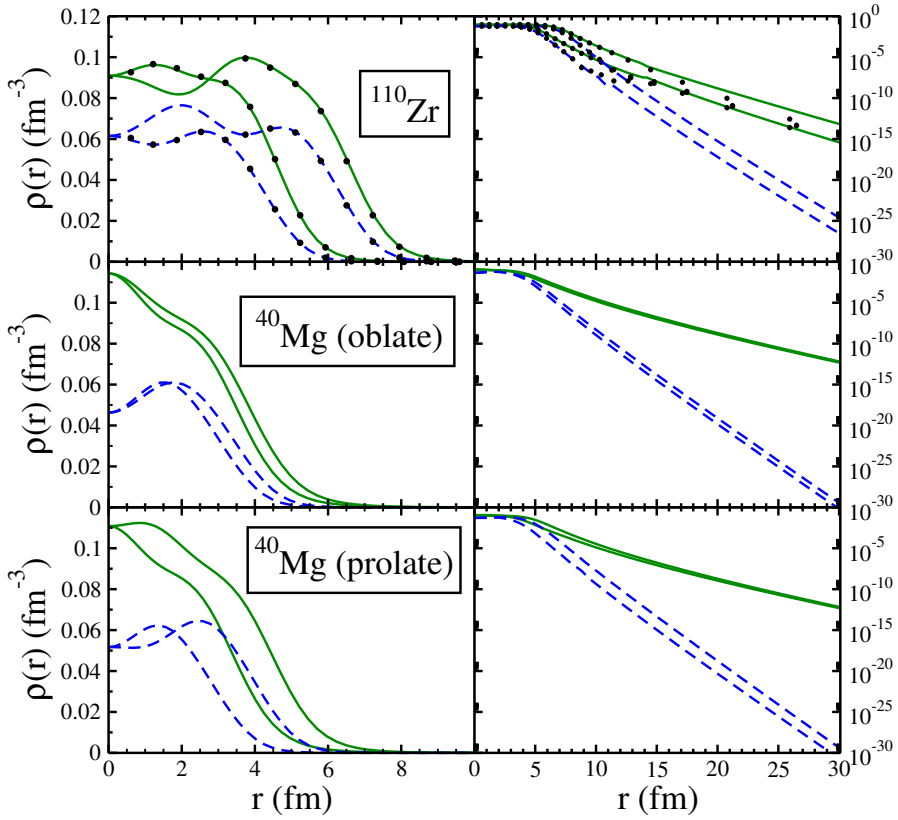

Figure 1. (color online) The neutron and proton densities of the prolately deformed nucleus ^{110}Zr ($\beta = 0.40$), respectively calculated by the HFB/PTG (respectively solid and dashed lines) and HFB/THO (circles) methods in normal (top left) and logarithmic (top right) scale. They are given along the long and short axes of deformation, easily identified from the figure. The neutron and proton densities of ^{40}Mg calculated by the HFB/PTG method for two states with different deformations (oblate $\beta = -0.09$ and prolate $\beta = 0.26$) in normal (middle and bottom left) and logarithmic (middle and bottom right) scale are also provided with the same line convention.

Table 1. Comparison of ground state properties of ^{110}Zr calculated with the HFB/Box, HFB/PTG and HFB/THO approaches. The rms radii are in fm, quadrupole moments are in barn, and all other quantities are in MeV.

	HFB/Box	HFB/PTG	HFB/THO
Q_{tot}	12.088	12.53	12.303
Δ_n	0.480	0.626	0.562
E_n^{pair}	-1.53	-3.015	-2.05
r_n	4.82	4.836	4.831
r_p	4.55	4.560	4.556
E_{tot}	-893.93	-893.952	-893.711

use of the PTG basis. This comparison also confirms the presence of deformation effects even in the far asymptotic region.

4. Conclusions

The HFB/PTG method is based on configuration-space diagonalization of the HFB Hamiltonian in the complete set of analytical PTG and Bessel/Coulomb wave functions, thus restoring the correct asymptotic properties of the HFB wave functions. The PTG potential is chosen to fit the nuclear HF potential and effective mass. The resulting PTG wave functions are close to the bound and continuum states of the related HF potential while the resonance states are substituted by the bound PTG states. Partial waves of high angular momentum are very well represented by Bessel/Coulomb wave functions. The examples shown, with a strongly deformed nucleus ^{110}Zr and ^{40}Mg with prolate and oblate deformations, compare well with coordinate space and THO results and thus have demonstrated the efficiency of the HFB/PTG method.

Acknowledgments

The authors acknowledge Japan Society for the Promotion of Science for awarding The Invitation Fellowship for Research in Japan (Long-term) to M. S. and The JSPS Postdoctoral Fellowship for Foreign Researchers to N. M., which make our collaboration possible. This work was supported by the JSPS Core-to-Core Program "International Research Network for Exotic Femto Systems." This work was carried out as a part of the U.S. Department of Energy under Contracts Nos. DE-FG02-96ER40963 (University of Tennessee), DE-AC05-00OR22725 with UT-Battelle, LLC (Oak Ridge National Laboratory), and DE-FG05-87ER40361 (Joint Institute for Heavy Ion Research), the UNEDF SciDAC Collaboration supported by the U.S. Department of Energy under grant No. DE-FC02-07ER41457.

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