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Relativistic Hartree-Fock-Bogoliubov predictions of superheavy magic nuclei

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Abstract. The occurrence of spherical shell closures in the superheavy nuclei region is explored in the framework of the relativistic Hartree-Fock-Bogoliubov theory (RHFB), and also with the simpler version of relativistic mean field with quasiparticles, in other words the relativistic Hartree-Bogoliubov (RHB) approximation. Both theoretical frameworks are often used for nuclei in the known regions of the nuclear chart. Shell closures characterized in terms of two-nucleon gaps indicate the magic regions. The results depend slightly on the effective Lagrangians used, but the magic numbers beyond ^{208}Pb are generally predicted to be $Z = 120$, 138 for protons and $N = 172$, 184, 228, 258 for neutrons. Shell effects are sensitive to various terms of the mean-field, such as the spin-orbit coupling, the scalar and effective masses. This explains the (relatively small) variations in the predictions, depending on the effective Lagrangians employed. The most complete model (RHFB) favors the nuclide ^{304}120 as the next spherical doubly-magic nucleus beyond ^{208}Pb.

1. Introduction

In modern nuclear physics, a challenging frontier remains in exploring the mass and charge limits of the superheavy nuclei (SHN) with proton numbers $Z \geqslant 104$. In the past years, many efforts have been devoted to identifying the position of the so-called stability island of the SHN, which depends on the balance of various contributions to the nuclear binding energy [1]. Experimentally, superheavy elements (SHE) have been synthesized up to $Z = 118$ [2]. The increasing survival probabilities of the measured SHE from $Z = 114$ to 118 seem to indicate enhanced shell effects with increasing Z and therefore a possible proton magic shell in the superheavy region. This would correspond to the position of the superheavy island, in the region $Z \geqslant 120$ [3].

It is thus interesting to explore with various microscopic models the doubly closed-shell systems within a spherical symmetry assumption. The shells are essentially determined by the spin-orbit (SO) splittings, and by the nucleon effective masses. On the other hand, the occurrence of shell closures could be somehow connected with approximate degeneracies of pseudo-spin (PS) partners [4, 5]. In the non-relativistic self-consistent mean field theory [6, 7], the SO splittings depend directly on an extra SO parameter in the energy density functional. In the covariant density functional (CDF) theory, such as the relativistic Hartree-Bogoliubov

(RHB) [8, 9] or the relativistic Hartree-Fock-Bogoliubov (RHFB) [10] approaches, the SO potential is naturally brought about by the same Lorentz scalar and vector fields which create the central potential. The number of independent degrees of freedom is thus reduced, and this could be an advantage for exploring unknown regions. Furthermore, in the more complete RHFB version of the CDF theory where the Lorentz $\rho - N$ tensor coupling can be included, the SO effects are found to be somewhat enhanced by this coupling [5], a feature which is not present in the simple RHB. This is one of the main motivations for undertaking the present study within the RHFB frame.

Aiming at the possible magic shells in the superheavy region, we investigate the superheavy nuclides covering $Z = 110 - 140$ and we compare the predictions of RHFB with those of RHB results where Fock terms are not explicitly considered. This short contribution is based on a recently published paper [11] where a more detailed discussion can be found. This contribution is organized as follows. In Sec. 2 we briefly introduce the RHFB theory. The occurrence of superheavy magic shells as well as the evolutions of the predicted shell closures are discussed in Sec. 3. A brief summary is presented in Sec. 4.

2. The Relativistic Hartree-Fock-Bogoliubov model

We briefly sketch the theoretical framework used here to describe the ground states of nuclei, and we apply it to spherically symmetric systems. The model consists of a Lagrangian $\mathscr{L}$ containing two parts. The first part $\mathscr{L}_{free}$ is a sum of terms describing the free nucleon field, free meson and photon fields. The second part $\mathscr{L}_I$ represents the nucleon-nucleon interaction mediated by the meson-nucleon and photon-nucleon couplings. This interaction Lagrangian can be expressed as:

$$\mathscr{L}_I = \bar{\psi}\Big(- g_\sigma \sigma - g_\omega \gamma^\mu \omega_\mu - g_\rho \gamma^\mu \vec{\rho}_\mu \cdot \vec{\tau} + \frac{f_\rho}{2M} \sigma_{\mu\nu} \partial^\nu \vec{\rho}^\mu \cdot \vec{\tau} - \frac{f_\pi}{m_\pi} \gamma_5 \gamma_\mu \partial^\mu \vec{\pi} \cdot \vec{\tau} - e\gamma^\mu A_\mu \frac{1-\tau_3}{2}\Big)\psi, \tag{1}$$

where ψ denotes the nucleon field whereas σ, ω_μ, $\vec{\rho}_\mu$, $\vec{\pi}$, and A_μ stand respectively for the isoscalar-scalar, isoscalar-vector, isovector-vector, isovector-pseudovector and photon fields. It can be noticed from Eq.(1) that, in this model the meson field $\vec{\rho}_\mu$ can be coupled to the nucleonic field ψ in two different ways, by vector-coupling with a coupling strength g_ρ, and by tensor-coupling with a coupling strength f_ρ. This Lagrangian is the most complete relativistic model to date. All meson-nucleon couplings g_i anf f_i are density-dependent, and their values have been adjusted in previous studies [5].

Following the standard variational procedure, one can obtain the field equations of the nucleon, mesons and photon, namely the Dirac, Klein-Gordon and Proca equations. The corresponding Hamiltonian H in nucleon space can be obtained through a Legendre transformation, as it is done, e.g., in Ref.[12]. This allows one to express H in terms of nucleonic operators only:

$$H = \sum_{\alpha\beta} c^\dagger_\alpha c_\beta T_{\alpha\beta} + \frac{1}{2} \sum_{\alpha\alpha'\beta\beta'} c^\dagger_\alpha c^\dagger_\beta c_{\beta'} c_{\alpha'} \sum_\phi V^\phi_{\alpha\beta\beta'\alpha'}, \tag{2}$$

where $T_{\alpha\beta}$ is the nucleon kinetic energy operator, and $V^\phi_{\alpha\beta\beta'\alpha'}$ stands for different types of two-body interactions mediated by the mesons (photon):

$$T_{\alpha\beta} = \int d\boldsymbol{r} \bar{\psi}_\alpha(\boldsymbol{r}) \left(-i\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} + M\right) \psi_\beta(\boldsymbol{r}), \tag{3}$$

$$V^\phi_{\alpha\beta\beta'\alpha'} = \int d\boldsymbol{r} d\boldsymbol{r}' \bar{\psi}_\alpha(\boldsymbol{r}) \bar{\psi}_\beta(\boldsymbol{r}') \Gamma_\phi D_\phi(\boldsymbol{r}, \boldsymbol{r}') \psi_{\beta'}(\boldsymbol{r}') \psi_{\alpha'}(\boldsymbol{r}), \tag{4}$$

and ϕ denotes the various meson (photon)-nucleon coupling channels, namely the σ-S, ω-V, ρ-V, ρ-T and ρ-vector-tensor (ρ-VT), π-PV and A-V couplings. The expressions of the Γ_ϕ and D_ϕ can be found in Ref.[12].

The pairing correlations are treated self-consistently by the RHFB method (see, e.g., Ref.[10]).

In this work, the integro-differential RHFB equations are solved by using a Dirac Woods-Saxon basis [13] with a radial cutoff $R = 28$ fm. The numbers of positive and negative energy states in the basis expansion for each single-particle (s.p.) angular momentum (l, j) are chosen to be 44 and 12, respectively.

3. Results and Discussion

The numerical applications have been carried out in RHFB approach with the parameter sets PKA1 [5] and the PKOi series (i=1, 2, 3) [14, 15] for the RHFB calculations, and PKDD [16] and DD-ME2 [17] Lagrangians for the RHB calculations. The DD-ME2 model is one of the most frequently used RMF Lagrangians, and we choose to compare with the PKDD parametrization to have an indication of the model dependence of the predictions. The PKOi parameter sets are the first density-dependent RHFB models in the literature whereas PKA1 is an improved version containing also a Lorentz tensor ρ-nucleon coupling.

The pairing fields are calculated with the finite-range Gogny force D1S [18] with a rescaling strength factor f, which is introduced to compensate for level-density differences among various mean field approaches. It is indeed known that pairing related quantities, such as odd-even mass differences and moments of inertia, are systematically overestimated in the RHFB calculations of heavy nuclei with the original Gogny pairing force [19]. Therefore, a renormalization factor $f = 0.9$ is applied to reproduce the odd-even mass differences in Pb isotopes.

In ordinary nuclei, the magicity is generally well marked, e.g., by a sizable shell gap along the isotopic or isotonic chains. In SHN, the shell effects are not so clearly visible. To identify the occurrence of shell closures in the superheavy region, we use the so-called two-nucleon gaps - δ_{2p} for protons and δ_{2n} for neutrons - namely the differences of two-nucleon separation energies of the neighboring isotopes or isotones which provide us with an efficient evaluation of the shell effects [20, 21]:

$$\delta_{2p}(N,Z) = S_{2p}(N,Z) - S_{2p}(N,Z+2), \tag{5}$$

$$\delta_{2n}(N,Z) = S_{2n}(N,Z) - S_{2n}(N+2,Z). \tag{6}$$

The peak values of δ_{2p} or δ_{2n} are essentially determined by the sudden jump of S_{2p} or S_{2n}, respectively. This constitutes a good indication of the emergence of closed shells.

To have further understanding on the model deviations, we compare the s.p. spectra obtained by the selected mean field functionals. Taking the predicted doubly magic SHN $^{304}120_{184}$ as an example, Fig. 1 shows the proton (left panel) and neutron (right panel) canonical s.p. spectra. It is found that PKA1 provides the most evident magicity at $Z = 120$ and $N = 184$, respectively, although these shell closures are relatively weaker than in ordinary nuclei. For the neutron shell $N = 184$, it is essentially determined by the degeneracy of two PS partners $\{2h_{11/2}, 1j_{13/2}\}$ and $\{4s_{1/2}, 3d_{3/2}\}$, respectively above and below the shell. For the latter, the PS partners are predicted to be almost degenerate by all the models considered, while for the former, the PS partners have high angular momentum and some differences among models are observed: PKA1 predicts a weak PS splitting, at variance with the predictions of the other Lagrangians.

It is interesting to discuss the structure of the s.p. levels for the proton shell closure $Z = 120$. As shown in the left panel of Fig. 1 the proton shell closure coincides with a large PS splitting, $\{3p_{3/2}, 2f_{5/2}\}$, whereas the SO doublet $\{3p_{1/2}, 3p_{3/2}\}$ above the shell is almost degenerate. The shell gap at $Z = 120$ can therefore be interpreted as a manifestation of a large PS splitting and a weak SO splitting. In fact as shown in Fig. 2, the evolution of proton (left plot) and neutron

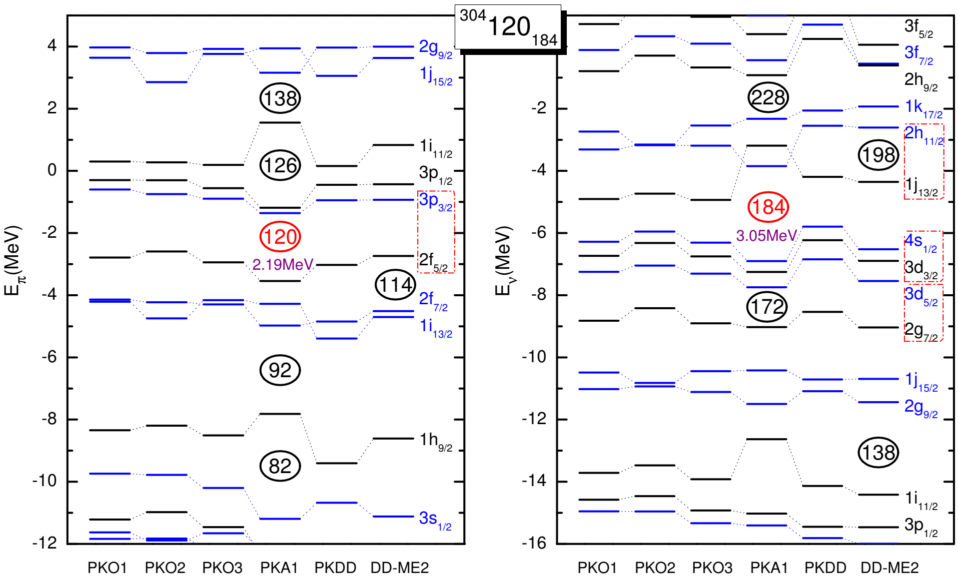

Figure 1. Proton (left panel) and neutron (right panel) single-particle spectra in the $^{304}120$ nuclide. The results with PKOi and PKA1 correspond to RHFB calculations, those with PKDD and DD-ME2 are obtained in RHB approximation.

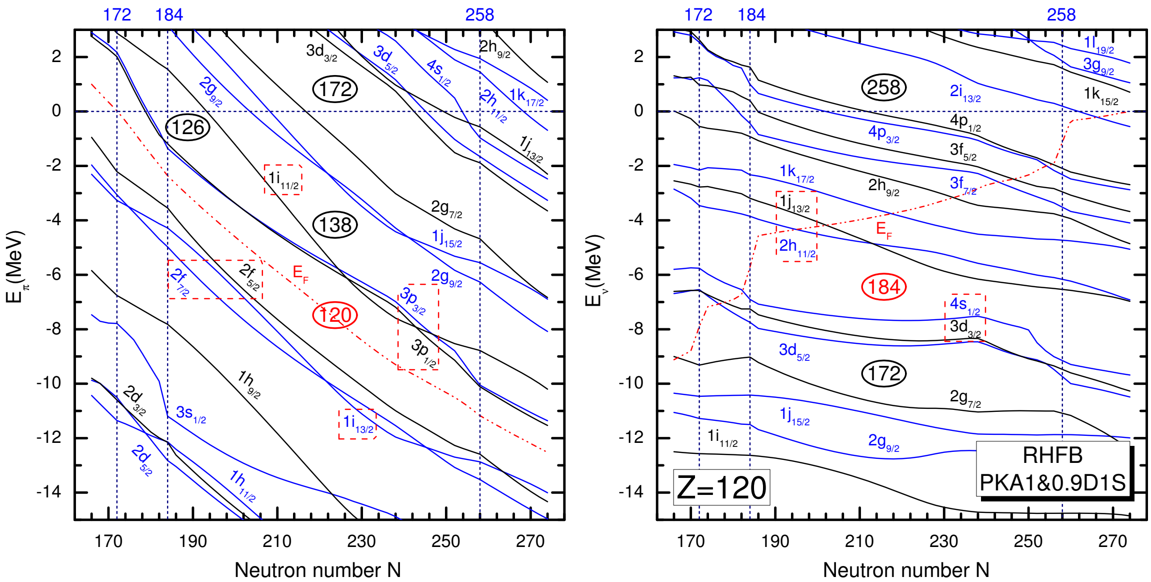

Figure 2. Proton (left plot) and neutron (right plot) single-particle energies along the isotopic chain of $Z = 120$. The results are extracted from the calculations of RHFB with the effective Lagrangian PKA1 and the D1S pairing force rescaled by a factor 0.9.

(right plot) s.p. energies along the $Z = 120$ isotopic chain determined by PKA1-RHFB model, it is also found that the spin partners $3p$ are almost degenerated and the SO splittings between the $2f$ states are not so distinct as generally expected. Coincident with the relation between the SO effects and PS symmetry conservation pointed out in Ref. [22], the reduced SO effects may lead to enlarged splitting between PS partners (i.e., $3p_{3/2}$ and $2f_{5/2}$).

4. Summary

In summary, the occurrence of spherical shell closures for SHN and the physics therein have been investigated using the RHFB theory with density-dependent meson-nucleon couplings, in comparison with the predictions of some RHB models. The shell effects are quantified in terms of two-nucleon gaps $\delta_{2n(p)}$. The results indicate that the nuclide $^{304}120_{184}$ could be the next spherically doubly magic nuclide beyond ^{208}Pb. It is also found that the shell effects in SHN are sensitive to the values of both scalar mass and effective mass, which essentially determine the spin-orbit effects and level density, respectively, and consistently the splittings between PS partners are essentially affects, which is also found to be tightly related with the emergence of superheavy magic shells. Additionally the analysis on the shell evolution as well as the density profile indicate that the emergence or disappearance of shell closure is tied up with the evolution of the central and spin-orbit mean fields, a feature that covariant mean field models may describe in a more unified way as compared to non-relativistic energy density functional (EDF) approaches. A further advantage of the RHFB framework is that exchange (Fock) terms are explicitly treated rather than approximately included by readjusted direct (Hartree) contributions as it is done in RHB (this is particularly true for the Coulomb exchange energy which is basically absent in RHB).

In this work, we have discussed the shell closure effects only at the mean field level, with the aim of comparing the predictions of different relativistic models. A more complete study would require, of course, to examine the changes brought about by the effects of particle-vibration coupling (see, e.g., Ref.[23]).

Experimental measurement of Q_α for at least one isotope of $Z = 120$ nucleus would help to set a proper constraint in determining the shell effects of SHN and to test further the reliability of the models as well. One also has to admit that for a more extensive exploration one needs to take into account the deformation effects.

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