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Ground State Structure of Hs Super-heavy Isotopes*

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Abstract: The ground state properties of Hs nuclei studied in the framework of the relativistic mean field theory revealed that more stable isotopes are located on the proton abundant side of the chain. The last stable nucleus to the proton drip line is ^{256}Hs. The most stable unknown Hs nucleus may be ^{268}Hs. The density dependent delta interaction pairing is used to improve the BCS pairing correction, which results in more reasonable single-particle energy level distributions and nucleon occupation, and it is shown to be available to describe the properties of nuclei in the superheavy region.

Key words: superheavy nucleus; nuclear structure; pairing

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So far about 85 superheavy elements (SHEs) with $Z=104$—118 (except $Z=117$), i.e., 14 SHEs have been produced by cold fusion reactions with lead or bismuth[1] as the target, or by hot fusion reactions with ^{48}Ca bombarding actinide targets[2] in experiments. However, there is a large gap of unknown isotopes between the neutron deficit super heavies obtained in cold fusion and the heaviest isotopes formed in hot fusion, especially, the latter isotopes underwent the spontaneous fission before reaching known nuclei. In order to have an overview of the island of super heavy nucleus (SHN), to study the structure and property of these unknown isotopes is very important.

The harsium nucleus ($Z=108$, Hs) was first identified as the isotope ^{265}108, produced in a ^{208}Pb (^{58}Fe, 1n) reaction[3]. Up to now, the $^{264-267, 269, 270, 277}$Hs isotopes have been known. Especially, it is worthy to note that the ^{270}Hs isotope, synthesized via reaction ^{248}Cm (^{26}Mg, 4n), was recently reported[4] as a doubly magic deformed nucleus by the GSI group. The experiment data provided an important point for theoretical models and clearly showed the enhanced nuclear stability at neutron number $N=162$ and proton number $Z=108$, which is the unique sub-double magic superheavy nucleus produced so far. The study of the structures and decay properties, and stabilities of the unknown nuclei in the Hs chain, is useful to give some information as how to synthesize and detect these nuclei, and at which characters they may connect with the decay chain of upper heavier nuclei, so that to fill the gap between the neutron deficient super heavies obtained in cold fusion and the heaviest isotopes formed in

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hot fusion.

Within the relativistic mean field(RMF) theory the ground state properties of the even Hs nuclei such as the binding energies, deformations, the radii of charge and neutron, alpha decay energy, neutron separation energy, the determination of the neutron drip line nucleus, single particle levels near the Fermi surface and so on are studied. The deformation in the present work is treated by that the nuclear spinors and meson fields are expanded in an axially deformed harmonic-oscillator basis with 20 shells taken into account as described in Refs. [5—7]. The quadrupole constrained calculations[5—7] have been performed in order to determine the ground-state deformations. A simple and commonly used method to deal with the paring interaction is Bardeen-Cooper-Schrieffer (BCS) theory, which considers the pairing interaction as a perturbation. However, Dobaczewski et al. have pointed out that the BCS approximation breaks down, if one has finite occupation probabilities for levels in the continuum[8]. We know that the most distinct phenomena for nuclei near the drip line are the weak binding and the appearance of the resonant states in the continuum, which are also the common phenomena for superheavy nuclei since their proton Fermi surfaces are usually close to the positive and some protons will be distributed in the positive levels by BCS treatment. Two important points for the microscopic study of the pairing interaction are the roles of finite range and of density dependence. The finite-range effect can be modelled by an explicit velocity dependence. Early calculations[9, 10] for nuclear matter predicted a very weak $^1S_0$ pairing at the saturation point (k_f=1.35 fm^{-1}), so it was concluded that strong pairing correlations in finite nuclei had to be due to interactions at the nuclear surface. The surface delta interaction (SDI) was thus used to deal with the problem[11, 12], however, the density dependent delta inter action(DDDI) is a more realistic density-dependent pairing force[13]. In this work, we incorporate the DDDI into the deformed RMF theory to calculate the pairing matrix element for the proton and neutron orbitals of even Hs isotopes as the following[14, 15]:

$$V = -V_0\left[1-\left(\frac{\rho(\boldsymbol{r})}{\rho_0}\right)^{\gamma}\right]\delta(\boldsymbol{r}_1-\boldsymbol{r}_2), \qquad (1)$$

where $\rho(\boldsymbol{r})$ is the isoscalar nucleon density, $\gamma=1$ and $\rho_0=0.16$ fm^{-3} (the saturation density of symmetric nuclear matter). The strength of the delta function interaction is taken as 850 MeV · fm^3 for neutrons and protons, which can give reasonable pairing gaps. As in the seniority pairing calculations, we consider only spin-singlet neutron-neutron, and proton-proton pairing. Based on the single-particle spectrum calculated with the RMF method, for either neutrons or protons, the pairing matrix elements may be written as

$$\begin{aligned}\overline{V}_{i\bar{i}j\bar{j}} &= \langle i\bar{i} \mid V \mid j\bar{j}\rangle - \langle i\bar{i} \mid V \mid \bar{j}j\rangle \\ &= -V_0\int \mathrm{d}^3 r\left[1-\left(\frac{\rho(\boldsymbol{r})}{\rho_0}\right)^{\gamma}\right]\times \\ &\quad(\psi_i^{\dagger}\psi_{\bar{i}}^{\dagger}\,\psi_j\psi_{\bar{j}} - \psi_i^{\dagger}\psi_{\bar{i}}^{\dagger}\,\psi_{\bar{j}}\,\psi_j).\end{aligned} \qquad (2)$$

It is necessary to prevent the unrealistic pairing of highly excited states, and to confine the region of influence of the pairing potential to the vicinity of the Fermi surface, thus a smooth cutoff factor is used as in Ref. [16]. For comparison, we have also carried out the calculations in the RMF+BCS model with a constant pairing interaction (RMF(CPI)). The pairing strengths, G_n= 15.0 MeV/A and G_p=20.0 MeV/A and the pairing window $\varepsilon_i-\lambda \leqslant 2(41\ A^{-1/3})$ MeV[6] have been adopted in the work. The NL-Z2 parameter set has been used and the values have been taken from Ref. [17].

Our calculation with DDDI pairing reveals 1.679 MeV neutron gap at neutron number N= 162 with β_2= 0.242, and 1.298 MeV proton gap at proton number Z = 108 with the quadrupole deformation β_2=0.262, so that the deformed double shell structure is produced.

In Fig. 1 the calculated binding energy per nucleon (BE/A) in this work is shown. The results are in good agreement with those from the macro-microscopic finite range droplet model (FRDM)[18] and the RMF(CPI) model. It is indicated that the bigger BE/A values lie in the range from $N=154$ ($A=262$) to $N=162$ ($A=270$). The nucleus, which has the maximum binding energy per nucleon for a given Z is the most stable nucleus against fission, and is related to the minimum Q value of fission[19]. Naturally, the bigger the nuclear binding energy per nucleon is, the stable the nucleus is against fission in the chain. Our calculated results revealed that the known nucleus $^{264, 266, 270}$Hs have the bigger binding energies per nucleon as 7.296, 7.298, and 7.295 MeV, respectively. So they are the more stable ones against fission among the chain. The bigger binding energy of ^{270}Hs confirmed that it is the deformed double sub-magic nucleus. These nuclei are mostly located on the neutron deficient side. When $A>270$ with increasing neutron numbers the BE/A values decreasing, and adding more neutrons doesn't seem to be able to increase the stability against fission. The experiment detected that ^{277}Hs goes to spontaneous fission, and so does the isotopes heavier than ^{277}Hs.

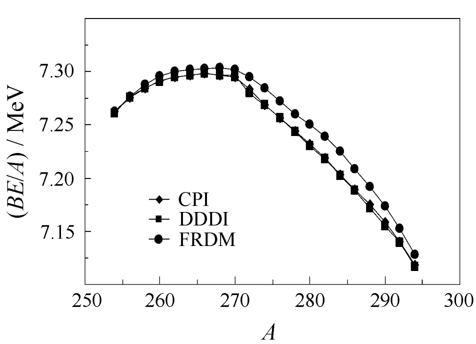

Fig. 1 The binding energy per particle for Hs isotopes.

The alpha-decay energies Q_α calculated using RMF theory with DDDI and CPI pairing and some available experimental data are plotted in Fig. 2. One observes minimum Q_α values at $N=162$ and $N=184$, respectively, and the shell effects are more distinct in the results of the DDDI model. And it is seen that the results from DDDI fit the known experimental data well and better than those from CPI. Generally, with increasing neutron number, the Q_α decreases, indicating increasing alpha-decay half life. One can estimate that at $A=277$ ($N=169$) the nucleus has a similar Q_α value as the nucleus $A=270$ ($N=162$) has, but we know from above, the nucleus $A=277$ ($N=169$) goes to fission. At this point of view it does not seem to hold the promise to have stable nucleus with $A>277$. In stead, on the neutron deficient side of the nucleus $A=277$ ($N=169$), the unknown nuclei look optimistic to be synthesized. The most optimistic candidate is ^{268}Hs with $N=160$.

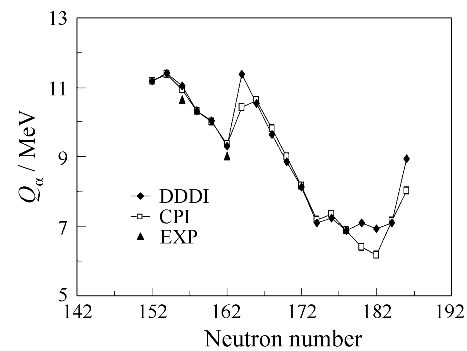

Fig. 2 The Q_α values for Hs isotopes.

The calculated ground-state quadrupole deformation parameter β_2 is plotted in Fig. 3 and the deformations calculated with FRDM and CPI are also shown for comparison. From the calculation with DDDI pairing the synthesized nuclei $^{264-267, 269, 270, 277}$Hs are all well deformed, and with increasing neutron number the ground-state shape has no sudden change from prolate to oblate. The deformation magnitudes and the tendency are in coincidence with the results from Ref. [20]. With increasing A the shape turns into spherical one as the nucleus approaches the magic neutron number $N=184$ ($A=292$) and then becomes oblate. But bigger descent of the deformation from $N=162$ and 184 to the next nuclei can clearly be seen, indicating the shell closures. At $N=162$, $\beta_2=0.250$, this reveals the deformed sub-closure, and for it the three showed results are very agreeable. Results after A

$=276$ from FRDM, and after $A=286$ from CPI are not so smooth, but three results are in coincidence again at $N=176(A=284)$, which is a small sub-magic number again.

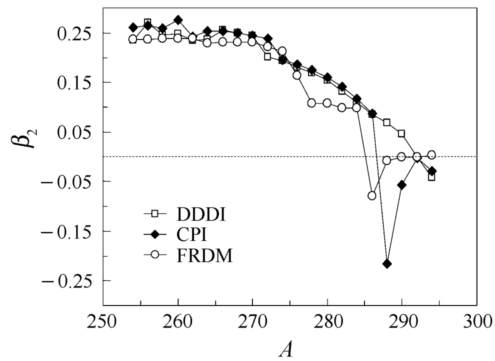

Fig. 3 The ground-state quadrupole deformation parameter as a function of the mass number of Hs nuclei.

In order to get further insight into shell effects, the two-neutron-separation energies by RMF(DDDI) for Hs isotopes have been plotted in Fig. 4. The results of the RMF(CPI) and FRDM model have also been shown for comparison. The

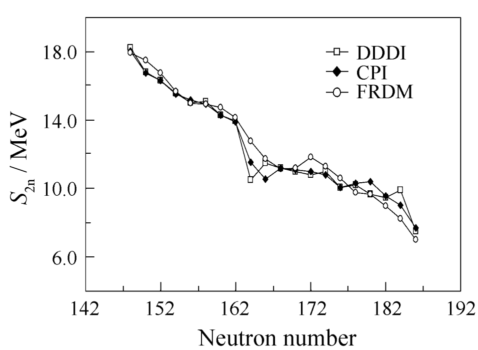

Fig. 4 Two-neutron separation energy S_{2n} for Hs isotopes.

two-neutron separation energy S_{2n} is evaluated from the binding energies of the two neighboring even isotopes with N and $N-2$ neutrons: $S_{2n}(Z, N)=B(Z, N)-B(Z, N-2)$. From the figure, it can be seen that a strong kink in the S_{2n} values is clearly visible at $N=162$ and 184, and a slight kink at $N=174$. In addition, the phenomenon is more evident in the DDDI calculations. The neutron drip line can go very far due to the absence of repulsive force, but those nuclei will not be stable against fission as we mentioned above.

To determine the drip-line nuclei the separation energy for an additional neutron or proton from the drip-line nuclei should be equal to or less than zero. As mentioned above, the super-heavy nuclei Hs can contain a lot of neutrons from the binding energy point of view, however, very neutron abundant Hs nuclei are not stable against fission. We are thus interested in proton drip-line nucleus. In Fig. 5 one proton separation energy for Hs isotopes is shown as a function of the neutron number, where the blocking method is adopted to deal with unpaired odd protons. As the neutron number decreases nucleus is getting closer to proton drip line. The one proton separation energy for ^{254}Hs is becoming negative, one may thus conclude that nucleus ^{256}Hs is the last bound nucleus.

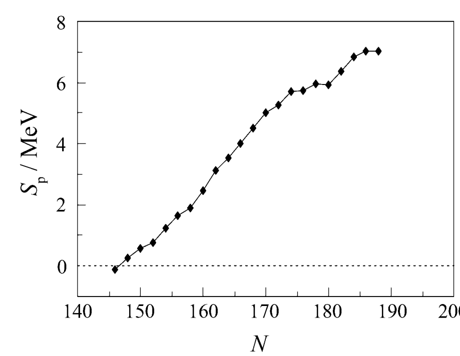

Fig. 5 Single proton separation energy S_p for Hs isotopes.

In order to confirm the drip line Hs nucleus the energy level diagram of nucleus ^{254,256}Hs is shown in Fig. 6. The last two protons of ^{254}Hs in Fig. 6 are at $\frac{9}{2}^+$[624](with 99.9% probability), which are already located in the unbound region with energy 0.334 1 MeV. While that for ^{256}Hs the last two protons are distributed at the state $\frac{1}{2}^+$ [651](100%) with energy −0.35 MeV. Therefore ^{256}Hs might be determined as the last proton stable nucleus. The conclusion is in coincidence with the result from one proton separation energy.

Conventional pairing calculations are carried out by using the BCS method with a constant pairing interaction. This method is, however, not ap-

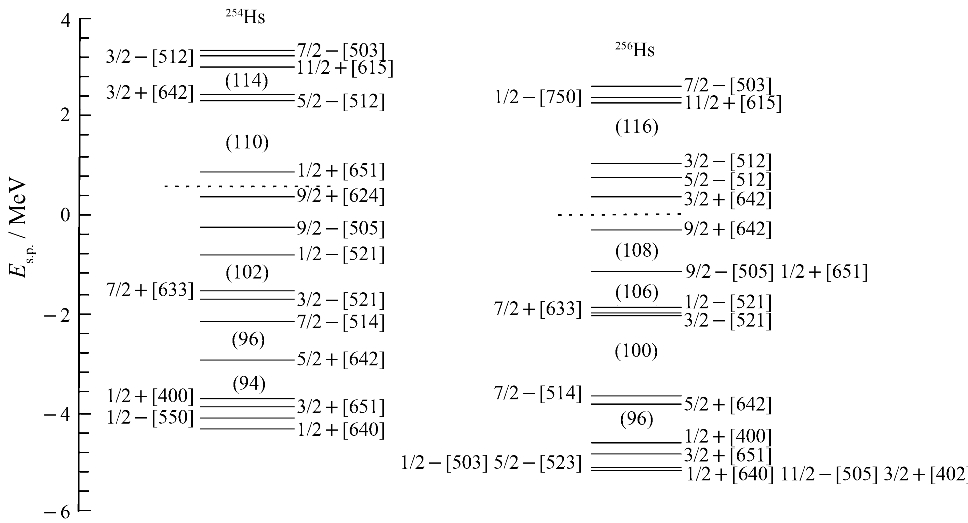

Fig. 6 The energy level diagram of nucleus ^{254,256}Hs.

plicable to the case of nuclei whose nucleon Fermi surface is close to the zero energy, since the positive states in the continuum for such nuclei are important, and the conventional BCS theory does not treat those positive states. In DDDI pairing treatment, the interaction between different paired nucleons is state-dependent, and the positive states, whose wave functions are concentrated in the nuclear region, also contribute to the pairing matrix elements. This results in more reasonable single particle energy level distributions and nucleon occupations. In this context, we studied the continuum levels and the particle occupation probabilities on the levels by using the constant pairing interaction(CPI) and the DDDI, respectively. The nucleon occupation numbers N_{occu} in the positive energy states for Hs are plotted in Fig. 7(a). It is seen that the nucleon occupation numbers N_{occu} in the positive energy states by the DDDI are generally equal to zero, while for CPI are not, especially for nuclei $A < 260$ the N_{occu} for CPI are much larger than those for DDDI. For magic nucleus ^{270}Hs, the $N_{occu} = 0$ for both cases due to the compact nucleon distribution in sub-double closure levels. When $A < 260$, the N_{occu} increase steeply for CPI pairing, which may indicate the failure of the theory. While for DDDI pairing N_{occu} increase steeply until $A <$ 256. The figure confirmed the necessity of the DDDI treatment. In Fig. 7(b), the corresponding Fermi surface is shown as a function of mass number A. One may find that more protons distribute in the positive levels when the Fermi surface is getting closer to zero. And the CPI always gives higher Fermi surface than that in DDDI.

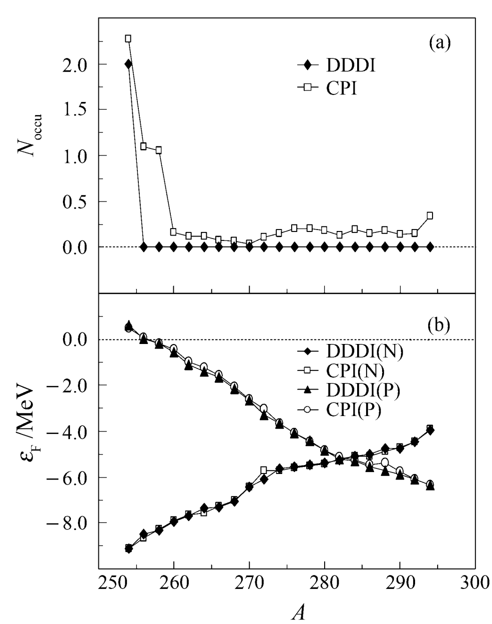

Fig. 7 The total nucleon occupation numbers N_{occu} in the positive-energy states(a) and Fermi energy for Hs isotopes (b).

In summary, the ground state properties of Hs nuclei were studied to give an overview to the isotope chain. It is seen that more stable isotopes are located on the proton abundant side of the chain. The last stable nucleus to the proton drip line is ^{256}Hs. The most stable unknown Hs nucleus may be ^{268}Hs. The proton Fermi surfaces of Hs nuclei are close to zero, the BCS treatment with CPI excites protons to the continuum, and causes the failure for pairing correction. The use of the DDDI to the BCS method has provided us a possibility to take into account the effects of the positive continuum states and on this basis to study the energy level distributions, occupations and the ground state properties in RMF theory with deformation in a self-consistent way. This theory and the resulting calculations describe the properties of nuclei in the superheavy nucleus well. In DDDI, the interaction between different paired nucleons is state dependent, the positive states whose wave functions are concentrated in the nuclear region, also contribute to the pairing matrix elements. This results in more reasonable single-particle energy level distributions and nucleon occupation. Therefore the theory by DDDI is generated to be available to describe the properties of nuclei in the superheavy region.

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