

Global α -decay study based on the mass table of the relativistic continuum Hartree-Bogoliubov theory*

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Abstract: The α -decay energies (Q_α) are systematically investigated with the nuclear masses for $10 \leq Z \leq 120$ isotopes obtained by the relativistic continuum Hartree-Bogoliubov (RCHB) theory with the covariant density functional PC-PK1, and compared with available experimental values. It is found that the α -decay energies deduced from the RCHB results present a similar pattern to those from available experiments. Owing to the large predicted Q_α values (≥ 4 MeV), many undiscovered heavy nuclei in the proton-rich side and super-heavy nuclei may have large possibilities for α -decay. The influence of nuclear shell structure on α -decay energies is also analysed.

Keywords: α -decay, RCHB theory, mass table, shell structure

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1 Introduction

The discovery of nuclear radioactivity one century ago may be considered as the beginning of nuclear physics [1]. Up to now, several nuclear decay modes have been observed experimentally, including α -decay, β -decay, orbital electron capture, spontaneous fission, proton decay and neutron decay [2]. One of the most important decay modes is α -decay, the investigation of which plays an essential role in exploring nuclear structure, especially for nuclei in the heavy and super-heavy nuclear regions [2].

One crucial characteristic quantity of an α -emitter is the α -decay energy Q_α , which is defined as

$$Q_\alpha = E_B(Z-2, N-2) + E_B(2, 2) - E_B(Z, N), \quad (1)$$

where $E_B(Z, N)$ is the binding energy for the nucleus with proton number Z and neutron number N . With the α -decay energies, a number of empirical formulae have been proposed for the half-lives of nuclei [3–7]. One of the necessary conditions for a nucleus to spontaneously emit an α -particle is that the α -decay energy Q_α must be positive. Consequently, in order to investigate the α -decay energies, the precise nuclear masses are needed. Experimentally, nuclear masses of more than 2000 nuclei have been measured thanks to the application of cyclotron,

storage ring and Penning trap facilities [8]. However, α -decay is also expected to happen in the large unknown region of the nuclear chart, which is still beyond experimental capabilities for the foreseeable future. Therefore, a systematic investigation of α -decay energies has to rely on robust theoretical nuclear mass models.

Theoretical investigations of nuclear masses can be classified into the following two categories. The first consists of macroscopic-microscopic models, such as the liquid drop model (LDM) [9], finite-range droplet model (FRDM) [10], extended Thomas-Fermi plus Strutinsky integral with shell quenching (ETFSI-Q) model [11] and Weizsäcker-Skyrme mass model (WS) [12–17]. The second is composed of microscopic models, for example, the Hartree-Fock-Bogoliubov (HFB) model [18–20] based on density functional theory (DFT), which is believed to have a reliable extrapolation to the unknown regions.

Nowadays, covariant density functional theory (CDFT) has attracted extensive attention because of the successful description of many nuclear phenomena [21–28]. It can provide a natural inclusion of the nucleon spin degree of freedom, resulting in the nuclear spin-orbit potential that emerges automatically with the empirical strength in a covariant way. It provides a new saturation mechanism for nuclear matter [29], reproduces well

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the measured isotopic shifts in the Pb region [30], reveals more naturally the origin of pseudospin symmetry [31, 32] as a relativistic symmetry [33–43], and predicts the spin symmetry in the anti-nucleon spectrum [44, 45]. It can also include nuclear magnetism [46], i.e., a consistent description of currents and time-odd fields, which plays a crucial role in nuclear magnetic moments [47–50] and nuclear rotations [51–54]. The CDFT is a reliable and useful model for nuclear structure study across the whole nuclear chart.

The first CDFT mass table calculated 2000 even-even nuclei with $8 \leq Z \leq 120$ [55], but without treating pairing correlations. Later, using the Bardeen-Cooper-Schrieffer (BCS) method, the ground-state properties of 1315 even-even nuclei with $10 \leq Z \leq 98$ were calculated [56]. In 2005, by employing the state-dependent BCS method with a delta pairing force, the first systematic study of the ground-state properties for about 7000 nuclei was performed [57]. More recently, the RHB framework was used for a systematic study of ground state properties of all even-even nuclei from the proton to neutron drip lines [58, 59].

It is widely considered that pairing correlation has a critical influence on open shell nuclei [24]. Among the methods in dealing with pairing correlation, the Bogoliubov quasiparticle transformation is generally used for exotic nuclei which can include the continuum appropriately when treated in the coordinate representation [60]. As an extension of the relativistic mean field and the Bogoliubov transformation in the coordinate representation, relativistic continuum Hartree-Bogoliubov (RCHB) theory provides a fully self-consistent description of both the continuum and the bound states as well as the coupling between them [61–63]. The halo in ^{11}Li has been described [61, 63] and the giant halos in light and medium-heavy nuclei were predicted [60, 62, 64]. In addition, generalizations to the odd-nucleon system [65, 66] and deformed nuclei [67–69] were developed.

To investigate the impact of the continuum on the nuclear chart, the RCHB theory is used to systematically calculate nuclear masses for $8 \leq Z \leq 120$ isotopes by assuming spherical symmetry. Taking the nuclear chart ranging from O to Ti as an example, the influence of the continuum on nucleon drip-lines has been investigated in Ref. [70]. It shows that although the proton drip-lines predicted with various mass models, such as FRDM [10], WS3 [14], HFB-21 [20] and TMA [57], are roughly the same and basically agree with observation, the neutron drip-line predicted by RCHB theory with the covariant density functional PC-PK1 [71] is extended further into the neutron-rich region than other mass models due to the continuum couplings. Therefore, it is interesting to systematically study the nuclear ground-state properties, such as nuclear mass and radius, by using the mass table

provided by RCHB theory. Meanwhile, it is also possible to systematically study nuclear decay modes related to the nuclear masses.

In this paper, the α -decay energies will be systematically investigated based on the RCHB mass table for $8 \leq Z \leq 120$ isotopes [72], calculated in RCHB theory with the covariant density functional PC-PK1. The RCHB results are compared with available experimental values. The influence of nuclear shell structure on α -decay energies is also investigated.

2 Theoretical framework

Starting from the effective Lagrangian density

$$\mathcal{L} = \mathcal{L}^{\text{free}} + \mathcal{L}^{\text{4f}} + \mathcal{L}^{\text{hot}} + \mathcal{L}^{\text{der}} + \mathcal{L}^{\text{em}}, \quad (2)$$

where

$$\mathcal{L}^{\text{free}} = \bar{\psi}(i\gamma_\mu \partial^\mu - m)\psi, \quad (3)$$

$$\begin{aligned} \mathcal{L}^{\text{4f}} = & -\frac{1}{2}\alpha_S(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi) \\ & - \frac{1}{2}\alpha_{\text{TV}}(\bar{\psi}\boldsymbol{\tau}\gamma_\mu\psi)(\bar{\psi}\boldsymbol{\tau}\gamma^\mu\psi), \end{aligned} \quad (4)$$

$$\begin{aligned} \mathcal{L}^{\text{hot}} = & -\frac{1}{3}\beta_S(\bar{\psi}\psi)^3 - \frac{1}{4}\gamma_V[(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)]^2 \\ & - \frac{1}{4}\gamma_S(\bar{\psi}\psi)^4, \end{aligned} \quad (5)$$

$$\begin{aligned} \mathcal{L}^{\text{der}} = & -\frac{1}{2}\delta_S\partial_\nu(\bar{\psi}\psi)\partial^\nu(\bar{\psi}\psi) - \frac{1}{2}\delta_V\partial_\nu(\bar{\psi}\gamma_\mu\psi)\partial^\nu(\bar{\psi}\gamma^\mu\psi) \\ & - \frac{1}{2}\delta_{\text{TV}}\partial_\nu(\bar{\psi}\boldsymbol{\tau}\gamma_\mu\psi)\partial^\nu(\bar{\psi}\boldsymbol{\tau}\gamma^\mu\psi), \end{aligned} \quad (6)$$

$$\mathcal{L}^{\text{em}} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - e\frac{1-\tau_3}{2}\bar{\psi}\gamma^\mu\psi A_\mu, \quad (7)$$

one can derive the RHB equation for the nucleons [73],

$$\begin{pmatrix} h_D - \lambda & \Delta \\ -\Delta^* & -h_D^* + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}, \quad (8)$$

where

$$h_D(\mathbf{r}) = \boldsymbol{\alpha} \cdot \mathbf{p} + V(\mathbf{r}) + \beta(M + S(\mathbf{r})), \quad (9)$$

and find the solution self-consistently. With the spherical symmetry, the RCHB theory solves the RHB equations in coordinate space. For the detailed formalism and numerical techniques, see Ref. [63] and references therein. In the present calculations, we follow the procedures in Refs. [63, 65] and solve the RCHB equations in a box with size $R=20$ fm and step size 0.1 fm. In addition, we use the density functional PC-PK1 [71] for the particle-hole channel, while for the particle-particle channel, the density-dependent delta pairing force

$$V(\mathbf{r}_1, \mathbf{r}_2) = V_0\delta(\mathbf{r}_1 - \mathbf{r}_2)\frac{1}{4}[1 - \boldsymbol{\sigma}_1\boldsymbol{\sigma}_2] \left(1 - \frac{\rho(\mathbf{r}_1)}{\rho_0}\right), \quad (10)$$

is employed. In equation (10) the saturation density $\rho_0 = 0.152 \text{ fm}^{-3}$ and the pairing strength $V_0 = 685.0 \text{ MeV} \cdot \text{fm}^3$ is fixed by reproducing experimental odd-even mass differences of $Z = 20, 50, 78, 92$ isotope chains and $N = 20, 50, 78, 92$ isotone chains, respectively. The contribution from the continuum is restricted within a cutoff energy $E_{\text{cut}} = 100 \text{ MeV}$ and cutoff angular momentum $j_{\text{max}} = \frac{19}{2} \hbar$.

3 Results and discussion

By using the binding energies provided in the RCHB theory with the density functional PC-PK1 [71], the Q_α values of 9035 predicted bound nuclei with $10 \leq Z \leq 120$ [72] are obtained with Eq. (1). It is found that the values of 3703 nuclei, plotted with different colors in Fig. 1(a), are positive. Among these nuclei, the Q_α values of 1629 nuclei are less than 4 MeV, of 1299 nuclei are within 4–8 MeV, of 734 nuclei are within 8–12 MeV, and of 41 nuclei are larger than 12 MeV. Several systematic features can be found from Fig. 1(a): 1) From a global view, most nuclei with positive Q_α values are located in

the upper-left side of the nuclear chart; 2) For a given isotope chain, Q_α generally decreases with the increase of neutron number N ; 3) For a given isotone chain, Q_α generally increases with the increase of proton number Z ; 4) The Q_α value can be greatly influenced by the existing shell structure, which can be clearly seen from the sudden increase of Q_α when Z or N cross the magic numbers 28, 50, 82 and 126; 5) The lightest nucleus predicted to have positive Q_α value in the RCHB mass table is ^{20}Ne ($Q_\alpha = 0.14 \text{ MeV}$), and then several $Z \approx N$ nuclei in the $A \sim 60$ mass region; 6) Nuclei with very large Q_α values ($> 4 \text{ MeV}$) are mostly the heavy or superheavy neutron-deficient nuclei; 7) Remarkably, in the superheavy mass region around $Z \sim 120$, positive Q_α can be even extended to the neutron-rich region.

Analogously, the experimental Q_α values are obtained with Eq. (1) from the evaluated mass data in AME2012 mass table [74] and those of 1067 nuclei, plotted in Fig. 1(b), are found to be positive. In particular, there are 719 nuclei observed experimentally with α -decay radioactivity at present [75], marked with green crosses in Figs. 1(a) and 1(b). It should be emphasized

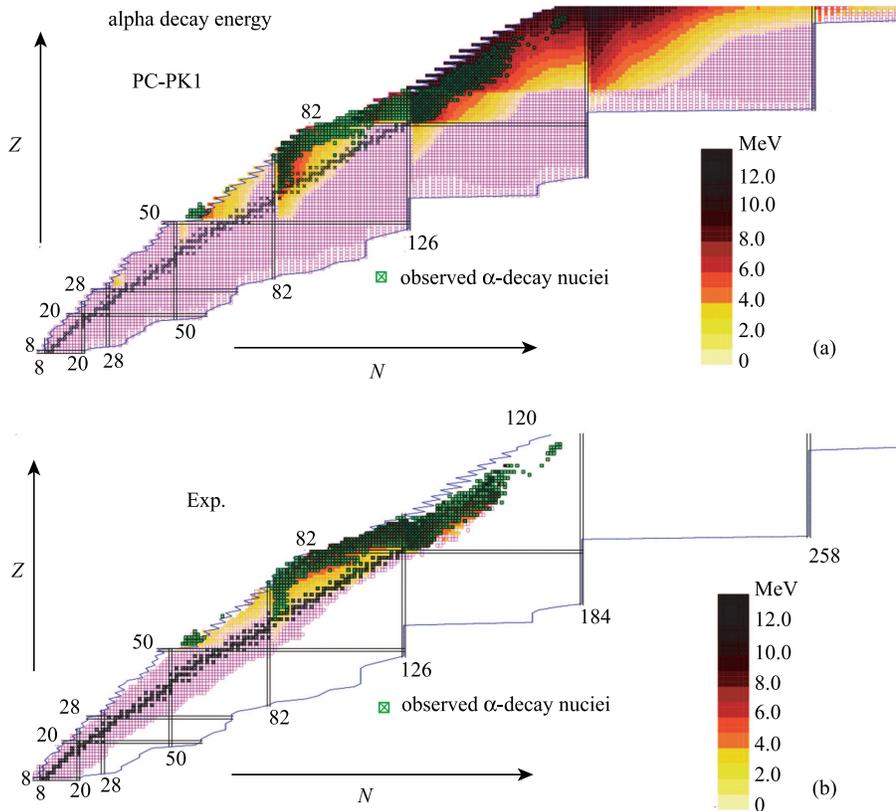


Fig. 1. (color online) α -decay energies Q_α for nuclei with $10 \leq Z \leq 120$, provided by (a) RCHB theory with the density functional PC-PK1 [71] and (b) available experimental values [74]. Blue lines are proton and neutron drip-lines predicted by the RCHB theory. The nuclei predicted to be bound in the present work and observed experimentally are represented as squares. The 719 nuclei observed experimentally with α -decay radioactivity are marked with green crosses.

that the aim is not to compare theoretical and experimental Q_α values in detail, but rather to investigate the schematic evolution of the α -decay energies.

Although the general features of α -decay are well known, for completeness, the following remarks are noted here from Fig. 1(b): 1) The lightest nucleus presently found to have α -decay radioactivity is ^{105}Te [75], and $A \sim 100$ marks the lightest mass region with α -decay radioactivity; 2) Globally, α -decay is mainly observed in the neutron deficient nuclei with $N \geq 84$; 3) In the region $N \geq 126$, most of the nuclei are found to have α -decay radioactivity and particularly, almost all observed superheavy nuclei ($Z \geq 110$) have α -decay radioactivity; 4) Due to the Coulomb barrier and the competition of other decay modes, not all nuclei with positive Q_α values are observed to have α -decay radioactivity in the ground state. Among the 719 nuclei observed with α -decay radioactivity, ^{187}Re is the one with the smallest Q_α value (1.66 MeV), and about 70 percent of nuclei have Q_α values larger than 4.0 MeV; 5) There are 68 nuclei with Q_α values larger than 4.0 MeV not observed to have α -radioactivity in the ground state, which, however, have been found to decay by other modes, such as β^+ , EC, β^- decays or spontaneous fission.

When comparing the two panels of Fig. 1, the following features can be found. First, although spherical symmetry is assumed, the positive α -decay energies deduced from the RCHB results still present a similar pattern as those from available experimental values. It is noted that for the magic number nuclei ($Z = 8, 20, 28, 50, 82$ or $N = 8, 20, 28, 50, 82, 126$), the root-mean-square (rms) deviation of binding energies between RCHB calculation and experimental data is 2.157 MeV and the rms deviation of Q_α between the RCHB calculation and experimental data is 2.024 MeV. The macroscopic - microscopic mass model [10–17]

has achieved great success in describing binding energy, with the rms deviation with respect to all the available mass data reaching 0.298 MeV [15]. Compared with the macroscopic-microscopic model, the RCHB theory contains only a few parameters which are determined by fitting to some specific nuclei. In this sense, the rms deviations of the RCHB calculations are acceptable.

Second, in Fig. 1(a) most of the neutron-deficient nuclei in the heavy and superheavy regions are predicted to have Q_α values larger than 4 MeV, therefore it is expected these nuclei should have large possibilities for α -decay, consistent with the region of observed nuclei with α -radioactivity.

Third, in the unexplored superheavy nuclear region with $N > 184$ and $Z > 92$, there is a triangle-like region for nuclei with $Q_\alpha > 4$ MeV or even > 10 MeV, indicating the possibility of α -radioactivity for these neutron rich nuclei.

Fourth, 80 exotic nuclei which are measured experimentally, mainly in the neutron-deficient region near $Z = 50$ and $Z = 82$, are located beyond the proton drip-line of the RCHB mass table and are absent in the present prediction. This needs to be further examined in the future, for instance by taking into account the deformation effect and Wigner term [76].

To closely inspect the evolution of α -decay energies with proton and neutron numbers, a comparison between the calculated and experimental Q_α values in two specific mass regions ($Z = 50-82, N = 50-126$) and ($Z = 82-120, N = 82-184$) is given in Fig. 2. The shell effect can be clearly seen here. For example, a sudden Q_α change can be seen when the neutron number crosses $N = 126$ or the proton number crosses $Z = 82$. As a magic nucleus provides more stability, according to Eq. (1), the Q_α value of a magic nucleus is much smaller than that of a nucleus with two more protons or neutrons.

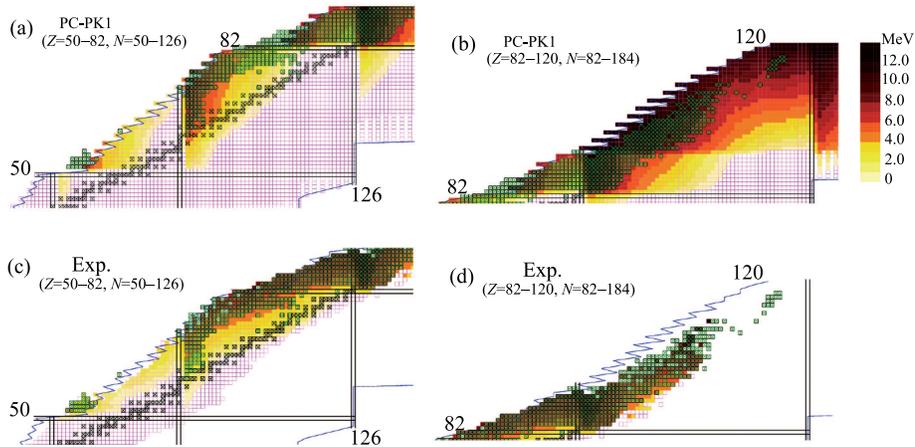


Fig. 2. (color online) Comparison between calculated and experimental Q_α values in the nuclear regions of ($Z = 50-82, N = 50-126$), and ($Z = 82-120, N = 82-184$).

The calculated and experimental α -decay energies Q_α for N (Z) = 80, 82, 84 isotone (isotope) chains are respectively shown in Fig. 3(a) and (b), and good agreement between them can easily be found. The influence of shell closure on the decay energies Q_α are illustrated in two aspects. First, as shown in the plots, a sudden increase of Q_α exists after the magic number $Z = 50$ ($N = 126$). Second, by comparing the three isotone (isotope) chains N (Z) = 80, 82, 84, both the calculated and experimental values of Q_α at N (Z) = 84 are clearly larger than the corresponding values at N (Z) = 80, 82.

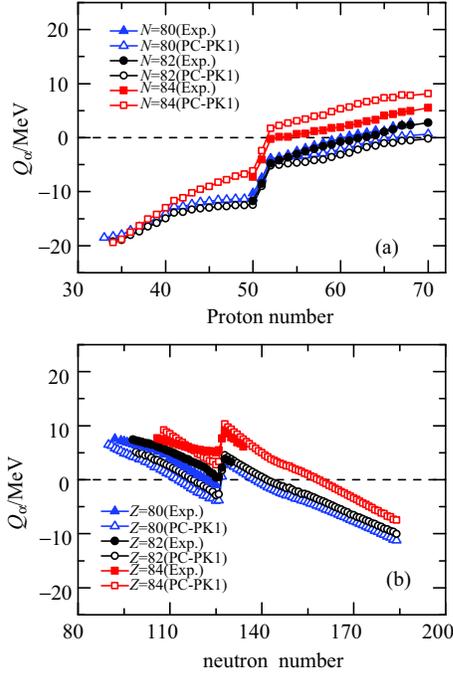


Fig. 3. (color online) α -decay energies Q_α for (a) $N = 80, 82, 84$ isotone chains; (b) $Z = 80, 82, 84$ isotopic chains.

Therefore, the sudden increase of the Q_α value along Z or N can be used as a probe for possible shell closures. In Fig. 4, the theoretical and experimental α -decay energies Q_α as functions of Z (N) are plotted for all the isotopic (isotonic) chains. As shown in Fig. 4, the sudden increases exist at the traditional proton magic numbers $Z = 20, 28, 50, 82$, and the neutron magic numbers $N = 8, 20, 28, 50, 82, 126$. Similar sudden increases of the theoretical Q_α value can also be clearly found at $Z = 16, 40, 92$, $N = 184, 258$, where $Z = 16$ has been proved as a magic number close to the neutron drip line [77, 78]; $Z = 40$ is generally considered as a sub-shell; $Z = 92$ is considered as a pseudo-shell in the relativistic mean field calculations; and $N = 184, 258$ are possibly the new magic numbers in the superheavy mass region, as suggested in the previous RCHB calculations [79] and the relativistic Hartree-Fock-Bogoliubov calculations [80].

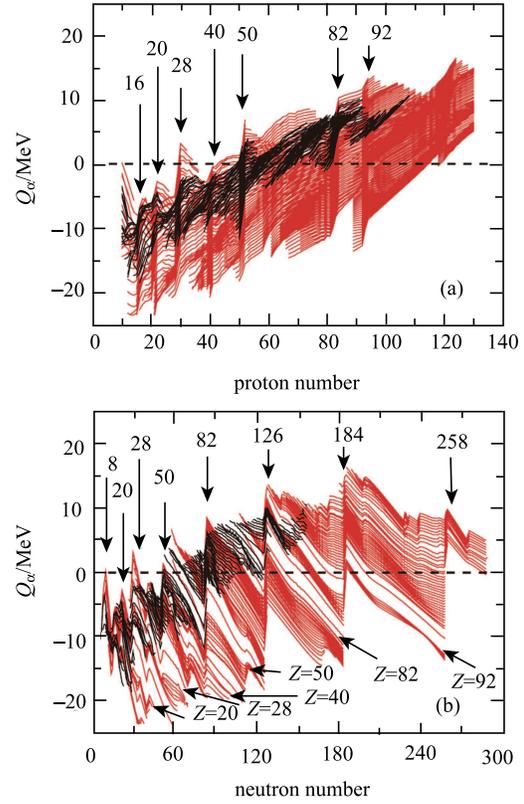


Fig. 4. (color online) α -decay energies Q_α as functions of (a) proton and (b) neutron numbers. The red lines represent the results of the RCHB theory with the covariant density functional PC-PK1; the black lines denote the experimental values from Ref. [74].

It is of particular interest to investigate the α -decay energies of superheavy nuclei, as α -decay is the most important decay mode for superheavy nuclei. In Fig. 5, the Q_α values for $110 \leq Z \leq 130$ isotopes are shown. The gap between $Z = 120$ and $Z = 122$ isotopic chains is larger than the others, which indicates that $Z = 120$ is a possible candidate for a proton magic number. As for

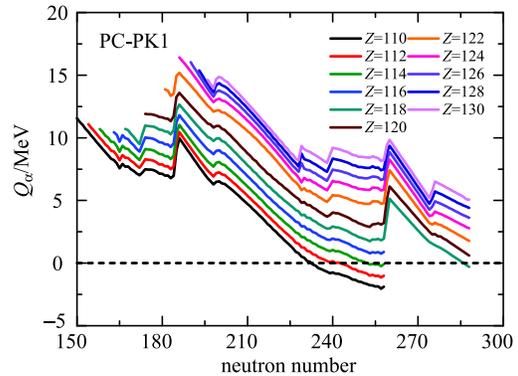


Fig. 5. (color online) α -decay energies Q_α for $Z = 110$ to 130 isotopic chains as functions of neutron number.

the possible proton magic number $Z = 114$ [81, 82], the gap between $Z = 114$ and $Z = 116$ isotopic chains is not so obvious as that for the $Z = 120$ isotopic chain. Furthermore, except the possible neutron magic number $N = 184$ and 258 which are mentioned in Fig. 4, the sudden increases at $N = 198, 228, 238$ and 274 can also be found in Fig. 5, which indicates the possible shell structures.

4 Summary and perspective

In conclusion, the α -decay energies with the RCHB mass table have been systematically studied. The Q_α values calculated by RCHB theory with the covariant density functional PC-PK1 agree well with experimental values. It is shown by available experimental values that α -decay is mainly observed in the proton-rich and heavy nuclear regions, and the values of observed Q_α^{exp} for most α -decay nuclei are larger than 4 MeV. In addition, illustrated by the calculated results, most of the decay energies Q_α predicted in the proton-rich heavy and super-heavy nuclear regions are larger than 4 MeV, which may indicate a large possibility for them to have

α -decay. By plotting α -decay energies Q_α for $N(Z) = 80, 82, 84$ isotone chains (isotope chains) calculated by RCHB theory and experimental values, the influence of shell effect on α -decay energies has also been investigated in detail. It is found that an abrupt change of Q_α exists when crossing over each magic number. Furthermore, by plotting α -decay energies with proton number Z and neutron number N respectively, the traditional magic numbers are reproduced by the sudden increase of Q_α there, and possible new magic numbers $N = 184$ and 258 are predicted.

In future, the RCHB mass table can be used to calculate the decay energies of C and O clusters, and study them in a similar way. In addition, deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc) can be used to study α -decay energies, and investigate the influence of deformation on the α -decay energies.

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