# Exact treatment of pairing correlations in Yb isotopes with covariant density functional theory *

LIU Lang(刘朗)[1;1)] ZHAO Peng-Wei(赵鹏巍)[2;2)]

[1] School of Science, Jiangnan University, Wuxi 214122, China
[2] State Key Laboratory of Nuclear Physics and Technology, School of Physics, Peking University, Beijing 100871, China

**Abstract:** The effects of pairing correlation in Yb isotopes are investigated by covariant density functional theory with pairing correlations and blocking effects treated exactly by a shell model like approach (SLAP). Experimental one- and two-neutron separation energies are reproduced quite well. The traditional BCS calculations always give larger pairing energies than those given by SLAP calculations, particularly for the nuclei near the proton and neutron drip lines. This may be caused because many of the single particle orbits above the Fermi surface are involved in the BCS calculations, but many of them are excluded in the SLAP calculations.

**Key words:** pairing correlation, Yb isotopes, covariant density functional theory, shell-model-like approach

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## 1 Introduction

Covariant density functional theory (CDFT) is one of the most important microscopic models due to its successful description of many nuclear phenomena [1–5]. Most recently, the theoretical framework of CDFT and its applications for nuclear ground states and excited states, as well as a couple of topics in interdisciplinary fields, have been reviewed in Ref. [6]. There are a number of attractive features in CDFT, especially in its practical applications in the self-consistent relativistic mean-field (RMF) framework. It naturally gives the spin-orbit potential and the relativistic effects are responsible for the pseudospin symmetry [7–12] in the nuclear single-particle spectra and the spin symmetry in the anti-nucleon spectrum [13, 14]. Moreover, it is of particular importance that the CDFT includes nuclear magnetism [15] (i.e., a consistent description of currents and time-odd fields), which plays an important role in nuclear rotations [16–19].

Pairing correlation plays an essential role in many nuclear properties, such as binding energies, moment of inertia, electromagnetic transition, low-lying collective modes, etc. RMF theory must be supplemented with a proper treatment of the pairing correlations to realistically describe the open shell nuclei. In the RMF model, the Bardeen-Cooper-Schrieffer (BCS) approximation and Bogoliubov transformation have become standard literatures to treat pairing correlations, in both stable and exotic nuclei. Since the approximation product of the quasiparticle wave functions in quasiparticle formalism breaks the gauge symmetries connected with the particle number, a particle number conserving (PNC) method has been proposed [20, 21] and employed successfully to describe odd-even differences in moments of inertia (MOI's) [22], the nonadditivity in MOI's [23], the identical bands [24, 25], the nuclear pairing phase transition [26], the high-spin states and high-$K$ isomers in the rare-earth, and the actinide region and superheavy nuclei [27–31]. Recently, this method has been used to investigate the effect of pairing in antimagnetic rotation [32]. This approach has been later combined with the RMF theory, known also as relativistic mean field theory with shell-model-like approach (RMF+SLAP), and successfully applied to describe both the ground states and excitation spectra of Ne [33, 34], Sn [35], and C [36] isotopes. Moreover, the $\alpha$-cluster structures of light nuclei have also been discussed in the framework of RMF+SLAP [37, 38].

In contrast to the conventional BCS or Bogoliubov approaches, the pairing Hamiltonian is solved directly in a truncated Fock space in SLAP [39, 40]. The particle number is thus conserved and Pauli blocking effects are taken into account exactly. Moreover, the RMF+SLAP provides a self-consistent framework to investigate the paring correlation without particle number violation.

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1) E-mail: liulang@jiangnan.edu.cn
2) E-mail: pwzhao@pku.edu.cn

Therefore, it would be very interesting to make a comparison between the SLAP and BCS approach in such a self-consistent framework.

In this work, by taking $Z=70$ isotopes as an example, the ground-state properties are investigated with RMF+SLAP and RMF+BCS models, respectively. In particular, the one- and two-neutron separation energies, pairing energies, and the single-particle occupation probability are discussed in detail.

## 2 Theoretical framework

The theoretical framework of RMF is explained in detail in Refs. [1–4]. In Ref. [20], the PNC method is introduced following the idea of shell model. The formulism of the combination of the RMF model and the shell-model-like approach can be found in Ref. [33]. In the following, we briefly present the framework of the RMF+SLAP model.

The starting point of the RMF theory is an effective Lagrangian density where nucleons are described as Dirac spinors, which interact via the exchange of several mesons (the isoscalar scalar $\sigma$, the isoscalar vector $\omega$, and isovector vector $\rho$) and the photon [2–4]. The detailed formulation of this Lagrangian density can be found in Refs. [2–4].

The classical variation principle leads to the Dirac equation

$$\{\mathrm{i}\alpha\cdot\nabla+V(\boldsymbol{r})+\beta[M+S(\boldsymbol{r})]\}\psi_i=\varepsilon_i\psi_i, \tag{1}$$

for the nucleons and the Klein-Gordon equations

$$\begin{cases} [-\Delta+m_\sigma^2]\sigma(\boldsymbol{r})=-g_\sigma\rho_\mathrm{s}(\boldsymbol{r})-g_2\sigma^2(\boldsymbol{r})-g_3\sigma^3(\boldsymbol{r}), \\ [-\Delta+m_\omega^2]\omega^\mu(\boldsymbol{r})=g_\omega j^\mu(\boldsymbol{r})-g_4(\omega^\nu\omega_\mathrm{v})\omega^\mu(\boldsymbol{r}), \\ \left[-\Delta+m_\rho^2\right]\rho^\mu(\boldsymbol{r})=g_\rho j^\mu(\boldsymbol{r}), \\ [-\Delta A^\mu(\boldsymbol{r})]=ej_\mathrm{p}^\mu(\boldsymbol{r}), \end{cases} \tag{2}$$

for the mesons. Here, the potentials $V(\boldsymbol{r})$ and $S(\boldsymbol{r})$ are connected in a self-consistent way to the various meson fields $\sigma(\boldsymbol{r})$, $\omega(\boldsymbol{r})$, and $\rho(\boldsymbol{r})$, which can be obtained from Klein-Gordon equations with the source terms $\rho_\mathrm{s}(\boldsymbol{r})$, $j^\mu(\boldsymbol{r})$, $\boldsymbol{j}^\mu(\boldsymbol{r})$, and $j_\mathrm{p}^\mu(\boldsymbol{r})$, for further details see Refs. [2–4]. Following the definition of the Dirac spinors in Ref. [33], the densities can be represented as

$$\rho_{\mathrm{s,v}}=2\sum_{i>0}n_i[(|f_i^+|^2+|f_i^-|^2)\mp(|g_i^+|^2+|g_i^-|^2)], \tag{3}$$

where $f_i$ and $g_i$ represent, respectively, the large and small components of the Dirac state $i$, and the corresponding occupation probability is denoted by $n_i$.

Based on the single-particle levels and wave functions obtained from the RMF theory, SLAP is adopted to treat the pairing correlations. The Hamiltonian reads

$$\begin{aligned} H &= H_{\mathrm{s.p.}}+H_{\mathrm{pair}} \\ &= \sum_\nu \varepsilon_\nu a_\nu^\dagger a_\nu - G\sum_{\mu,\nu>0}^{\mu\neq\nu} a_\mu^\dagger a_{\bar{\mu}}^\dagger a_{\bar{\nu}} a_\nu, \end{aligned} \tag{4}$$

with $\varepsilon_\nu$ the single-particle energy obtained from the RMF and $G$ the constant average pairing strength.

As shown in Ref. [33], the multi-particle-configurations (MPC) are constructed as a basis to diagonalize the Hamiltonian in Eq. (4). In realistic calculation, the MPC space has to be truncated and a cutoff energy $E_\mathrm{c}$ is introduced. Only the configurations with energies $E_i-E_0\leqslant E_\mathrm{c}$ are chosen to diagonalize the Hamiltonian $H$ in Eq. (4), where $E_i$ and $E_0$ are the energies of the $i$th configuration and the lowest configuration, respectively [39, 40]. According to the obtained wave functions, one can readily have occupation probability of the $i$th level (see Eq. (15) in Ref. [33]). The SLAP is thus connected to the RMF theory by substituting the obtained occupation probability into Eq. (3) to calculate the various densities.

## 3 Results and discussion

In this work, the effective interaction PK1 [41] is adopted. The Dirac equation Eq. (1) and the Klein-Gordon Eq. (2) are solved by expansion in the harmonic oscillator basis with 18 major shells. The oscillator frequency of the harmonic oscillator basis is fixed as $\hbar\omega_0=41A^{-1/3}$ MeV. The cutoff energy $E_\mathrm{c}$ of the MPC space in RMF+SLAP calculation is fixed as $E_\mathrm{c}=15$ MeV with the corresponding pairing strengths $G_\mathrm{n}=51/A$ MeV and $G_\mathrm{p}=58/A$ MeV normalized to the experimental odd-even mass differences [42]. The dimension of MPC under this truncation is less than 1000, for both neutron and proton. Similarly, a pairing window with $\epsilon_i-\lambda\leqslant 2\hbar\omega_0$ [2] with the pairing strengths $G_\mathrm{n}=22/A$ MeV and $G_\mathrm{p}=31/A$ MeV are adopted in the RMF+BCS calculations, where $\lambda$ denotes the chemical potential.

In Fig. 1, the odd-even mass differences $\Delta_\mathrm{n}$ of Yb isotopes calculated by RMF+BCS and RMF+SLAP with PK1 effective interaction are shown in comparison with the experimental data [42]. Here, the odd-even mass differences are extracted from the three point formula for both experimental and theoretical values. It is found that, with the chosen pairing strengths and the corresponding cut-off energies, both RMF+BCS and RMF+SLAP calculations reliably reproduce the experimental odd-even mass differences.

In Fig. 2, the one- and two-neutron separation energies calculated by RMF+BCS and RMF+SLAP with PK1 are compared with the data [42]. It is shown that both RMF+BCS and RMF+SLAP can reproduce the one- and two-neutron separation energies quite well. In particular, both RMF+BCS and RMF+SLAP can describe the behavior of the shell gap of $S_\mathrm{n}$ and $S_{2\mathrm{n}}$ near $A=152$ and the staggering of $S_\mathrm{n}$.

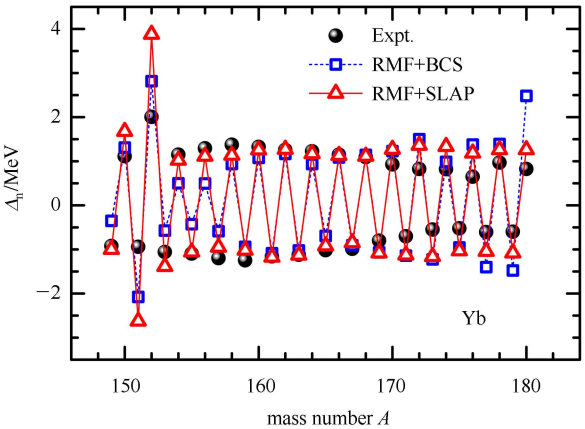


Fig. 1. (color online) Odd-even mass differences of Yb isotopes calculated by RMF+SLAP (open triangles) and RMF+BCS (open squares) with PK1 in comparison with the data (full circles).

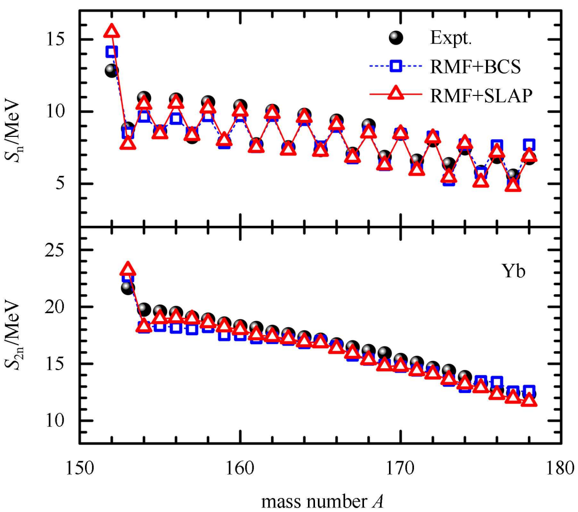


Fig. 2. (color online) Calculated one- (top panel) and two-neutron separation energies (bottom panel) with RMF+SLAP (open triangles) and RMF+BCS (open squares) with PK1 in comparison with the data (full circles).

Fig. 3 shows the pairing energies of neutron, proton, and total of the ground state for Yb isotopes calculated by RMF+BCS and RMF+SLAP with PK1. The pairing energy for the ground state is evaluated by $\langle\psi_{\text{g.s.}}|H_{\text{pair}}|\psi_{\text{g.s.}}\rangle$ in the framework of RMF+SLAP, where $\psi_{\text{g.s.}}$ is the ground state wave function for the nuclei and $H_{\text{pair}}$ is defined in Eq. (4). In the case of the neutron, both RMF+BCS and RMF+SLAP results are almost zero when mass number is around 152. However, the differences between these two methods enhance dramatically with the increasing of neutron number. Moreover, the RMF+BCS results present stronger staggering than that of RMF+SLAP since RMF+BCS cannot treat blocking effect strictly and in consequence overestimates pairing effect. For the proton both calculations provide almost the same pairing energies for the nuclei near $A=180$, but large deviations are shown in the neutron-deficient side. For the total pairing energy, therefore, one can see that the RMF+BCS calculations always give larger pairing energies than the RMF+SLAP calculations, particularly for the nuclei near the proton and neutron drip lines.

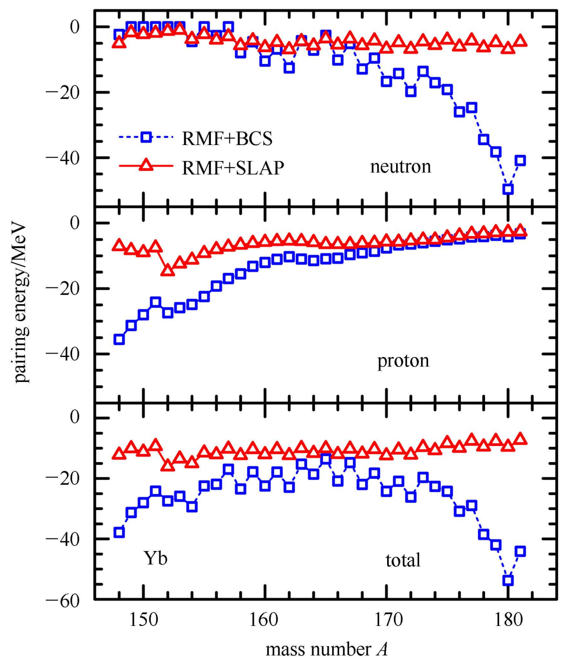


Fig. 3. (color online) Calculated pairing energies of neutron (top panel), proton (middle panel), and the total (bottom panel) of Yb isotopes calculated by RMF+SLAP (open triangles) and RMF+BCS (open squares) with PK1.

In order to understand the behavior of the pairing energies shown in Fig. 3, the neutron and proton single particle occupation probabilities of $^{148}$Yb, $^{166}$Yb, and $^{180}$Yb calculated by RMF+SLAP and RMF+BCS with PK1 are shown in Fig. 4. For the neutron occupation probability, the RMF+SLAP provides almost the same results as RMF+BCS for the nuclei $^{148}$Yb and $^{166}$Yb. However, it can be seen that the occupation probability of $^{180}$Yb from RMF+BCS spreads more widely than that from RMF+SLAP. On the contrary, the situation of proton is opposite. The occupation probability of $^{148}$Yb from RMF+BCS spreads more widely than that from RMF+SLAP. It is clear that a wider occupation distribution leads to a stronger pairing correlation. The behavior of pairing energies shown in Fig. 3 can be explained self-consistently by the single particle occupation in Fig. 4.

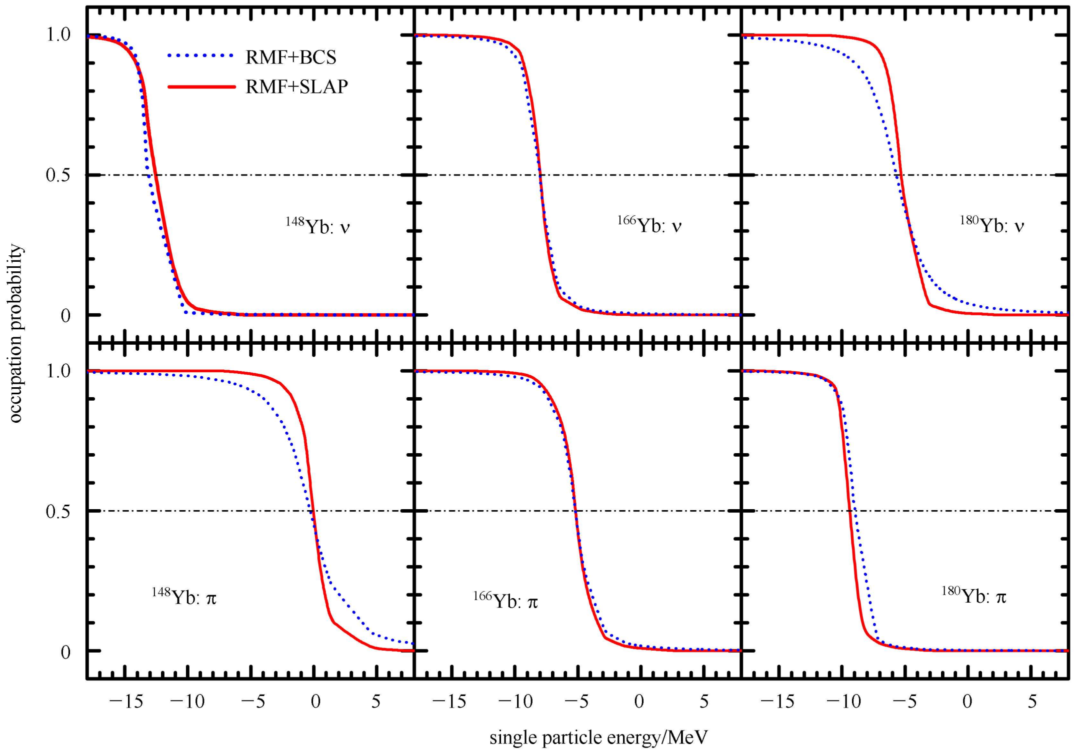


Fig. 4. (color online) Neutron (upper rows) and proton (bottom rows) single particle occupation probabilities of $^{148}$Yb (left columns), $^{166}$Yb (middle columns), and $^{180}$Yb (right columns) calculated by RMF+SLAP (solid lines) and RMF+BCS (dashed lines) with PK1.

It has been discussed in Ref. [20] that the pairing correlation is overestimated in BCS due to the non-conservation of the particle number. Now, the question is why this large deviation between BCS and SLAP occurs mainly in those nuclei near the drip line? The reason is mainly due to the different recipes adopted in the truncation of RMF+BCS and RMF+SLAP. In the case of RMF+BCS, more single particle orbits above Fermi surface are involved because the pairing window is larger. However, in the framework of RMF+SLAP, only the configurations with energies $E_i$–$E_0 \leqslant E_c$ are chosen, and consequently many configurations composed of single particle orbits above Fermi surface are excluded.

## 4 Summary

In summary, the pairing correlation of the ground state for Yb isotope is investigated by RMF+BCS and RMF+SLAP models with PK1 effective interaction. The pairing strengths $G_\tau$ are normalized to the experimental odd-even mass differences [42] with the truncations. It is found that both RMF+BCS and RMF+SLAP models can reproduce the one- and two-neutron separation energies quite well. However, the RMF+BCS calculations always give larger pairing energies than those given by RMF+SLAP calculations, particularly for the nuclei near proton and neutron drip lines. This phenomenon has been analyzed in terms of the single particle occupation probability, which shows that RMF+BCS presents wider distribution of occupation probability around drip line nuclei. We discuss two kinds of truncations and find that multi-particle configuration truncation presents a more reliable pairing window than a single particle truncation in the BCS. Finally, it should be also mentioned that it would be very interesting to perform a similar investigation by different effective interactions, such as point-coupling functionals [43] or by solving the deformed Dirac equation in Woods-Saxon basis [44].

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## References


1 Serot B D, Walecka J D. Adv. Nucl. Phys., 1986, **16**: 1
2 Gambhir Y K, Ring P, Thimet A. Ann. Phys. (N. Y.), 1990, **194**: 132
3 Ring P. Prog. Part. Nucl. Phys., 1996, **37**: 193
4 MENG Jie, Toki H, ZHOU Shan-Gui et al. Prog. Part. Nucl. Phys., 2006, **57**: 470
5 Vretenar D, Afanasiev A V, Lalazissis G A, Ring P. Phys. Rep., 2005, **409**: 101
6 MENG Jie, GUO Jian-You, LI Jian et al. Prog. Phys., 2011, **31**: 199
7 Ginocchio J N. Phys. Rep., 2005, **414**(4–5): 165
8 MENG Jie, Sugawara-Tanabe K, Yamaji S et al. Phys. Rev. C, 1998, **58**(2): R628
9 LIANG Hao-Zhao, ZHAO Peng-Wei, ZHANG Ying et al. Phys. Rev. C, 2011, **83**(4): 041301
10 LI Fang-Qiong, ZHAO Peng-Wei, LIANG Hao-Zhao. Chinese Phys. C (HEP & NP), 2011, **35**: 825
11 LIANG Hao-Zhao, SHEN Shi-Hang, ZHAO Peng-Wei et al. Phys. Rev. C, 2013, **87**: 014334
12 LU Bing-Nan, ZHAO En-Guang, ZHOU Shan-Gui. Phys. Rev. C, 2013, **88**: 024323
13 ZHOU Shan-Gui, MENG Jie, Ring P. Phys. Rev. Lett., 2003, **91**: 262501
14 HE Xiao-Tao, ZHOU Shan-Gui, MENG Jie et al. Euro. Phys. J. A, 2006, **28**: 265
15 Koepf W, Ring P. Nucl. Phys. A, 1989, **493**(1): 61
16 Afanasjev A V, Ring P, König J. Nucl. Phys. A, 2000, **676**: 196
17 ZHAO Peng-Wei, ZHANG Shuang-Quan, PENG Jing et al. Phys. Lett. B, 2011, **699**(3): 181
18 ZHAO Peng-Wei, PENG Jing, LIANG Hao-Zhao et al. Phys. Rev. Lett., 2011, **107**: 122501
19 ZHAO Peng-Wei, PENG Jing, LIANG Hao-Zhao et al. Phys. Rev. C, 2012, **85**: 054310
20 ZENG Jin-Yan, CHENG Tan-Sheng. Nucl. Phys. A, 1983, **405**: 1
21 ZENG Jin-Yan, JIN Tai-Hao, ZHAO Z J. Phys. Rev. C, 1994, **50**: 1388
22 ZENG Jin-Yan, LEI Yi-An, JIN Tai-Hao et al. Phys Rev. C, 1994, **50**: 746
23 LIU Shu-Xin, ZENG Jin-Yan. Phys. Rev. C, 2002, **66**: 067301
24 ZENG Jin-Yan, LIU Shu-Xin, LEI Yi-An et al. Phys. Rev. C, 2001, **63**: 024305
25 LIU Shu-Xin, ZENG Jin-Yan, ZHAO En-Guang. Phys. Rev. C, 2002, **66**: 024320
26 WU Xi, ZHANG Zhen-Hua, ZENG Jin-Yan et al. Phys. Rev. C, 2011, **83**: 034323
27 LIU Shu-Xin, ZENG Jin-Yan, YU L. Nucl. Phys. A, 2004, **735**: 77
28 ZHANG Zhen-Huan, LEI Yi-An, ZENG Jin-Yan. Phys. Rev. C, 2009, **80**: 034313
29 HE Xiao-Tao, YU Shao-Ying, ZENG Jin-Yan et al. Nucl. Phys. A, 2005, **760**: 263
30 ZHANG Zhen-Hua, HE Xiao-Tao, ZENG Jin-Yan et al. Phys. Rev. C, 2012, **85**: 014324
31 ZHANG Zhen-Hua, MENG Jie, ZHAO En-Guang et al. Phys. Rev. C, 2013, **87**: 054308
32 ZHANG Zhen-Hua, ZHAO Peng-Wei, MENG Jie et al. Phys. Rev. C, 2013, **87**: 054314
33 MENG Jie, GUO Jian-You, LIU, Lang et al. Front. Phys. China, 2006, **1**: 38
34 GUO Jian-You, MENG Jie, ZHANG Shuang-Quan. Nucl. Phys. Rev., 2004, **21**: 355
35 LIU Lang, MENG Jie, ZHANG Shuang-Quan. HEP & NP, 2006, **30**: 299 (in Chinese)
36 WANG Pei-Wei, CHEN Hong, LI Jia-Xing et al. HEP & NP, 2006, **30**(Supp. Ⅱ): 94 (in Chinese)
37 LIU Lang, WANG Peng-Wei, CHEN Hong et al. HEP & NP, 2006, **30**(Supp. Ⅱ): 227 (in Chinese)
38 LIU Lang, ZHAO Peng-Wei Chinese Phys. C (HEP & NP), 2012, **36**: 818
39 WU Chong-Shi, ZENG Jin-Yan. Phys. Rev. C, 1989, **39**: 666
40 Molique H, Dudek J. Phys. Rev. C, 1997, **56**: 1795
41 LONG Wei-Hui, MENG Jie, Giai N V et al. Phys. Rev. C, 2004, **69**: 034319
42 WANG Meng, Audi G, Wapstra A H et al. Chinese Phys. C (HEP & NP), 2012, **36**: 1603
43 ZHAO Peng-Wei, LI Zhi-Pan, YAO Jiang-Ming et al. Phys. Rev. C, 2010, **82**: 054319
44 ZHOU Shan-Gui, MENG Jie, Ring P et al. Phys. Rev. C, 2010, **82**: 011301(R)