Covariance Propagation in R-Matrix Model Fitting*

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Abstract This work is done for improving the current international standard cross section of nuclear reaction. The features of covariance propagation in R-matrix model fitting for ^{7}Li, ^{11}B and ^{16}O systems are researched systematically with Code RAC, and the results about propagation of non-diagonal elements of covariance matrix are presented. It is found that in R-matrix model fitting, short-energy-range parameters result in relatively smaller covariance propagation coefficient (CPC), medium and long-energy-range parameters produce relatively larger CPC. Especially the medium-energy-range component of systematic error plays very important role in propagation of covariance. In the evaluation procedure of nuclear data both long-energy-range component (LERC) and medium-energy-range component (MERC) of systematic error should be considered in experimental data-base file. Furthermore, these conclusions are suitable for the similar model fitting in other science fields.

Key words error propagation, covariance, r-matrix fitting, nuclear reaction cross section

1 Introduction

As some fields of modern science and technology are developing towards high precision and synthetical analysis, the research on error propagation and covariance become more and more important[1]. For example. a nuclear measurement[2] requires standard cross section with high precision. So we have systematically researched the error propagation features with R-matrix model fitting for ^{7}Li, ^{11}B and ^{16}O systems. The basic formula, simulation data, calculation procedure, and some regularities of propagation for standard error have been published in Ref. [3] This letter will describe the result about propagation of non-diagonal element of covariance matrix, it follows the terms, formula and signs defined in Refs. [3,4].

We have calculated out tens of thousands covariance data of the cross sections of ^{6}Li(n, α), ^{10}B(n, α_0), ^{10}B(n, α_1) and ^{16}O(n, n) ^{16}O with R-Matrix Code RAC[5], the sub-sets of simulative data used are 300, 340 and 800 data points respectively. The numbers of covariance matrix elements are from 90000 to 640000.

In R-matrix theory, intrinsic wave function can be expressed by operator Green Function[6]

$$G = \sum_{\lambda} \frac{|\lambda\rangle\langle\lambda|}{E_{\lambda} - E}, \tag{1}$$

The values of G rely strongly on the energy E, so the parameters of R-matrix can be divided into three kinds in accordance with their dependency on energy. The first one is long-energy-range parameter, e.g. channel radii, background parameters; the second one is middle-energy-range parameter, e.g. the parameters of wider energy level; the third one is short-energy-range parameter, e.g. the parameters of narrow energy level. Different kinds of parameters make the covariance propagation have different features. The property of parameter of R-matrix rely strongly on the structure of cross section of ^{6}Li(n, α), ^{10}B(n, α_0), ^{10}B(n, α_1) and ^{16}O(n, n) (refer to Fig.1.).

2 Analysis of covariance propagation

For convenience, a collection made up of coordinate points that have the same value of correlation coefficient (CC) is called as 'correlation coefficient curve' (CCC);

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the quotient of a element of calculated covariance matrix and it's corresponding element of covariance matrix of simulation data is called 'covariance propagation coefficient' (CPC); Let $Y_i = Y_i^2 / U_i^2$ in which Y_i^2 is total systematic variance and U_i^2 is total variance; for a given Y_i^2, let $M_i = M_i^2 / Y_i^2$ in which M_i^2 is medium-energy-range component (MERC) of systematic error.

It was found that propagation of covariance depends on the intrinsic features of R-matrix parameters and the error distribution of simulation data.

2.1 Intrinsic features of R-matrix parameters for propagation of covariance

When non-diagonal element of covariance matrix of simulation data is set as zero (that is $Y = 0$), the non-diagonal element of calculated covariance matrix is not zero. In this situation there is no CPC exist, the feature of covariance propagation can be studied with the calculated value of CC. Fig.2, Fig.3 and Fig.4 show the CC figures of ^{6}Li (n, α) and ^{16}O (n, n) ^{16}O respectively when all the error is regarded as statistical error ($Y = 0$), they actually show the intrinsic features of error propagation for R-matrix parameters. In these figures the digital numbers show the values of CC for the most adjacent lines.

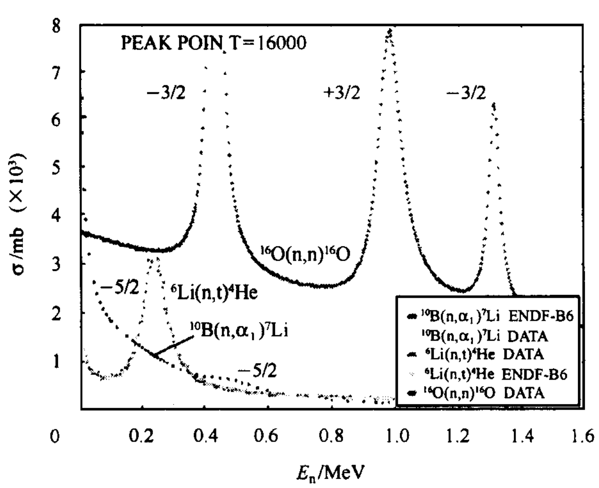

Fig.1. Cross section of ^{6}Li(n, α), ^{10}B(n, $α_0$), ^{10}B(n, $α_1$) and ^{16}O(n,n).

Fig.2 is the CCC of ^{6}Li (n, α), its characteristic is that near the energy coordinate (0.25, 0.25) there is a symmetrical closed or half closed curve collection (called 'closed collection' for short), the CC value at the center part of closed collection is about −0.2 and about 0 for

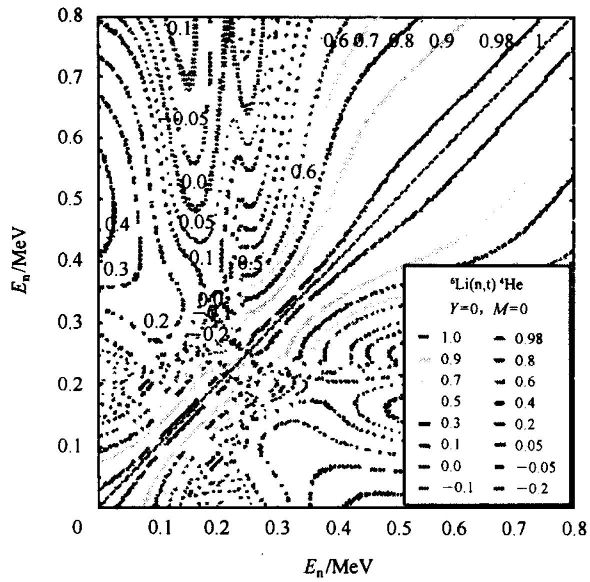

Fig.2. CCC of ^{6}Li(n, α) ($Y = 0$).

marginal part. From Fig.1 it can be seen that the closed collection is just corresponding to the resonance energy level −5/2. This is the result of corporate action of the parameters of this energy level and other parameters, but the parameters of the level −5/2 play a main role.

In the initiative part of diagonal area, correlation curves distribute parallel around the diagonal line in a radiant shape (called 'parallel collection' for short) and the value of CC decreases from 1 to about 0.5. The cross section of ^{6}Li(n, α) in this area is mainly generated by the background parameters of S wave. In another half part of diagonal area, correlation curves also distribute parallel around the diagonal line in radiant shape, and the value of CC decreases from 1 to about 0.5. This is caused by background parameters of distant energy levels.

The CC figure of ^{16}O(n,n) ^{16}O is the most reprehensive one. For the sake of being clear only the part for 0—1.6 MeV is shown in Fig.3. In cross section of ^{16}O(n, n) ^{16}O (See Fig.1), there are three very strong resonance (corresponding energy zone is called 'apex zone' for short), in this energy zone they result in three closed collections in diagonal area and, the middle one correspond level +3/2 is shown in Fig.4 in detail. The value of CC in the central part of this closed collection is about −0.95 and about 0.1 for marginal part. For the energies in the vicinity of 'extraordinary point' or 'vertex point'. the value of CC are negative and the correlation is very

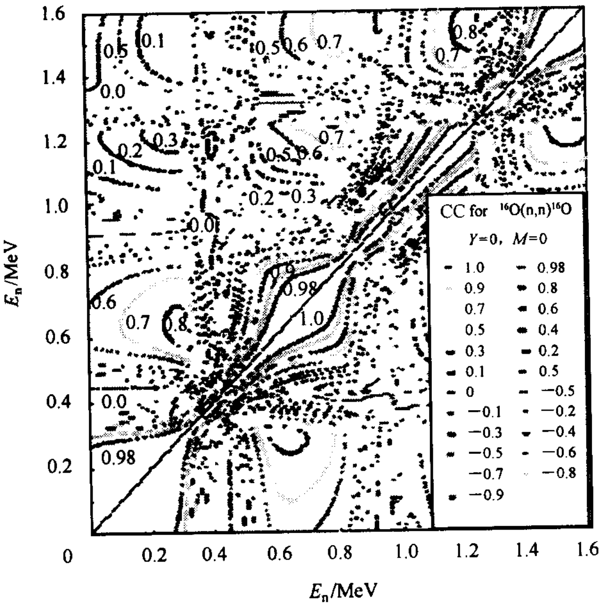

Fig.3. CCC of $^{16}O(n,n)^{16}O$ ($Y=0$)

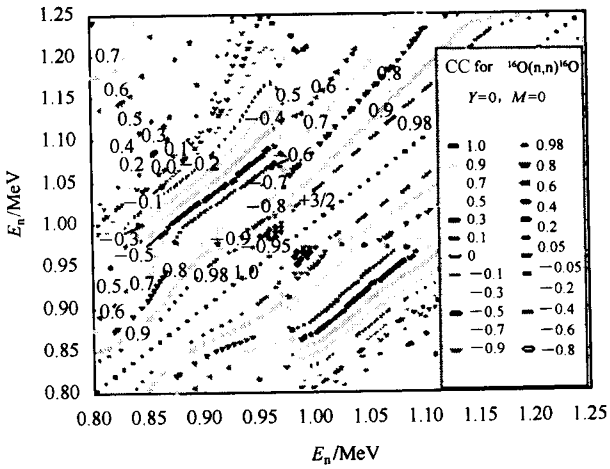

Fig.4. CCC of $^{16}O(n,n)^{16}O$ on the energy area of +3/2 level ($Y=0$).

strong so that it has a tendency to approach −1.0, this is due to there just exist $^{16}O(n,n)^{16}O$ channel.

From the figures above it can be seen that if there are obvious 'apex zone' and 'incline zone' in integrated cross section fitted, the value of CC that related energy points in 'apex zone' are relatively lower, forming horizontal and vertical 'vales'; the value of CC of two energy points in 'incline zone' are relatively higher, forming 'plateaus' which are separated by the 'vales'.

The characteristic of CCC for $^{10}B(n,\alpha_0)$ and $^{10}B(n,\alpha_1)$ (refer to Fig.5 and Fig.6) is that in diagonal area, CCC distributes parallel around the diagonal line throughout all energy zones and values of CC decrease from 1 to about 0. Out of diagonal area there are several smaller closed curve collections. They just correspond with the resonance energy levels. From the curves of cross section of $^{10}B(n,\alpha_1)$ in Fig.1, it can be seen the background parameters and parameters of wide distant energy levels play a primary role, the parameters of some weak energy levels in that energy zone play a secondary role. The parameters of weak resonance energy level are not able to produce closed collection in diagonal area, and just able to produce small closed collections out of diagonal area.

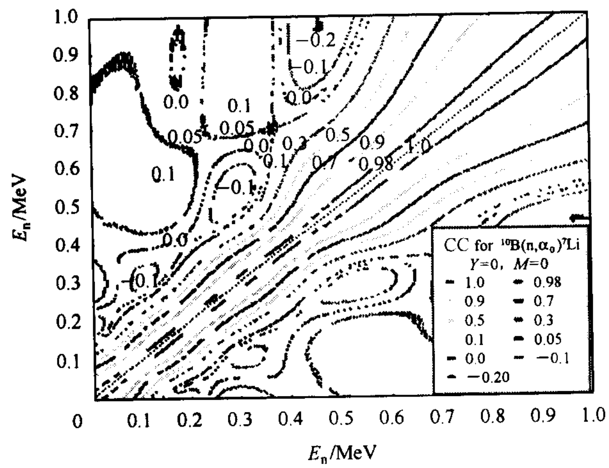

Fig.5. CCC of $^{10}B(n,\alpha_0)^7Li$ ($Y=0$).

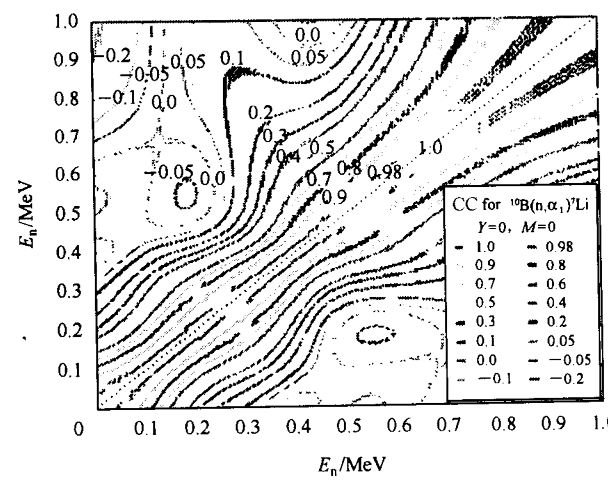

Fig.6. CCC of $^{10}B(n,\alpha_1)^7Li$ ($Y=0$).

General speaking, in R-matrix model fitting, short-energy-range parameters result in relatively lower CPC, it playing a role something like 'sieving covariance'; long-energy-range parameters produce relatively higher CPC and therefore should be used in computation as few as possible.

2.2 Effect of error distribution of simulation data for propagation of covariance

In order to research the effect of error distribution of data for propagation of covariance, the covariance or CPC that associated with $E_n = 0.2$ MeV for $^6Li(n, \alpha)$ is shown in Fig.7 to Fig.12.

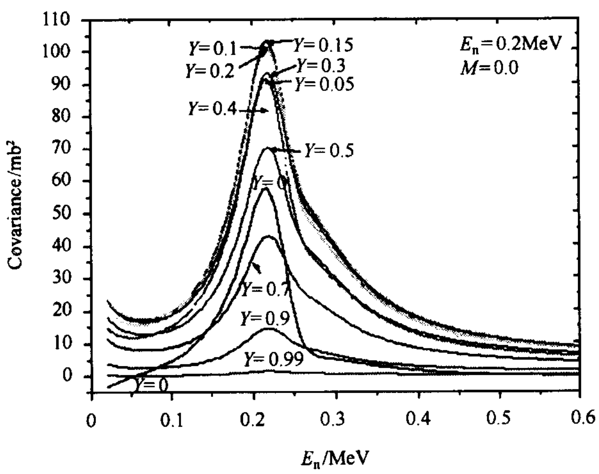

Fig.7. Covariance of $^6Li(n, \alpha)$ ($M = 0$).

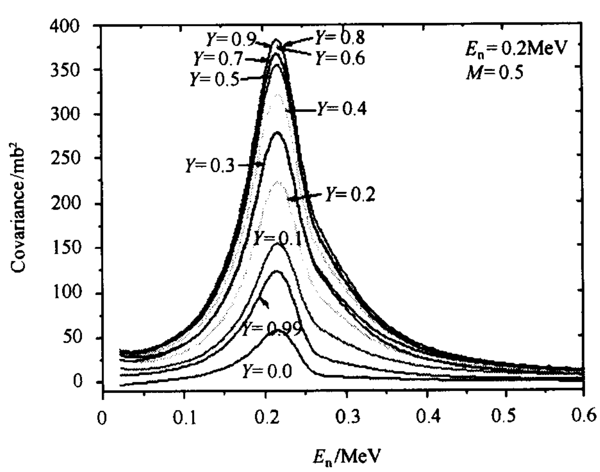

Fig.8. Covariance of $^6Li(n, \alpha)$($M = 0.5$).

Fig.7 shows the covariance for $M = 0$ and Y increased from 0 to 0.99. The curve marked with $Y = 0$ refers to the covariance for total systematic error being zero; the covariance looks relative smaller. If Y has a little increasing (e.g. $Y = 0.05$) the corresponding covariance increased a lot; when Y reaches 0.15 the covariance got maximum value, this is due to the contribution of total systematic error increased. When Y larger than 0.15 the covariance decreased with Y increasing; the covariance for $Y = 0.99$ is very small, the peak value just is about 1.46 mb^2. Those explain that in R-matrix model fitting, if all error is considered as statistic error the evaluated covariance will be relative lower if all error is considered as long-energy-range component (LERC) of systematic error the evaluated covariance will be very small.

Fig.8 shows the covariance for $M = 0.5$ and Y increased from 0 to 0.99. The curve marked with $Y = 0.0$ refers to the covariance for total systematic error being zero. For Y smaller than 0.9 the covariance increased with Y increasing, when Y reaches 0.9 the covariance got maximum value, for Y larger than 0.9 the covariance decreased with Y increasing; When $Y = 0.99$ the peak value is about 110mb^2. Making comparison of Fig. 8 with Fig.7 it can be found that the covariance for $M = 0.5$ is remarkably larger than that for $M = 0$. Those explain that the MERC of systematic error plays very important function for propagation of covariance.

Fig.9 shows the covariance for $Y = 0.99$ and M increased from 0 to 0.99. The curve marked with $M = 0.0$ refer to the covariance for medium-energy-range component (MERC) of systematic error being zero. The covariance increased with M increasing, and looks very sensitive to the change of M when M are smaller than 0.4. In real experimental data the most possible value of M is located in this range. When M reaches 1.0 the covariance got maximum value.

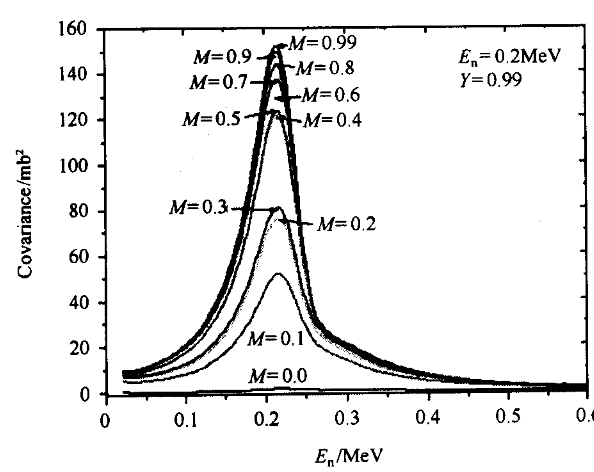

Fig.9. Covariance of $^6Li(n, \alpha)$ ($Y = 0.99$).

2.3 Propagation of covariance for real situation

The real error of experimental data must include both statistical error and systematic error; the systematic errors usually include LERC and MERC; it's reasonable to suppose that both Y and M taking the values about 0.3 are close to real situation.

Fig.10 shows the covariance for $Y = 0.3$ and M increased from 0 to 0.99. The curve marked with $M = 0.0$ refers to the covariance for medium-energy-range component (MERC) of systematic error being zero. The covariance increased with M increasing, when M reaches 1 the covariance got maximum value. Those explain that in R-matrix fitting if the MERC of systematic error of experimental data is not considered the evaluated covariance will be relatively lower.

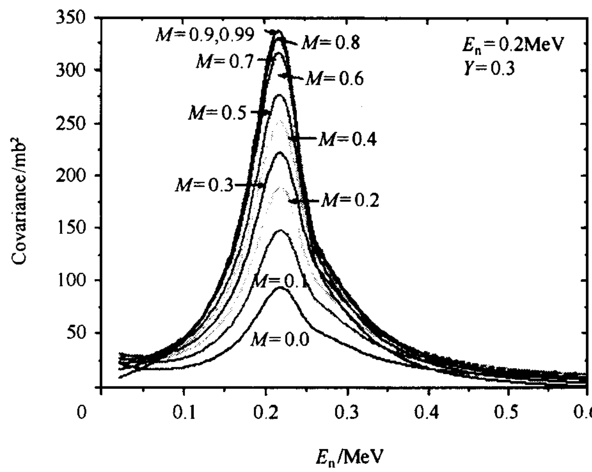

Fig.10. Covariance of ^{6}Li(n, α)($Y = 0.3$).

Fig.11 shows the covariance of ^{6}Li(n, α) for Y = 0.2, 0.3, 0.4 and M = 0.2, 0.3, 0.4 respectively. In this range of Y and M. the covariance increased when both Y and M increased. An interesting thing is that if

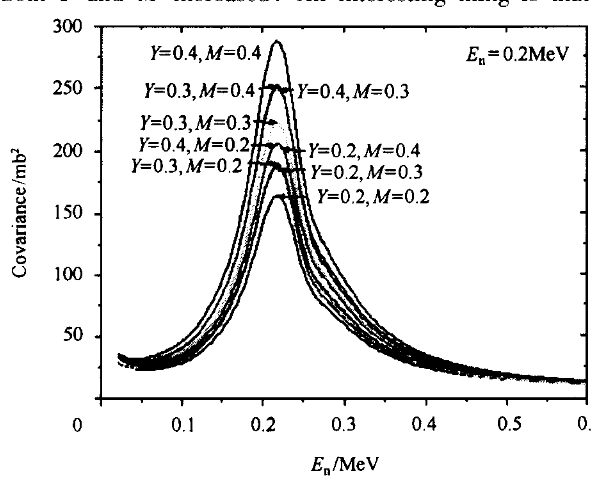

Fig.11. Covariance of ^{6}Li(n, α).

the value of Y and the value of M exchanged each other the covariance is very closed. This explains that in evaluation procedure both LERC and MERC of systematic error of experimental data should be considered correctly.

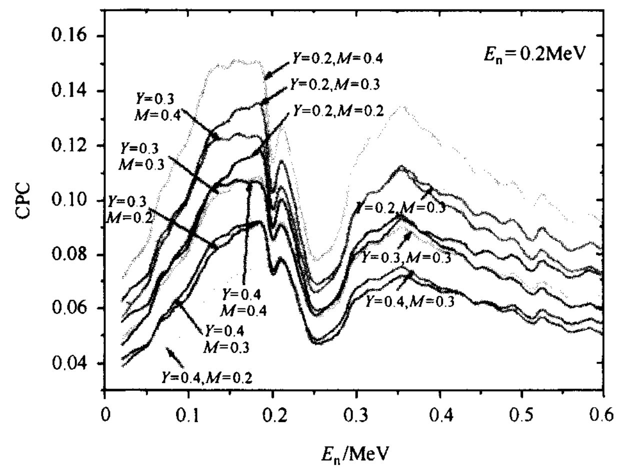

Fig.12. CPC of ^{6}Li(n, α).

Fig.12 shows the CPC of ^{6}Li(n,α) associated with E_n = 0.2 MeV for Y = 0.2, 0.3 0.4 and M = 0.2, 0.3, 0.4 respectively. It can be found that in this range of Y and M, for a given Y the CPC increased with M increasing; for a given M the CPC decreased with Y increasing. An interesting thing is that the CPC is dependent on the ratio of M/Y, CPC increased with M/Y increasing, for different M and Y, if the values of M/Y are close each other the CPC are closed each other. The narrow 'vales' at 0.2 MeV represent the propagation coefficient of standard error; the wider 'vales' at 0.25 MeV reflect the effect of resonance parameters of the narrow energy level −5/2.

3 Conclusions

In R-matrix model fitting, short-energy-range parameters result in relatively smaller covariance propagation coefficient (CPC), it play a role something like 'sieving covariance'; the correlation coefficient curves (CCC) form closed or half-closed collections. The medium and long-energy-range parameters produce relatively larger CPC, the CCC form 'parallel collection'.

In R-matrix model fitting, the CPC is more sensitive to medium-energy-range component (MERC) of systematic error than to long-energy-range component (LERC) of systematic error; the MERC of systematic error plays very important function for propagation of covariance. In the evaluation procedure of nuclear data both LERC and MERC of systematic error should be considered in database file.

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R矩阵模型拟合中的协方差传递*

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摘要　对^{7}Li, ^{11}B和^{17}O系统的R矩阵模型拟合进行了系统的协方差传递特性研究;揭示出部分协方差传递的规律性,发现系统误差的中程相关项在协方差传递中起到非常重要的作用.

关键词　误差传递　协方差　R矩阵　核反应截面

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