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DWBA Calculation of the Neutron Angular Distribution of ^{7}Li (n,n') Reaction[+]

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Abstract

The ^{7}Li first level inelastic scattering neutron angular differential cross sections in the energy range from 8 to 10MeV were calculated in this work. The calculations was performed by a zero-range approximation DWBA code DWUCK4. The calculated results were compared with the corresponding measured data. The comparison results show that the DWBA can be used for calculation of the data.

1. Introduction

Some reasons are leading our attention to the measurement and the calculation of the inelastic neutron angular distribution of ^{7}Li(n,n')(477.6keV). The first reason is that the nuclear data of ^{7}Li are very important because of the developments of the controlled nuclear fusion reactor. Especially, the cascade neutron inelastic scattering process is considerable in the triton generation reaction ^{7}Li(n,n't)α. ^{7}Li is of 92.5 percent abundance in the natural lithium. So the angular differential cross section(ADX) is important for neutron transport calculations in the reactor blanket. But because of the time resolution limit of the TOF technique, the ^{7}Li first level inelastic scattering neutrons are very difficult to be separated from the elastic scattering neutrons when the incident energy is higher than 6MeV. up to now, the measurement data for the ^{7}Li first level inelastic neutron angular distribution are very few. The second reason is that there is no suitable mono-energy neutron source in

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neutron energy range from 9 to 13 MeV, which makes the measurement even more difficult in the neutron energy region. In 1986, Dr. H. Liskien and his co-worker developed the Doppler broaden and shifted gamma ray measurement method for measuring the neutron angular distribution with the incident energy below 8.5MeV[1]. The primary results were also got in the energy region 8.5 ~ 10MeV[2].Comparing the data with the earlier calculated data, the consistencies are not satisfactory[1]. So a new theoretical calculations are necessary. Therefore,the efforts were made both in experiment measurements and the theoretical calculations in our laboratory. The direct process is dominant for the reaction ^{7}Li(n,n')(477.6keV) at rather high incident energy. The usual model for calculations of the direct inelastic scattering cross section are the DWBA and the Coupled Channel Approximation(CCA). In this work, the calculations was performed with the code DWUCK4[3] based on the zero-range approximation DWBA. The code was programed by Dr. P. D. Kunz(Colorado Univ.) and got from RSIC, ORNL, USA. In order to do the calculation better, we added a subroutine to the code DWUCK4, which was used for automatically searching the optical potential parameters, residual interaction potential parameters and the deformation parameter β. Some original subroutines were changed slightly to fit the parameters searching. Using the code, the ADX of the reaction ^{7}Li(n,n')(477.6keV) in the energy range from 8 to 20 MeV were calculated. The calculated data were compared with some measured data from 8 to 10 MeV. In the energy region 8 to 14 MeV, the elastic plus inelastic(the first level) ADX were also calculated and the results were compared with experiment data. The comparisons show that the DWBA can basically be used for description of the reaction.

2. Principle

The interaction between the incident particle and the target nuclei can be divided into two parts. One of them is the average potential that includes the coulomb potential, which can cause the large distortion of the incident wave, but do not induce the nuclear reaction. The other is the residual interaction which induced the reaction. Suppose the incident channel is α and the exit channel is β, then the Hamiltonian of

the reaction system can be written as

$$H = H_\alpha + V_\alpha + U_\alpha = H_\beta + V_\beta + U_\beta \qquad (1),$$

where H_α and H_β are the corresponding channel Hamiltonian, U_α, U_β and V_α, V_β are the average potentials and the residual interaction potential of the corresponding channel respectively. The transition amplitude of the nuclear reaction can be expressed as[4]

$$T = \langle \phi^-_\beta | V_\beta | \Phi^+_\alpha \rangle \qquad (2).$$

where $\phi^{-}{}^{*}_{\beta}(\vec{r}, \vec{k}_\beta) = \phi^+_\beta(\vec{r}, -\vec{k}_\beta)$, and $\phi^+_\beta(\vec{r}, \vec{k}_\beta)$ satisfied the Schrödinger equation

$$(H_\beta + U_\beta + E_0)\phi^+_\beta(\vec{r}, \vec{k}_\beta) = 0 \qquad (3),$$

where E_0 is the center of mass total energy for the reaction system. That means, $\phi^+_\beta(\vec{r}, \vec{k}_\beta)$ is the distorted wave of the exit channel, $|\Phi^+_\alpha\rangle$ is the scattering resolution of the Schrödinger equation $H|\Phi^+_\alpha\rangle = E_0|\Phi^+_\alpha\rangle$.
Using $|\phi^+_\alpha\rangle$ to replace $|\Phi^+_\alpha\rangle$, one gets the distorted wave Born approximation.

So the transition amplitude now has the form

$$T = \langle \phi^-_\beta | V_\beta | \phi^+_\alpha \rangle \qquad (4).$$

For the reaction A(a, b)B, expression (4) has the integrated form

$$T = J\int d\vec{r}_a \int d\vec{r}_b\, \phi^{-}{}^{*}_{\beta}(\vec{k}_\beta, \vec{r}_b) \langle Bb|V|Aa\rangle \phi^{(+)}_\alpha(\vec{k}_a, \vec{r}_a) \qquad (5).$$

The distorted wave satisfied the boundary condition:

$$\phi^{(+)}_\alpha(\vec{k}_a, \vec{r}_a) \xrightarrow[r\to\infty]{} e^{i\vec{k}\cdot\vec{r}} + f(\theta)\frac{e^{i\vec{k}\cdot\vec{r}}}{r} \qquad (6)$$

In order to simplify the calculations of integral of the space vectors, which needs 6 dimension integrals, DWUCK4 uses the zero range approximation, which suppose the outgoing particle is absorbed in the position of the incident particle location, so that

$$\vec{r}_b = \frac{A}{B}\vec{r}_a \qquad (7),$$

where A and B are the mass of the target and the residual nucleus respectively. For the inelastic scattering, we automatically have

$\vec{r}_a=\vec{r}_b$. Then we can make an expansion of the interaction matrix elements $\langle Bb|V|Aa\rangle$ into terms which corresponding the transfer to the nucleus of a definite angular momentum j, which is comprised of an orbital part l and spin part s. If the incident and outgoing particles have spins s_a and s_b, and the target and the residual nuclear spins are J_A and J_B respectively, we define

$$\vec{j} = \vec{J}_A - \vec{J}_B , \qquad \vec{s} = \vec{s}_a - \vec{s}_b , \quad \vec{l} = \vec{j} - \vec{s} \qquad (8).$$

Very often, in a definite transition only one set of j, l, s value is important[5]. According to the vector coupling (8), the expansion can be expressed as

$$\langle J_B M_B S_b m_b|V|J_A M_A S_a m_a\rangle = \sum_{l s j} B_{l s j} \langle J_A jM_A M_B - M_A | J_B M_B\rangle \langle s_b s m_b m_a - m_b | s_a m_a\rangle$$

$$\langle lsm\, m_a - m_b | j M_B - M_A\rangle f_{l s j}(r_a)\delta(\vec{r}_b - \frac{A}{B}\vec{r}_a) i^{-l} Y_l^{m*}(\hat{r}_a) \qquad (9),$$

where $B_{l s j}$ is a measure of the strength of the interaction, M_A, M_B, m_a and m_b are the corresponding z-component of the spin J_A, J_B, s_a and s_b, $m=M_B-M_A+m_b-m_a$.

If the optical potential includes the spin-orbit coupling, the distorted wave is a matrix in spin space. The time reversal relation is

$$\phi^-_{m',m}{}^*(\vec{k},\vec{r}) = (-)^{m-m'} \phi^+_{-m',m}(-\vec{k},\vec{r}) \qquad (10),$$

where m, m' are the third component of the particle spin before and after their interaction with the optical potential. Then $\phi^+_{m',m}(\vec{k},\vec{r})$ can be written as

$$\phi^+_{m',m}(\vec{k},\vec{r}) = \frac{\sqrt{4\pi}}{kr}\sum_{JL} i^l \langle LsMm|JM'\rangle\sqrt{2L+1}\,\phi_{JL}(k,r)\langle LsM'-m'm'|JM'\rangle$$

$$Y_L^{M'-m'}(\hat{r}) d^L_{0\,M'-m'} \qquad (11),$$

where d^L_{0m} is the rotation function for integer spin . The radial part of distorted wave functions satisfied the following equation:

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{L(L+1)}{r^2} - \frac{2\mu}{\hbar^2}(U+U_C+U_L^J)\right]\phi_{JL}(k,r) = 0 \qquad (12)$$

and the boundary condition is :

$$\phi_{JL}(k,0)=0,\quad \phi_{JL}(k,r)\xrightarrow[r\to\infty]{}\frac{[H^{*}_{L}(kr)-\eta^{J}_{L}H_{L}(kr)]\,e^{i\sigma_{L}}}{2i} \qquad (13),$$

where $H_L(kr)=G_L+iF_L$ is the outgoing wave coulomb function, η^J_L are the (complex)element of the scattering matrix. σ_L is the coulomb phase shift. The quantity $\frac{\eta^J_L-1}{2i}$ is the usual elastic partial scattering amplitude. Then the expression of the transition amplitude have the form

$$T=\frac{\sqrt{4\pi}}{k_a k_b}\frac{C^2}{AB}\sum_{lsj}\sqrt{2L+1}\,B_{lsj}\langle J_A\, j\, M_A M_B-M_A\,|\,J_B M_B\rangle S^{m_a m_b}_{lsj} \qquad (14),$$

where C is the sum of the mass of the transferred particle and nucleus, $S^{m_a m_b}_{lsj}$ is the quantity that includes the interaction shape factor and the internal freedom degree of the nucleus.
If the interaction is treated as perturbation, then the expression of the differential cross section can be written as:

$$\frac{d\sigma}{d\Omega}=\frac{\mu_a\mu_b}{(2\pi\hbar)^2}\frac{k_b}{k_a}\frac{1}{2J_A+1}\frac{1}{2s_A+1}\sum_{M_A M_B m_a m_b}\sum|T|^2$$

$$=\frac{2J_B+1}{2J_A+1}\frac{1}{4\pi}\frac{1}{E_a E_b}\frac{k_b}{k_a}\left(\frac{C^2}{AB}\right)^2\frac{1}{2s_a+1}\sum_{m_a m_b}\Big|\sum_{lsj}\sqrt{2l+1}\,B_{lsj}S^{m_a m_b}_{lsj}\Big|^2 \qquad (15)$$

The states most strongly excited by inelastic scattering are those recognized as involving collective motion of some kind, vibrational or rotational. The ^{7}Li ground($\frac{3}{2}^-$), the first excited(0.478MeV,$\frac{1}{2}^-$) and the second excited(4.63MeV,$\frac{7}{2}^-$) states belong to the rotational band with $K=\frac{1}{2}$[6,7]. So we think that the collective excitation play an important role in the ^{7}Li first excited state neutron inelastic scattering. Suppose the deformation for the first excited state is symmetry, the residual interaction potential with first order deformation has the form

$$V=-\beta_2\frac{R_0A^{1/3}}{a}V_0\frac{df_1}{dx}Y^0_2(\theta) \qquad (16),$$

where $x=\frac{r-R_0A^{1/3}}{a}$, θ is the angle between the particle scattering

direction and the nucleus symmetry axis. When the nucleus rotate π angle around the symmetry axis, the internal Hamiltonian represented by the attach-body coordinates remained constant. So the internal nuclear wave functions can be written as

$$\psi^{J}_{JMK} = \sqrt{\frac{2J+1}{16\pi^2}} \left[\chi^{j}_{k} D^{J\ *}_{KM} + (-1)^{J-j} \chi^{j}_{-K} D^{J\ *}_{-KM} \right] \qquad (17)$$

then we can get

$$\langle J_B M_B s_b m_b | V | J_A M_A s_a m_a \rangle = -\beta_2 \frac{R_0}{a} V_0 \frac{df_1}{dx} \sqrt{\frac{2J_A+1}{2J_B+1}} \langle J_A\, 1K0 | J_B K \rangle$$
$$\langle J_A\, 1M_A\ M_B - M_A | J_B M_B \rangle Y^{m}_{2}(\hat{r}_a) \qquad (18)$$

For the inelastic scattering, the spin transfer s=0, so j=1. The channel parity is conservative in the reaction. So the orbital momentum transfer l must be even. From (8), we can get j=l=2. Comparing (18) with expression (9), we may write $B_{l\,s\,j}$ as

$$B_{l\,s\,j} = B_{1\,0\,1} = \beta_2 \langle J_A\, 1K0 | J_B K \rangle \sqrt{\frac{2J_A+1}{2J_B+1}} \qquad (19).$$

According to (15),

$$\frac{d\sigma^{1}}{d\Omega} = \beta_2^2 \left| \langle J_A\, 1K0 | J_B K \rangle \right|^2 \sigma^{1}_{DW}(\theta) = 0.2\beta_2^2 \sigma^{1}_{DW}(\theta) \qquad (20),$$

where

$$\sigma^{1}_{DW}(\theta) = \frac{1}{4\pi} \frac{1}{E_a E_b} \frac{k_b}{k_a} \left(\frac{C^2}{AB}\right)^2 \frac{1}{2s_a+1} \sum_{m m_a m_b} \left| S^{m m_a m_b}_{l\,s\,j} \right|^2 .$$

The compound inelastic scattering is not included in the DWBA calculation. But when the incident energy is rather high, many exit channels are open, so the probability for the compound inelastic scattering is rather small.

3. Results and Discussions

The spherical optical potential parameters and the residual interaction potential parameters were automatically searched by a complex shape method[8]. The optical potential used in this work

is expressed as

$$V_{OM}=V_R f(x_{RO})+iV_I\frac{df(x_{IO})}{dx_{IO}}-V_{LS}\frac{1}{r}\frac{df(x_{RO})}{dr}\vec{L}\cdot\vec{S} \quad (21),$$

where $x_{RO}=\frac{r-R_{iO}A_T^{1/3}}{a_{iO}}$ $(i=R,I)$, $V_R=V_{RO}+C_{RO}E_c$, $V_I=V_{IO}+C_{IO}E_c$, E_c is the center of mass energy of the incident particle.

As the excitation energy of ^{7}Li first excited state is rather small, the optical potential parameters for the incident and the exit channel are taken as the same in this work. The adjustable parameters are: V_{RO}, C_{RO}, R_{RO}, a_{RO}, V_{IO}, C_{IO}, R_{IO}, a_{IO}, V_{LS}. The chi-square in the parameter auto-search code was constructed as

$$\chi_0^2=W_{TO}\sum_i\left[\frac{\sigma_{t.o.t.}^{ex}(E_i)-\sigma_{t.o.t.}^{t.h}(E_i)}{\Delta\sigma_{t.o.t.}^{ex}(E_i)}\right]^2+W_{IO}\frac{1}{N}\sum_{ij}\left[\frac{\sigma^{ex}(E_i,\theta_j)-\sigma^{t.h}(E_i,\theta_j)}{\Delta\sigma^{ex}(E_i,\theta_j)}\right]^2,$$

where, $\sigma_{t.o.t.}(E)$ is the ^{7}Li neutron total cross section and $\sigma(E,\theta)$ is the elastic plus the first inelastic scattering neutron ADX, $W_{TO}=0.05$, $W_{IO}=0.95$, N is the number of angle.

Because there are no experiment data for the ^{7}Li neutron elastic ADX $\sigma_0^{ex}(E,\theta)$ but for elastic plus the first inelastic scattering ADX $\sigma^{ex}(E,\theta)$ and the elastic scattering ADX is far greater than the inelastic scattering ADX in the energy range from 8 to 20MeV. So a set of rather suitable initial optical potential parameters and interaction potential parameters are adopted for calculations of the inelastic scattering ADX $\sigma_1^{t.h}(E,\theta)$, which remained unchanged during searching the optical potential parameters. The expression $\sigma^{t.h}(E,\theta)=\sigma_0^{t.h}(E,\theta)+\sigma_1^{t.h}(E,\theta)$ will not affect the quality of the searched optical potential parameters. The 7 energy points of the measurement elastic plus the inelastic scattering ADX and the evaluation total cross section with incident energy range from 8 to 14MeV were taken from H. H. Hogue et al[9] and the ENDF/BVI data file. During the searching, the weight factors W_{TO} and W_{IO} are taken to be 0.05 and 0.95 respectively. The chi-square and the searched optical parameters are listed in table 1(energy unit: MeV, length unit: fm).

Table 1. The searched Optical Parameters and chi-square χ_0^2

V_{RO}	R_{RO}	a_{RO}	C_{RO}	V_{IO}	R_{IO}	a_{IO}	C_{IO}	V_{LS}	χ_0^2
-40.66	1.31	0.74	0.43	25.72	1.18	0.47	0.39	28.4	1.79

The comparisons between experiment data and the calculations are shown in Fig. 1-2. From the results, We can find that the calculated elastic plus inelastic scattering ADX in the forward angle are increased with the incident energy in the range form 8 to 14MeV. We think it is reasonable. But the measurement ADX have not such tendency. The data at 0^{0} are around 700mb/sr.. Therefore the calculated data in forward angle at 8MeV are larger than the experimental and are relatively consistent well with the measurement data in energy range from 9 to 12 MeV. In energy region 13 to 14 MeV the calculated data became larger than the experimental. Generally speaking, the consistencies between the calculated and the experiment data are good. After the determination of the optical parameters, the interaction potential parameters and the deformation factor were adjusted and determined. The expression of the residual interaction potential has the form

$$V_{IN} = -\beta_2 A_T^{1/3}\left[\frac{R_{R1}}{a_{R1}}V_R'\frac{df(x_{R1})}{dx_{R1}} + i\frac{R_{R1}}{a_{R1}}V_I'\frac{df(x_{I1})}{dx^2_{I1}}\right] \quad (22),$$

where $x_{i1} = \dfrac{r - R_{i1}A_T^{1/3}}{a_{i1}}$ $(i = R, I)$, $V_R' = V_{R1} + C_{R1}E_C$,

$V_I' = V_{I1} + C_{I1}E_C$.

The adjustable parameters are β_2, V_{R1}, C_{R1}, R_{R1}, a_{R1}, V_{I1}, C_{I1}, R_{I1} and a_{I1}. The following form of chi-square were used during searching these parameters,

$$\chi_1^2 = W_{T1}\sum_i\left[\frac{\sigma_{int}^{th}(E_i) - \sigma_{int}^{ex}(E_i)}{\Delta\sigma_{int}^{ex}(E_i)}\right]^2 + W_{I1}\frac{1}{N}\sum_{ij}\left[\frac{\sigma_{in}^{th}(E_i,\theta_j) - \sigma_{in}^{ex}(E_i,\theta_j)}{\Delta\sigma_{in}^{ex}(E_i,\theta_j)}\right]^2 ,$$

where $\sigma_{int}(E)$ is the angle integrated inelastic cross section, $\sigma_{in}(E, \theta)$ is the normalization inelastic angular distribution. the measurement angle integrated cross sections were taken from Hogue et al[9] measured data and the the angular distribution data taken from references [1,2]. Total of 4 energy points(8, 8.25, 8.5, and 10 MeV) measurement data took part in the parameters searching. The weight factors W_{T1} and W_{I1} were taken to be 0.3 and 0.7 respectively. The searched parameters are listed in table 2.

Table 2. The searched β_2^2, the interaction potential parameters and the chi-square χ^2

β_2^2	V_R	R_{R1}	a_{R1}	C_{R1}	V_{I1}	R_{I1}	a_{I1}	C_{I1}	χ^2
1.50	-40.66	1.39	0.99	0.34	49.16	1.34	0.35	0.39	6.79

The deformation parameter β_2^2 determined by the calculation is 1.5, which is a little higher than the value in reference [6,7] (β_2^2=1.4). We think that the deformation parameter relies on the experimental data which are used for parameters searching. Using the determined parameters, the calculated results in the energy range from 8 to 20MeV are shown in Fig. 3-6. The comparisons between the calculated and the experiment data in the energy region 8-10MeV are also shown in Fig. 2. The comparisons show that the the calculated data have a good agreement with the experiment data at 8.5 and 10 MeV and the consistencies are not so good at 8 and 8.25MeV. The shapes for the calculated ADX in the energy region 8-8.5MeV are similar but rather different for the measurement ADX. We think that more measurement data will benefit the calculation.

4. Conclusion

From the above results and discussions , we can conclude that the DWBA can be used as a primary method to calculate the ^{7}Li neutron inelastic scattering ADX at rather high incident energy(e.g. $E_n \geq 8$MeV). Because the coupling between the ground and the first excited state may exist, we think the coupled channel calculation will be better for the reaction, that will be our work in near future.

5. Acknowledgements

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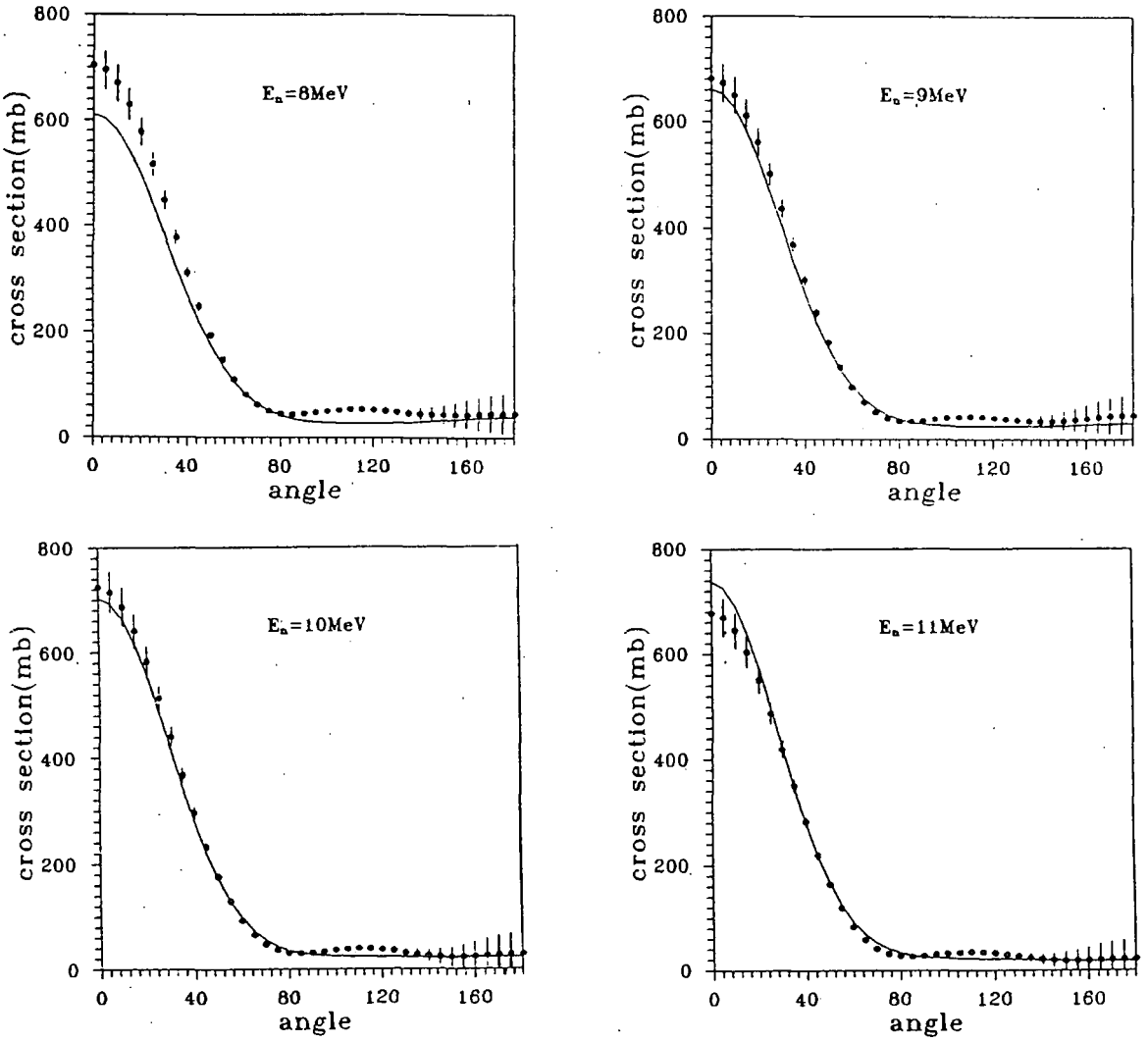


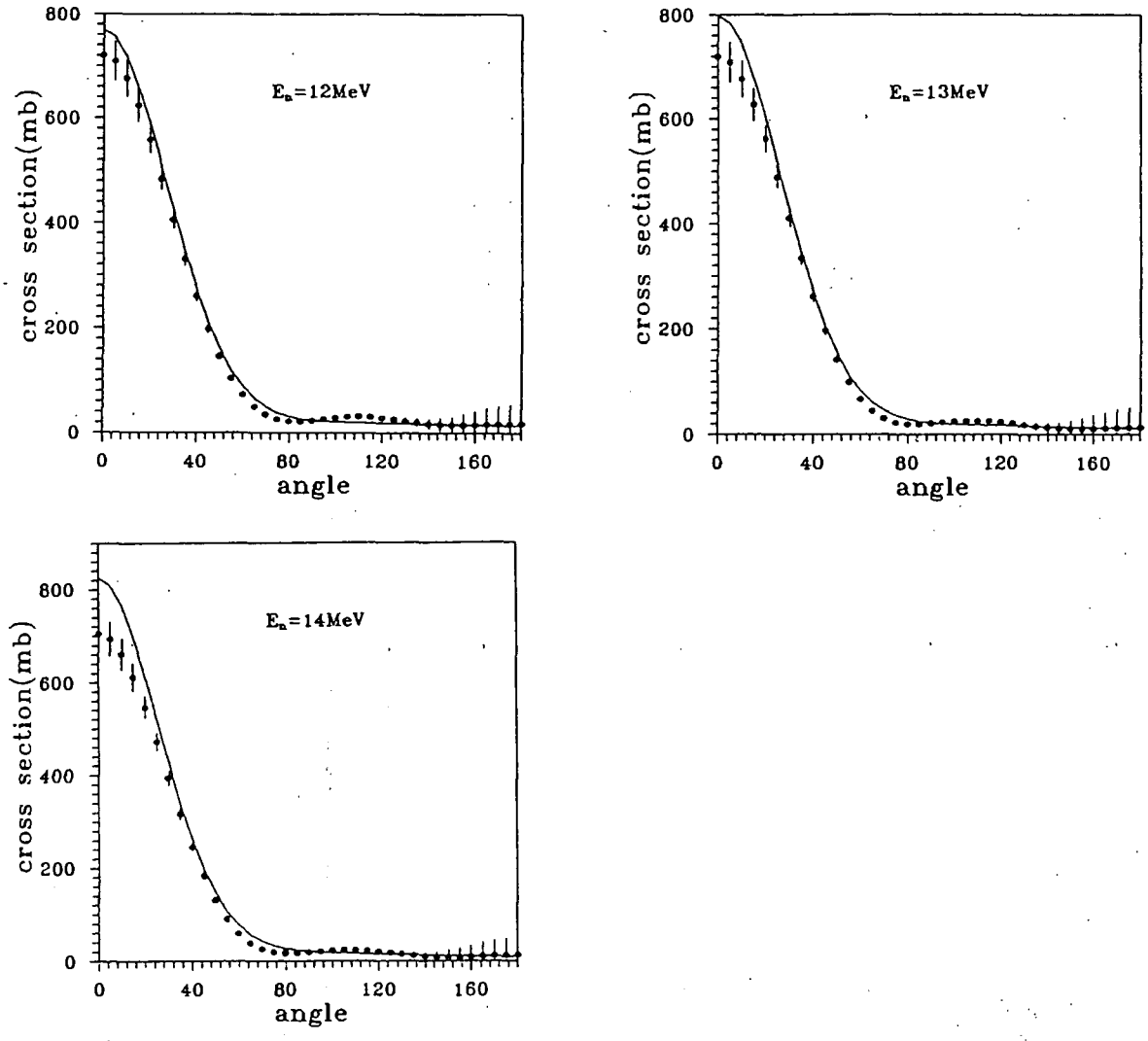
Fig. 1

Figure captions:

Fig.1-2. The comparisons between the calculated and the measured ^{7}Li elastic plus inelastic scattering neutron ADX in the energy range from 8 to 14MeV.

Fig.3. The comparisons between the calculated and the measured ^{7}Li inelastic scattering neutron ADX in the energy range from 8 to 10MeV.

Fig.4-6. The Calculated inelastic scattering neutron ADX in the energy range from 11 to 20MeV.


cross section(mb)
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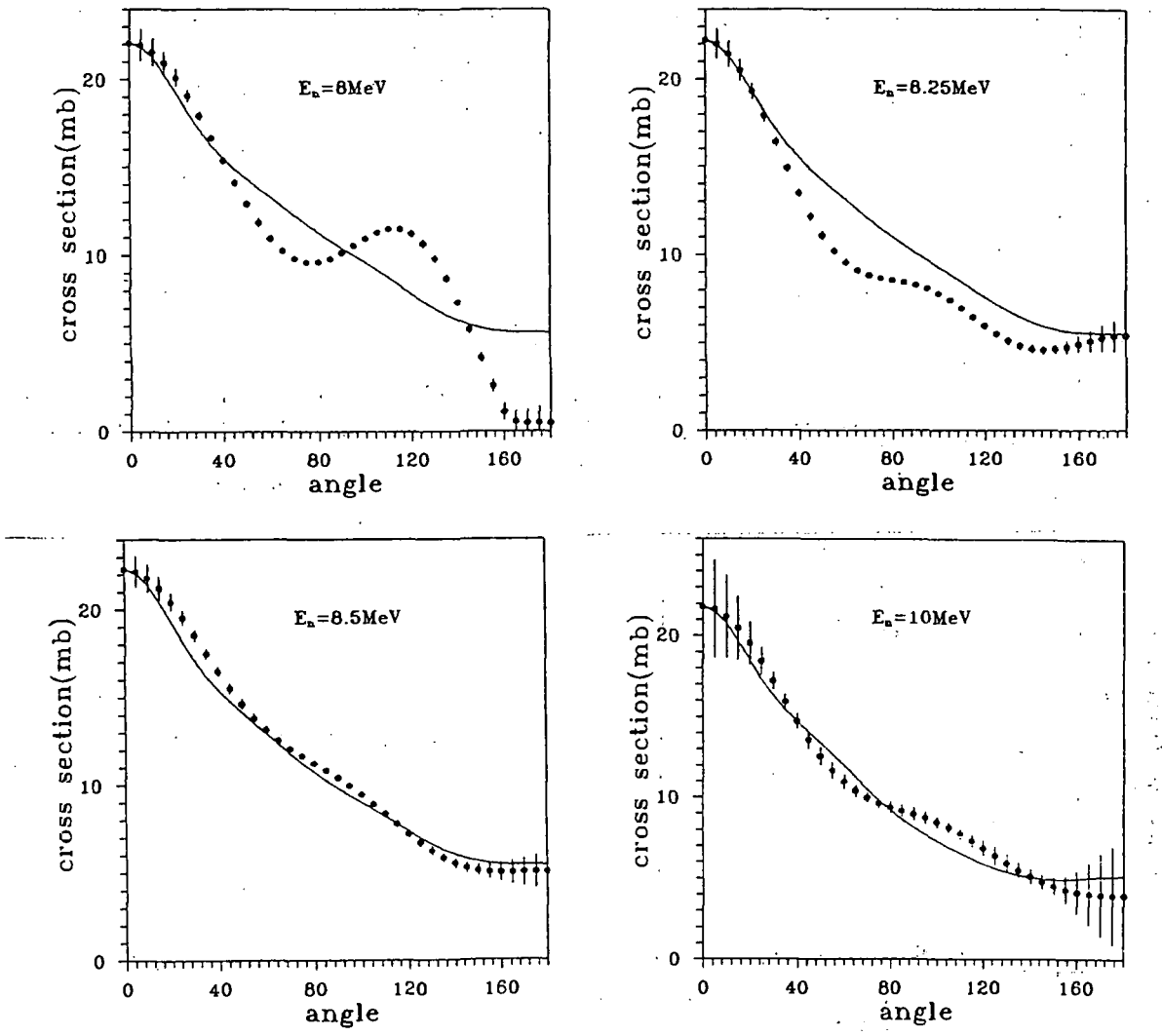
600
400
200
0
0
40
80
120
160
angle
E_n=12MeV
E_n=13MeV
E_n=14MeV

Fig.2


E_n=8MeV
E_n=8.25MeV
E_n=8.5MeV
E_n=10MeV
cross section(mb)
angle
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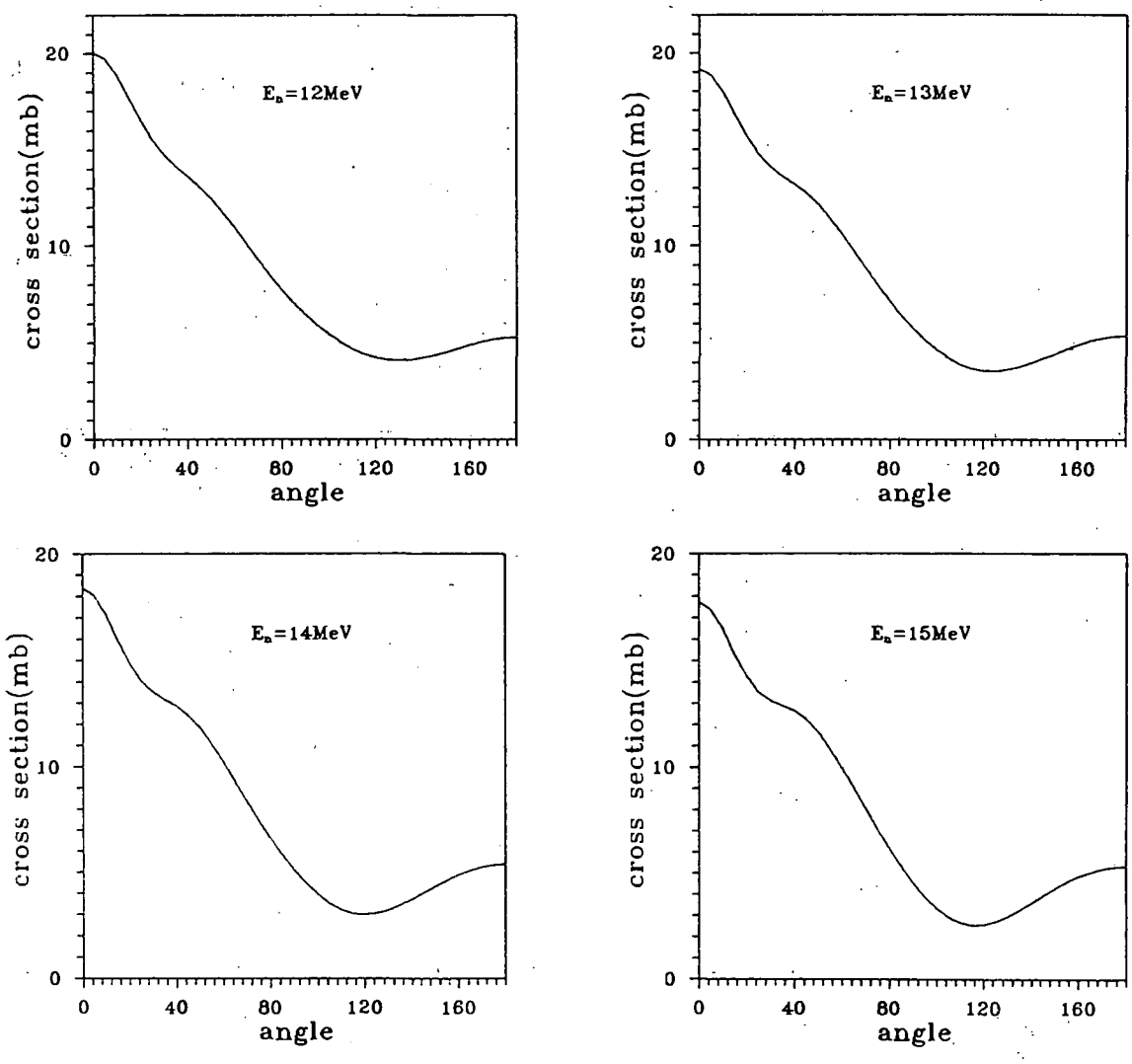
10
20
0
40
80
120
160

Fig. 3


cross section(mb)
20
10
0
E_n=12MeV
0
40
80
120
160
angle
cross section(mb)
20
10
0
E_n=13MeV
0
40
80
120
160
angle
cross section(mb)
20
10
0
E_n=14MeV
0
40
80
120
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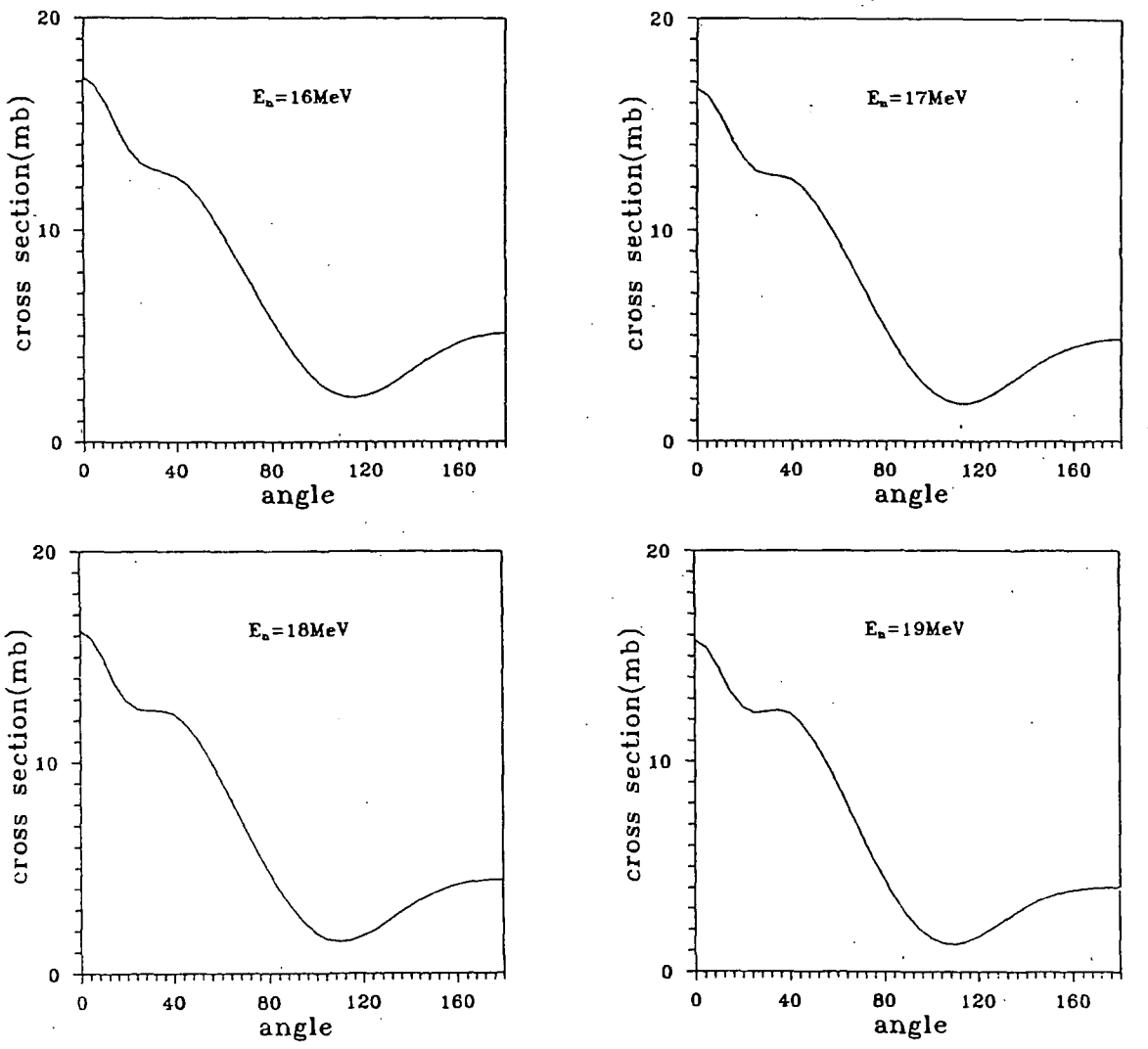
E_n=15MeV
0
40
80
120
160
angle

Fig. 4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0
cross section(mb)
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40
80
120
160
angle
E_n=17MeV
E_n=18MeV
E_n=19MeV

Fig. 5

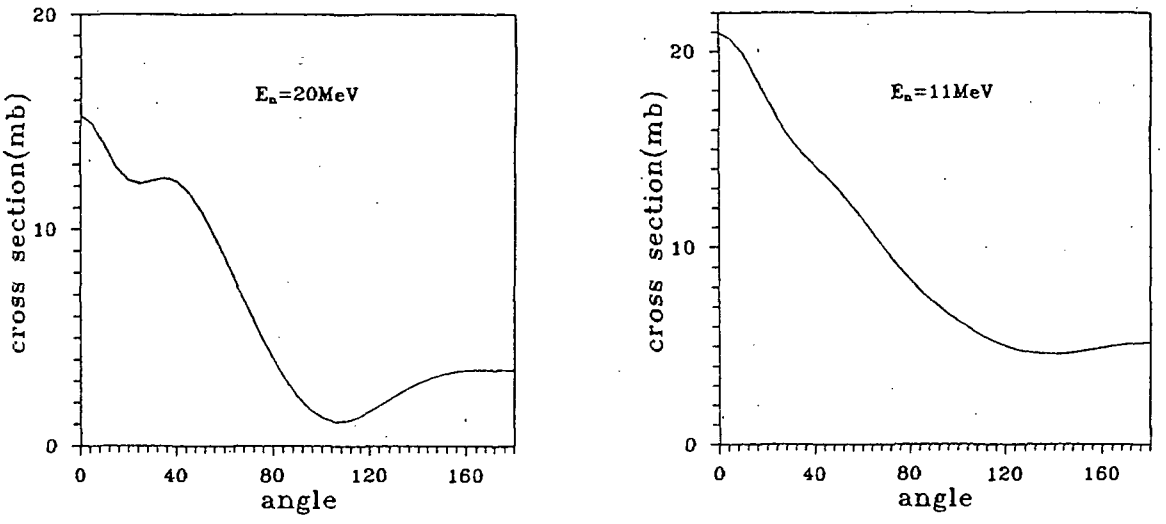

Fig. 6

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