Level Width Broadening Effect

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【**abstract**】*In file-6 for double-differential cross sections, the level width broadening effect should be taken into account properly due to Heisenberg' uncertainty. Besides level width broadening effect, the energy resolution in the measurements is also needed in fitting measurement procedure. In general, the traditional normal Gaussian expansion is employed. However, to do so in this way the energy balance could not be held. For this reason, the deformed Gaussian expansion functions with exponential form for both the single energy point and continuous spectrum are introduced, with which the normalization and energy balance conditions could be held exactly in the analytical form.*

Introduction

To set up file-6 for double-differential cross sections of light nuclei with the new approach[1], the Heisenberg' uncertainty relation, as a basic principle in quantum mechanics, should be taken into account properly. However, the shape of expansion for this uncertainty is not provided. Usually the traditional Gaussian expansion form is employed for the level width broadening expansion. However, the normal Gaussian expansion does not keep the normalization and energy balance. An additional factor is added in order to keep the normalization condition[1], while in this way the energy balance is still not held. Hence a deformed Gaussian expansion is introduced accordingly, with which either the normalization or the energy balance could be held satisfactorily. In general, the Heisenberg relation uncertainty needs to be considered only at low outgoing energies and large level widths. The representation of the deformed Gaussian expansion formula is presented in this paper. The normal Gaussian expansions are introduced in section 1, while the deformed Gaussian expansions are given in section 2. The relevant calculations are performed and discussed. The remarks are given in section 3.

1 Level-broadening Expansion with Normal Gaussian Form

Because of the level widths and energy resolution in the measurements, the measured data are always in a broadening form. Therefore, the broadening effect must be taken into account properly for fitting experimental measurements. For particle emission processes, the normalized Gaussian expansion reads

$$\mathrm{G}(\varepsilon,k)=\frac{1}{\sqrt{2\pi}\Gamma}\exp\left(-\frac{(\varepsilon-E)^2}{2\Gamma^2}\right) \tag{1}$$

ε refers to the expanded outgoing energy point, E stands for the individual energy from compound nucleus to level k of its residual nucleus with the width Γ. For the first emitted particle the width is given by

$$\Gamma=\sqrt{\Gamma_1^2+\Delta E} \tag{2}$$

However, for the second particle emission, E stands for the individual energy from level k_1 to level k_2, and the width is given by

$$\Gamma=\sqrt{\Gamma_1^2+\Gamma_2^2+\Delta E} \tag{3}$$

Γ_1 and Γ_2 refer to the level widths of level k_1 and level k_2, respectively. The ΔE[2] in Eq.(3) stands for the energy deviation including the finite-energy resolution of the neutron source, due mostly to the energy reduction of the deuterium beam in the neutron producing target, and the energy spread caused by the finite timing resolution in the time-of-flight method used in the measurements. Of course, ΔE=0 is used in the file-6 in the format of ENDF/B-6 outputting, in which the energy deviation from measurements should not be involved.

To keep the normalization condition, the normalized Gaussian expansion has the following form:

$$\mathrm{G}(\varepsilon,E)=\frac{\sqrt{2}}{\sqrt{\pi}\Gamma}\frac{\exp\left(-\frac{(\varepsilon-E)^2}{2\Gamma^2}\right)}{1+\mathrm{erf}\left(\frac{E}{\sqrt{2}\Gamma}\right)} \tag{4}$$

where erf in Eq.(4) is the error function. Only in the case of $E/\sqrt{2}\Gamma << 1$, the Eq.(4) has obvious value from that of Eq.(1).

In the case of continuous spectrum, the spectrum of the outgoing particle is written by $S(\varepsilon')$, with the energy region $\varepsilon_{\min} \le \varepsilon' \le \varepsilon_{\max}$, which often occur in the secondary particle emission processes, the normal Gaussian expansion at energy point ε reads [1]

$$S_{\mathrm{G}}(\varepsilon) = \frac{\sqrt{2}}{\sqrt{\pi}\Gamma} \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} \frac{\exp\left\{-\frac{(\varepsilon-\varepsilon')^2}{2\Gamma^2}\right\}}{1+\mathrm{erf}(\frac{\varepsilon'}{\sqrt{2}\Gamma})} S(\varepsilon')\mathrm{d}\varepsilon' \tag{5}$$

This expression keeps the value of the cross section unchangeable as shown by the following equation

$$\int_0^\infty S_{\mathrm{G}}(\varepsilon)\mathrm{d}\varepsilon = \int_{\varepsilon_{\min}^c}^{\varepsilon_{\max}^c} S(\varepsilon')\mathrm{d}\varepsilon' \tag{6}$$

The formulation mentioned above is employed in the model calculations of neutron induced light nuclear reactions for fitting the experimental data. It stresses that all error function appeared in Eqs. (4) and (5) is caused by the restriction of positive energy region. If energy region could be extended to negative values, then the error functions would be disappeared in these equations. Because of positive energy restriction, the energy balance is not held when using the above normal Gaussian expansion functions. As the matter of fact, the Eqs.(4) and (5) only keep the normalization condition.

2 Energy Balance

2.1 Single Energy Point Expansion

When the level broadening effect is taken into account by using the normal Gaussian expansion in the ENDF/B-6 format outputting, the energy balance is not held. For instance, for a given single value of energy E, the expansion formula (4) gives the energy as

$$\int_0^\infty \mathrm{G}(\varepsilon, E)\varepsilon\mathrm{d}\varepsilon \equiv E + \Delta E \tag{7}$$

here

$$\Delta E = \sqrt{\frac{2}{\pi}}\Gamma \frac{e^{-E^2/2\Gamma^2}}{1+\mathrm{erf}(\frac{E}{\sqrt{2}\Gamma})} \tag{8}$$

If let

$$x = \frac{E}{\sqrt{2}\Gamma} \tag{9}$$

then

$$\frac{\Delta E}{E} = \frac{1}{\sqrt{\pi}x}\frac{\mathrm{e}^{-x^2}}{1+\mathrm{erf}(x)} \tag{10}$$

Obviously, in eq.(10) the value of $\Delta E/E$ decreases rapidly with the increasing of x.

The calculated values of $\Delta E/E$ as the function of x are shown in Fig.1. From Fig.1 one can see that at low values of x the energy gain $\Delta E/E$ has very large percentage. Oppositely, for large values of x the energy gain has very small percentage. From Eq.(9) one can see that the low values of x correspond to the low energy or large width.

In the case of small values of x, the traditional normal Gaussian expansion could not work in the application.

From the point of view on the applications, when $\Delta E/E < 1\%$ the level broadening effect can be neglected. However, when $\Delta E/E > 1\%$ it is corresponding to $x \le 1.96$ or $E/\Gamma < 2.772$, the level broadening effect should be taken into account properly. In order to keep the energy balance, a correction factor $a\mathrm{e}^{-b\varepsilon}$ is needed to be introduced as a multiplier factor in the normal Gaussian expansion function (4), the parameters a and b could be obtained by the two conditions: (1) normalization, (2) energy balance.

Therefore, the deformed Gaussian expansion function has the form as

$$\widetilde{\mathrm{G}}(\varepsilon, E) = a\mathrm{G}(\varepsilon, E)\mathrm{e}^{-b\varepsilon} \tag{11}$$

① From the normalization condition

$$\int_0^\infty \widetilde{\mathrm{G}}(\varepsilon, E)\mathrm{d}\varepsilon = 1 \tag{12}$$

carrying out the integration over ε, the value of a can be obtained by

$$a = \mathrm{e}^{-b^2\Gamma^2/2+b\mathrm{E}} \frac{1+\mathrm{erf}(\frac{E}{\sqrt{2}\Gamma})}{1+\mathrm{erf}(\frac{E-b\Gamma^2}{\sqrt{2}\Gamma})} \tag{13}$$

If b=0 then a=1 is reasonable.

② From the energy balance condition

$$\int_0^\infty \widetilde{\mathrm{G}}(\varepsilon, E)\varepsilon\mathrm{d}\varepsilon = E \tag{14}$$

The expression of b is obtained by

$$b = \frac{\sqrt{2}}{\sqrt{\pi}\Gamma} \frac{\exp\left\{-\frac{(E-b\Gamma^2)^2}{2\Gamma^2}\right\}}{1+\mathrm{erf}\left(\frac{E-b\Gamma^2}{\sqrt{2}\Gamma}\right)} \tag{15}$$

Let $x = \frac{E}{\sqrt{2}\Gamma}$ and $y = \frac{b\Gamma}{\sqrt{2}}$, Eq.(15) becomes into the form as

$$y = \frac{1}{\sqrt{\pi}} \frac{\exp\{-(x-y)^2\}}{1+\mathrm{erf}(x-y)} \qquad (16)$$

and Eq.(13) becomes into the following form

$$a = \exp(2xy - y^2)\frac{1+\mathrm{erf}(x)}{1+\mathrm{erf}(x-y)}$$

Obviously, when $x \to \infty$ then $y \to 0$, means there is no correction at large values of x.

Using the optimum searching method numerically, the calculated results of $y(x)$ are shown in Fig.2.

From Fig.2 one can see that at small values of x, y have large values, which means that the correction effect is important. However, at large values of x, the values of y become very small, and the correction effect could be omitted.

Therefore, the deformed Gaussian expansion function reads

$$\widetilde{\mathrm{G}}(\varepsilon, E, b) = \frac{\sqrt{2}}{\sqrt{\pi}\Gamma} \frac{\exp\left\{-\frac{(\varepsilon - E + b\Gamma^2)^2}{2\Gamma^2}\right\}}{1+\mathrm{erf}\left(\frac{E-b\Gamma^2}{\sqrt{2}\Gamma}\right)} \qquad (17)$$

The numerical solutions of the Eq.(16) indicate that if $E/\Gamma > 2.772$, the level broadening effect could be ignored.

On the other hand the difference between the deformed Gaussian expansion function of Eq. (17) and the normal Gaussian expansion function of Eq.(4), as the examples, at E=3 MeV and $\Gamma = 1.5$ MeV, which corresponding to x=1.414, is shown in Fig.3, and at E=1 MeV and $\Gamma = 1$ MeV, which corresponding to x=0.7071, is shown in Fig.4, respectively.

In comparison with the normal Gaussian expansion as shown in Fig.3 and Fig.4, the deformed Gaussian expansion curve is moved to the low energy region, the correction effects to offset the energy gain due to the normal Gaussian expansion and to keep the energy balance. The smaller value of x is, the more composition is at the low energy region.

2.2 Continuous Spectrum Expansion

Based on the normal Gaussian expansion form of Eq. (5), the energy carried by a spectrum $S_{\mathrm{G}}(\varepsilon)$ is given by

$$\int_0^\infty S_{\mathrm{G}}(\varepsilon)\varepsilon \mathrm{d}\varepsilon = E + \Delta E \qquad (18)$$

Carrying out the integration over ε at first and using the integrated relation

$$\int_0^\infty \mathrm{e}^{-\frac{(\varepsilon-\varepsilon')^2}{2\Gamma^2}} \varepsilon \mathrm{d}\varepsilon = \Gamma^2 \mathrm{e}^{-\frac{\varepsilon'^2}{2\Gamma^2}} + \varepsilon' \sqrt{\frac{\pi}{2}}\Gamma\left[1+\mathrm{erf}\left(\frac{\varepsilon'}{\sqrt{2}\Gamma}\right)\right] \qquad (19)$$

The energy and energy gain are obtained, respectively.

The energy carried by the spectrum is given by

$$E = \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} S(\varepsilon')\varepsilon' \mathrm{d}\varepsilon' \qquad (20)$$

and the energy deviation is given by

$$\Delta E = \sqrt{\frac{2}{\pi}}\Gamma \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} \frac{\mathrm{e}^{-\frac{\varepsilon'^2}{2\Gamma^2}} S(\varepsilon')}{1+\mathrm{erf}(\frac{\varepsilon'}{\sqrt{2}\Gamma})} \mathrm{d}\varepsilon' > 0 \qquad (21)$$

In the case of normalized constant spectrum, which is expressed by $S(\varepsilon) = 1/(\varepsilon_{\max} - \varepsilon_{\min})$, Eqs. (20) and (21) have the simple form analytically as

$$E = (\varepsilon_{\max} + \varepsilon_{\min})/2 \qquad (22)$$

$$\Delta E = \frac{\Gamma^2}{\varepsilon_{\max} - \varepsilon_{\min}} \ln \frac{1+\mathrm{erf}(\frac{\varepsilon_{\max}}{\sqrt{2}\Gamma})}{1+\mathrm{erf}(\frac{\varepsilon_{\min}}{\sqrt{2}\Gamma})} \qquad (23)$$

The calculation for n+^{9}Be reactions indicates that the energy gain from the normal Gaussian expansion in the case of continuous spectrum becomes serious, all of the normal Gaussian expansions for the ring-type continuous spectra give large energy gain, even $\Delta E/E > 10$, except from K_1=3 (the second excitation level of ^{9}Be) to K_2=1 (the ground state of ^{8}Be). Thus, the deformed Gaussian expansion ought to be added in the continuous spectrum expansion of Eq.(5). As same as that of the single energy point expansion, the exponential form correction factor $a\mathrm{e}^{-b\varepsilon}$ is added in the normal Gaussian expansion function of Eq.(5). The parameters of a and b can also be obtained by the normalization condition and the energy balance condition, respectively.

Therefore, the deformed Gaussian expansion function of continuous spectrum has the form as

$$\widetilde{S}_{\mathrm{G}}(\varepsilon) = \frac{\sqrt{2}a\mathrm{e}^{-b\varepsilon}}{\sqrt{\pi}\Gamma} \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} \frac{\mathrm{e}^{-\frac{(\varepsilon-\varepsilon')^2}{2\Gamma^2}}}{1+\mathrm{erf}\left(\frac{\varepsilon'}{\sqrt{2}\Gamma}\right)} S(\varepsilon')\mathrm{d}\varepsilon' \qquad (24)$$

In order to get the values of the parameters a and b, the two following condition give two equations.

① From the normalization condition

$$\int_0^\infty \widetilde{S}_{\mathrm{G}}(\varepsilon)\mathrm{d}\varepsilon = 1 \qquad (25)$$

Carrying out the integration over ε the following relation can be given by

$$a\mathrm{e}^{b^2\Gamma^2/2}\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} S(\varepsilon')\mathrm{e}^{-b\varepsilon'}\frac{1+\mathrm{erf}\left(\dfrac{\varepsilon'-b\Gamma^2}{\sqrt{2}\Gamma}\right)}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'=1 \qquad (26)$$

This is the equation to get the parameter a. Obviously, if $b\to0$ then $a\to1$ this is reasonable.

② From the energy balance condition

$$\int_0^\infty \widetilde{S}_{\mathrm{G}}(\varepsilon)\varepsilon\mathrm{d}\varepsilon = E \qquad (27)$$

Substituting Eq.(24) into Eq.(27) and carrying out the integration over ε the following relation is obtained by

$$E=\sqrt{\frac{2}{\pi}}a\Gamma\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\frac{\mathrm{e}^{-\frac{\varepsilon'^2}{2\Gamma^2}}S(\varepsilon')}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'+a\int_{\varepsilon_{\min}}^{\varepsilon_{\max}} e^{\frac{b^2\Gamma^2}{2}-b\varepsilon'}S(\varepsilon')\varepsilon'\frac{1+\mathrm{erf}\left(\dfrac{\varepsilon'-b\Gamma^2}{\sqrt{2}\Gamma}\right)}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'-b\Gamma^2 \qquad (28)$$

Substituting Eq.(26) into Eq.(28) the equation of the parameter b is expressed by a very complex form

$$E+b\Gamma^2=\frac{\sqrt{\dfrac{2}{\pi}}\Gamma\mathrm{e}^{-\frac{b^2\Gamma^2}{2}}\displaystyle\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\frac{\mathrm{e}^{-\frac{\varepsilon'^2}{2\Gamma^2}}S(\varepsilon')}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'+\displaystyle\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\mathrm{e}^{-b\varepsilon'}S(\varepsilon')\varepsilon'\frac{1+\mathrm{erf}\left(\dfrac{\varepsilon'-b\Gamma^2}{\sqrt{2}\Gamma}\right)}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'}{\displaystyle\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\mathrm{e}^{-b\varepsilon'}S(\varepsilon')\frac{1+\mathrm{erf}\left(\dfrac{\varepsilon'-b\Gamma^2}{\sqrt{2}\Gamma}\right)}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'} \qquad (29)$$

Obviously, when the width $\Gamma\to0$ then we have $b\to0$ and $a\to1$.

Since the secondly emitted particle has the energy independent ring-type spectrum by the recoil effect[1], in this case the constant spectrum, Eq.(29) can be reduced to the following form

$$E+b\Gamma^2=\frac{\sqrt{\dfrac{2}{\pi}}\Gamma\mathrm{e}^{-\frac{b^2\Gamma^2}{2}}\displaystyle\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\frac{\mathrm{e}^{-\frac{\varepsilon'^2}{2\Gamma^2}}}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'+\displaystyle\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\mathrm{e}^{-b\varepsilon'}\varepsilon'\frac{1+\mathrm{erf}\left(\dfrac{\varepsilon'-b\Gamma^2}{\sqrt{2}\Gamma}\right)}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'}{\displaystyle\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\mathrm{e}^{-b\varepsilon'}\frac{1+\mathrm{erf}\left(\dfrac{\varepsilon'-b\Gamma^2}{\sqrt{2}\Gamma}\right)}{1+\mathrm{erf}\left(\dfrac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'} \qquad (30)$$

Let $x=\dfrac{\varepsilon'}{\sqrt{2}\Gamma}$ and $y=\dfrac{b\Gamma}{\sqrt{2}}$, x and y are dimensionless, the integration limits are changed into

$\varepsilon_{\min}\to x_{\min}$ and $\varepsilon_{\max}\to x_{\max}=\dfrac{\varepsilon_{\max}}{\sqrt{2}\Gamma}$. Therefore, Eq.(29) becomes into the form as

$$\frac{E}{\sqrt{2}\Gamma}+y=\frac{\dfrac{1}{\sqrt{\pi}}\mathrm{e}^{-y^2}\displaystyle\int_{x_{\min}}^{x_{\max}}\mathrm{e}^{-x^2}\frac{S(\sqrt{2}\Gamma x)}{1+\mathrm{erf}(x)}\mathrm{d}x+\displaystyle\int_{x_{\min}}^{x_{\max}}e^{-2xy}S(\sqrt{2}\Gamma x)x\frac{1+\mathrm{erf}(x-y)}{1+\mathrm{erf}(x)}\mathrm{d}x}{\displaystyle\int_{x_{\min}}^{x_{\max}}\mathrm{e}^{-2xy}S(\sqrt{2}\Gamma x)\frac{1+\mathrm{erf}(x-y)}{1+\mathrm{erf}(x)}\mathrm{d}x} \qquad (31)$$

In the case of normalized constant spectrum, Eq.(31) is reduced to the form as

$$\frac{E}{\sqrt{2}\Gamma}+y=\frac{\frac{\mathrm{e}^{-y^2}}{\sqrt{\pi}}\int_{x_{\min}}^{x_{\max}}\frac{\mathrm{e}^{-x^2}}{1+\operatorname{erf}(x)}\mathrm{d}x+\int_{x_{\min}}^{x_{\max}}\mathrm{e}^{-2xy}x\frac{1+\operatorname{erf}(x-y)}{1+\operatorname{erf}(x)}\mathrm{d}x}{\int_{x_{\min}}^{x_{\max}}\mathrm{e}^{-2xy}\frac{1+\operatorname{erf}(x-y)}{1+\operatorname{erf}(x)}\mathrm{d}x} \tag{32}$$

Obviously, if $y=0$ then Eq.(32) becomes into

$$E=\frac{\sqrt{2}\Gamma^2}{\varepsilon_{\max}-\varepsilon_{\min}}\int_{x_{\min}}^{x_{\max}}\frac{\mathrm{e}^{-x^2}}{1+\operatorname{erf}(x)}\mathrm{d}x+E \tag{33}$$

this equation could be held in any case, so that $y=0$ is always not the solution of Eq.(32). This condition is used for the numerical method to set the initial value of y.

If the integration limits region is tended to zero, i.e. $\varepsilon_{\min}=\varepsilon_{\max}\equiv E$, then Eq.(32) is reduced into

$$y=\frac{1}{\sqrt{\pi}}\frac{\exp\{-(x-y)^2\}}{1+\operatorname{erf}(x-y)} \tag{34}$$

Which is identical to Eq.(16). Thus, the correctness of Eq.(32) is proved.

For a given continuous spectrum of $S(\varepsilon)$, and its integration limits, as well as the width Γ, Eq.(29) can be solved rapidly with the optimum seeking method.

Finally the deformed Gaussian expansion function of continuous spectrum reads

$$\tilde{S}_{\mathrm{G}}(\varepsilon)=\sqrt{\frac{2}{\pi\Gamma^2}}\mathrm{e}^{\frac{b^2\Gamma^2}{2}-b\varepsilon}\frac{\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\frac{\mathrm{e}^{-\frac{(\varepsilon'-\varepsilon)^2}{2\Gamma^2}}}{1+\operatorname{erf}\left(\frac{\varepsilon'}{\sqrt{2}\Gamma}\right)}S(\varepsilon')\mathrm{d}\varepsilon'}{\int_{\varepsilon_{\min}}^{\varepsilon_{\max}}\mathrm{e}^{-b\varepsilon'}S(\varepsilon')\frac{1+\operatorname{erf}\left(\frac{\varepsilon'-b\Gamma^2}{\sqrt{2}\Gamma}\right)}{1+\operatorname{erf}\left(\frac{\varepsilon'}{\sqrt{2}\Gamma}\right)}\mathrm{d}\varepsilon'} \tag{35}$$

Let us take two examples:

1) The energy spectrum scope is from $\varepsilon_{\min}=0.5$ MeV to $\varepsilon_{\max}=1.5$ MeV with the width $\Gamma=1$ MeV. So the energy carried by the continuous spectrum is *E*=1 MeV, the energy deviation is $\Delta E=0.3$ MeV, and the ratio is $\Delta E/E$ =30%. Solving Eq.(30) and using Eq.(26) we have *a*=1.8078, *b*=0.51815 MeV^{-1}. The curves of the normal Gaussian expansion function of Eq.(5) and the deformed Gaussian expansion function of Eq. (35) are shown in Fig.5.

2) The energy spectrum scope is from $\varepsilon_{\min}=0.2$ MeV to $\varepsilon_{\max}=0.4$ MeV with the width $\Gamma=1$ MeV. So the energy carried by the continuous spectrum is *E*=0.3 MeV, the energy deviation is $\Delta E=0.2305$ MeV, and the ratio is $\Delta E/E$ =76.6%, with the result of *a*=2.7430, *b*=2.5169 MeV^{-1}. The curves of the normal Gaussian expansion function of Eq.(5) and the deformed Gaussian expansion function of Eq. (35) are shown in Fig.6.

In comparison with the normal Gaussian expansions, as shown in Fig.5 and Fig.6, the width broadening expansion of the deformed Gaussian expansions has more composition at low energy region obviously, which offsets the energy gain caused by the normal Gaussian expansion.

The calculations indicate that the smaller of the ratio E/Γ is, the more composition is at low energy region. The deformed Gaussian expansion could raise the low energy part of the continuous spectrum.

3 Remarks

In the new method for calculating neutron induced reaction data of light nuclei to set up file-6 for double-differential cross sections, all of the emissions are carried out from discrete levels to discrete levels, and the levels have their individual life-time, then the Heisenberg' uncertainty should be taken into account properly, because the uncertainty is surely involved in the measurements of outgoing particles. Usually the traditional normal Gaussian expansion form is employed in the fitting procedure [1], but to do so in this way the energy balance could not be held. For this reason the deformed Gaussian expansion functions are introduced to keep the energy balance for both single energy points and continuous spectra in CMS. The correction factor is in exponential form to avoid the negative values occuring in the expanded spectra, which often appear in the case of linear correction factor *a*+*bε*. Therefore, the deformed Gaussian expansion functions could be employed for making the energy balance hold for the double-differential cross sections of all kinds of outgoing particles in the file-6 when the level width broadening effect is taken into account. In addition, in order to keep the energy balance in LS, from the formulation in Ref.1, it turns out that any expansions are not needed for the partial wave except *l*=0 wave. To do so in this way, the energy scope of the outgoing neutron angular-energy spectra could be extended by the level width broadening expansions. However, in the region of high outgoing neutron energies of the spectra, the extended part in the angular-energy spectra could become isotropic, due to no any contribution in the angular-energy spectra without the level width broadening expansions for the partial waves with *l*>0. This is the condition to keep the energy balance in LS.

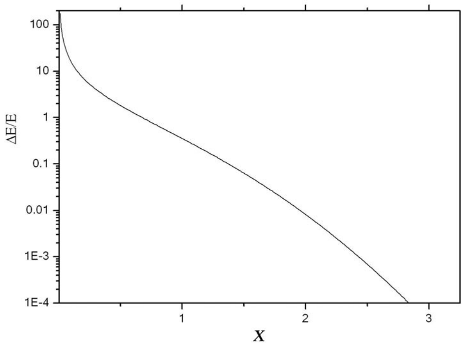

Fig.1 The energy gain $\Delta E/E$ vs x

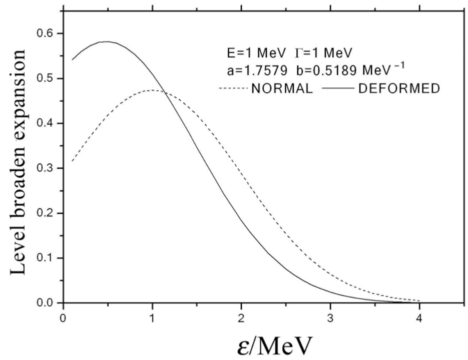

Fig.4 The level broadening expansioning at E=1 MeV Γ=1 MeV

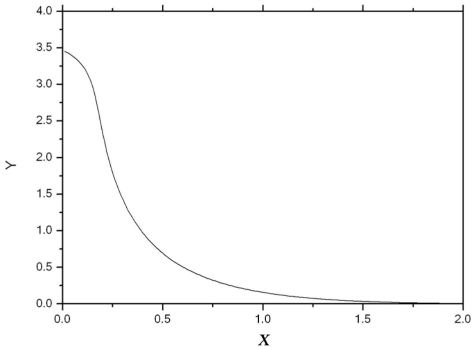

Fig.2 y vs x

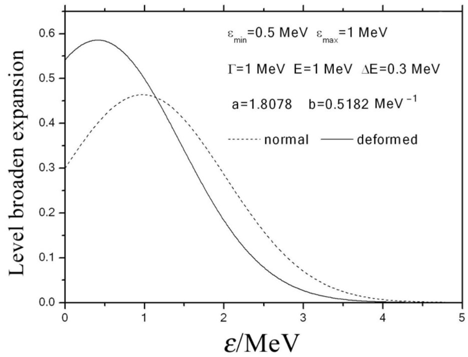

Fig.5 The width broadening of continuous spectrum

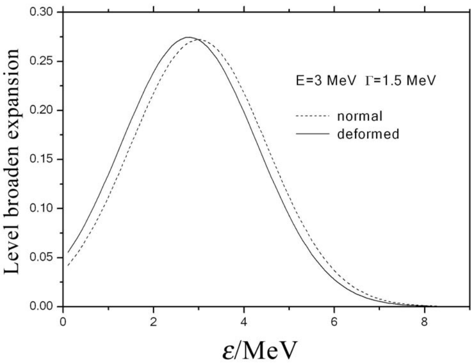

Fig.3 The level broadening expansion at E=3 MeV Γ=1.5 MeV

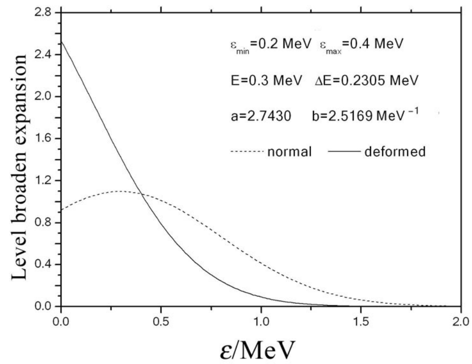

Fig.6 The width broadenning of continuous spectrum

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