LBL-23228 c.2

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Presented at the 25th International Winter Meeting
on Nuclear Physics, Bormio, Italy,
January 19–23, 1987

PARTICLE EVAPORATION SPECTRA WITH INCLUSION OF THERMAL SHAPE FLUCTUATIONS

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April 1987

NUCLEAR SCIENCE DIVISION

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

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Particle Evaporation Spectra with Inclusion of Thermal Shape Fluctuations

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Abstract

The origin of the substantial sub-Coulomb component observed in proton and ^{4}He evaporation spectra at high excitation energy is attributed to the thermal excitation of shape degrees of freedom. A critique of the Hauser-Feshbach theory as used in evaporation codes is presented. A new formalism including the thermal excitation of collective modes as well as quantal penetration in the framework of a transition state approach is derived.

Introduction

The dominant channels in compound nucleus decay involve the emission of light particles like neutrons, protons, and alphas. Expressions for the corresponding partial decay widths and specifically for the associated kinetic energy spectra go back to the ancient past of compound nucleus theory and have acquired since a patina of venerability sometimes confused with the mark of truth.

Despite the title of this paper, it is not our desire to criticize in depth the foundations of, say, the Hauser Feshbach theory,whose truth is easily verified as it involves solely the statistical assumption of compound nucleus and the use of the detailed balance or of microscopic reversibility. Rather we would like to show some pedants who have marred those venerable theories with the unwitty use of optical model transmission coefficients the possible dangers and errors of their ways as they move to higher and higher energies in the hopeful attempt of explaining the spectra of particles emitted in intermediate energy heavy ion collisions. In all fairness, their arduous and questionable work may not go totally unrewarded as it unveils, and may have done so already, some interesting physics in this new energy region.

Aside from the uncertainty associated with the characterization of the emitting sources in so far as their number, mass, charge and excitation energy are concerned, it seems fairly well established that in this high energy realm, light charged particles such as protons and alphas are emitted with kinetic energies extending far below the expected Coulomb energy. This observation has prompted a variety of explanations going from the incorporation of ground state deformations, to the ad-hoc introduction of deformation as a parameter to be fixed by the data, to the grand vision of particles being emitted from the "bloated stratosphere" (sic) of highly excited nuclei.

In what follows we are going to criticize the use of the standard formalism, consider possible ameliorations and, eventually offer a novel and consistent formalism incorporating thermal shape fluctuations and quantum penetration.

Elementary derivation of the standard formulae and the resistable evils of optical models

One of the main aspects that we find objectionable in the standard evaporation codes is the casual and unwitty use of the optical model for the evaluation of the inverse transition probabilities or cross sections. In order to show the deficiencies and dangers of such an approach we are going to rederive quickly the relevant equations and to point out under which conditions the use of an optical model may be warranted. For our purpose we need here only to derive the simplest form for the decay width.

Consider the compound nucleus as the initial state A and the residual nucleus plus evaporated particle as the final state B. The detailed balance principle says that:

$$\rho_A P_{A\to B} = \rho_B P_{B\to A} \qquad (1)$$

where $P_{A\to B}$ is the probability of going from A to B, $P_{B\to A}$ is the probability for the inverse transition, ρ_A and ρ_B are the respective statistical weights. The quantity ρ_A is just the compound nucleus level density $\rho(E)$. For ρ_B we can write

$$\rho_B = \rho_B{}^*(E\text{-}B\text{-}\varepsilon)\, h^{-3} V 4\pi p^2\, dp/d\varepsilon \qquad (2)$$

where $\rho_B{}^*(E\text{-}B\text{-}\varepsilon)$ is the level density of the residual nucleus at the appropriate excitation energy, p and ε are the momentum and energy of the emitted particle and V is a normalization volume that will drop out in the final expression for $P_{A\to B}$.

The inverse probability $P_{B\to A}$ is written typically in terms of the inverse cross section $\sigma(\varepsilon)$ and of the particle velocity v as

$$P_{B\to A} = \sigma_{inv}(\varepsilon) v/V \qquad (3)$$

Substituting we obtain

$$P_{A\to B} = h^{-3}\, \rho(E)^{-1}\, 4\pi\, 2m\, \sigma(\varepsilon)\, \varepsilon\, \rho^*(E\text{-}B\text{-}\varepsilon) \qquad (4)$$

By expanding the level density as

$$\ln \rho^*(E\text{-}B\text{-}\varepsilon) = \ln \rho^*(E\text{-}B) - (\partial \ln \rho^*/\partial\varepsilon)\, \varepsilon + \ldots \qquad (5)$$

One obtains

$$P_{A\to B} = h^{-3}\, \rho(E)^{-1}\, 4\pi\, 2m\, \rho^*(E\text{-}B)\, \sigma(\varepsilon)\, \varepsilon \exp(-\varepsilon/T) \qquad (6)$$

which shows the Maxwellian-like shape characterized by the temperature

$$T = (\partial \ln\rho^*/\partial\varepsilon\,|_{E\text{-}B}\,)^{-1} \qquad (7)$$

The writing of the inverse probability as in (3) is the cause of a common misunderstanding. In fact it is a common practice (and a source of potential troubles) to evaluatate $\sigma_{inv}(\varepsilon)$ by means of an optical model with parameters set to reproduce elastic scattering from a cold nucleus. Inspection of the detailed balance equation reveals that σ_{inv} is a rather peculiar cross section, namely it is the inverse cross section for a particle with energy ε approaching a nucleus excited with an energy E-B-ε in the same quantum state and thus with the same deformation of the nucleus left behind immediately after the emission of the particle. In contrast, the σ_{inv} commonly calculated with an optical model refers to a nucleus in its own ground state and with its ground state deformation, which may, at best, be relevant only for particle energies around $\varepsilon \cong$ E-B. These energies are practically never observed since most of the particles come out rather with energies $\varepsilon \cong$ T+V where V is the Coulomb barrier.

It follows that, in the most common case, the excitation energy of the residual nucleus may be so great as to make the relevance of the shape and optical potential of the ground state nucleus somewhat doubtful. Certainly the large excitation energy allows the nucleus the access to a broad range of deformations which may greatly influence the decay process. The commonly felt need to doctor the radius parameter of the optical potential in order to accommodate effects of this sort on one hand indicates the seriousness of the problem, on the other makes the extensive effort to calculate penetrability coefficients for each impact parameter appear rather futile.

On the way to a new solution

It is apparent that the distribution of deformations that the residual nucleus assumes spontaneously during the emission process, profoundly affects the kinetic energy spectra of charged particles through the associated changes of the Coulomb field. One could envisage a simple general procedure to account for such shape fluctuations. If the total potential energy is known as a function of shape

$$V = V(\text{shape})$$

then the thermal shape distribution can be calculated

$$S(\text{shape},T) = k \exp\left[-V(\text{shape})/T\right]$$

If one manages to calculate the energy spectrum P for each shape, then one can obtain the overall spectrum

$$P(\varepsilon,T) = \int S(\text{shape},T)\, P(\text{shape},T,\varepsilon)\, d(\text{shape})$$

The difficulty of the problem is now shifted to the calculation of P(shape,T,ε) for which some suggestions have been made.

This procedure, however, is unsatisfactory for a variety of reasons, one of which is that one should not consider the distribution in shapes of the residual nucleus by itself, but in the presence of the emitted particle, which, by virtue of its charge, can induce a shape polarization on the residual nucleus. It is possible to devise a fully consistent formalism which allows for the shape fluctuations and which does not rely on any specific model. Rather this formalism will ask for a minimum amount of information out of any given model proposed for the description of hot compound nuclei.

A transition state formalism for thermal spectra

We can try to write down the decay rate in analogy to the fission process, by searching first for a "saddle point" in deformation space. This saddle point could be searched, for instance, among the shapes corresponding to the small particle in near contact with the surface of the residual nucleus which in turn can have a variety of deformations. The relevant collective degrees of freedom can be catalogued as shown in fig. (1). The first class corresponds to the decay mode, which is unbound and similar to the fission mode. The second class includes the non-amplifying modes whose excitation energy is directly translated without amplification into kinetic energy at infinity. Two such modes could be the two orthogonal oscillations of the particle about the tip of the "spheroidal" residual nucleus. With these two modes, the particle can experience the whole distribution of Coulomb energies associated with a given deformation of the residual nucleus. The third class corresponds to the amplifying modes. In these modes the total potential energy remains rather flat about the minimum, while substantial changes occur in the Coulomb energy. As shown at the bottom of fig. (1), an oscillation about this mode involving an amount of energy on the order of the temperature corresponds to a variation in the monopole - monopole term of the Coulomb energy

$$\Delta E_C = 2\,(c^2/k)^{1/2} = 2\,(pT)^{1/2} \qquad (8)$$

where the coefficients c and k are defined by the quadratic expansion of the total potential energy associated with the mode z:

$$V(z) = B_0 + kz^2 \qquad (9)$$

and by the linearization of the Coulomb energy along the same mode:

$$E_{Coul} = E^0{}_{Coul} - cz \qquad (10)$$

The quantities B_0, $E^0{}_{Coul}$, c, k and p are defined at the minimum of the total potential energy and are as a consequence saddle point quantities.

After having identified and classified the normal modes at the saddle point, one can write down the decay width as

$$\Gamma^{(n)}d\varepsilon\,\Pi dx_i dp_i = [2\pi\rho(E)]^{-1}\,\rho^*[E-B_0-\varepsilon-\Sigma(a_i x_i^2+p_i^2/2m_i)]\,d\varepsilon\Pi(h^{-3}dx_i dp_i) \qquad (11)$$

where ε is the kinetic energy along the decay mode and a_i, m_i are the stiffnesses and the inertias of the bound modes.

With excellent accuracy one can expand ln ρ^* to obtain

$$\Gamma^{(n)}d\varepsilon\,\Pi dx_i dp_i = [2\pi\rho(E)]^{-1}\,\rho^*(E-B_0)\,\exp-[\varepsilon+\Sigma(a_i x_i^2+p_i^2/2m_i)]/T\,d\varepsilon\Pi(h^{-3}dx_i dp_i) \qquad (12)$$

where the saddle temperature T is given by

$$T = \partial \ln \rho^*/\partial x\,|_{x=E-B} \quad (13)$$

We are now going to consider three specific cases. The first and simplest chooses to treat only one decay mode and one amplifying mode in detail. The decay width becomes

$$\Gamma(\varepsilon,z)\, d\varepsilon dz \propto \exp -(\varepsilon+kz^2)/T\, d\varepsilon dz \quad (14)$$

Remembering that the final kinetic energy can be written as

$$E = E^0_{Coul}-cz+\varepsilon \quad (15)$$

we can rewrite the decay width as follows

$$\Gamma(\varepsilon,z) \propto \exp -(\varepsilon+(E- E^0_{Coul}-\varepsilon)^2/p)/T \quad (16)$$

or $\Gamma(\varepsilon,z) \propto \exp -(\varepsilon+(x-\varepsilon)^2/p)/T$ (17)

The final kinetic energy distribution is obtained by integrating over ε

$$P(E) \propto \int \exp\text{-}(\varepsilon+(x-\varepsilon)^2/p)/T\, d\varepsilon \quad (18)$$

or $P(E) = 1/2\, (\pi pT)^{1/2} \exp (p/4T) \exp\text{-}x/T \{\mathrm{erf}\, [(2E^0_{Coul}+p)/2(pT)^{1/2}] - \mathrm{erf}\, [(p-2x)/2(pT)^{1/2}]\}$

(19)

This formula elegantly allows for the following features:

1) the particle is emitted from the deformed saddle point configuration

2) shape fluctuations with the resulting Coulomb fluctuations are accounted for in a statistically consistent way.

The addition of two harmonic non-amplifying modes (potential energy only) like those illustrated in fig. (1) or of one non-amplifying mode (potential + kinetic energy) leads to a more general expression

$$\Gamma(\varepsilon,z) \propto \varepsilon \exp -(\varepsilon+(x-\varepsilon)^2/p)/T \quad (20)$$

which, after integration over ε gives:

$$P(E) = 1/2\, (\pi pT)^{1/2} \exp (p/4T) \exp -x/T\, [1/2(2x-p)\{\mathrm{erf}\, [(2E^0+p)/2(pT)^{1/2}] - \mathrm{erf}\, [(p-2x)/2(pT)^{1/2}]\} - (pT/\pi)^{1/2} (\exp - [(2E^0+p)^2/4pT] - \exp - [(p-2x)^2/4pT])]$$

(21)

This formula not only portrays the same features as the one derived above, but also allows for emission of the particle from any point of the surface (if the Coulomb potential is assumed to vary quadratically as the particle moves away from the pole toward the equator of the residual nucleus). It is not unexpected but interesting to notice that eq. (21) does not depend on any parameter associated with the potential or kinetic energy of the non-amplifying modes but depends only on their number. In this way the problem of the integration over the Coulomb field at the nuclear surface is elegantly bypassed.

A pleasing feature of these equations is the limit to which they tend for p=0

$P(E) \propto e^{-E/T}$ and $P(E) \propto E\, e^{-E/T}$

The latter form is the standard expression for the neutron spectra.

To summarize, so far we have calculated analytical expressions for the kinetic energy distributions which need only the following parameters to be extracted from any suitable model.

1) The monopole-monopole Coulomb energy E^0 of the relevant saddle shape.
2) the amplification parameter p.
3) the number of non-amplifying modes.

Inclusion of quantum penetration

So far the expressions that we have calculated are based exclusively on classical statistical mechanics and may be adequate to describe the evaporation of particles heavier than ^{4}He. However in view of the fact that this paper is specifically addressed to p and He emission, with particular attention to the low energy part of the spectra, it is important to deal with the problem of quantum barrier penetrability.

In general we can write for the probability of emission of a particle with final energy E:

$$P_{QM} = \int_{-\infty}^{+E} \Gamma(\varepsilon,E)\, F(\varepsilon)\, d\varepsilon \qquad (22)$$

where Γ is the decay width calculated as in (18) or (20), and $F(\varepsilon)$ is the barrier penetration probability. For analytic simplicity we have chosen the following form for $F(\varepsilon)$

$$F(\varepsilon) = 1/2\, e^{\alpha\varepsilon} \quad \varepsilon<0 \quad ; \quad F(\varepsilon) = 1/2\,(2-e^{-\alpha\varepsilon}) \quad \varepsilon>0$$

This function is continuous with its 1st derivative at $\varepsilon=0$. It contains only one parameter α, yet it has the qualitative features of penetration and reflection expected for a penetrability function.

With such a function, the integral in (22) can be evaluated analytically by parts.

For the first form (18) one obtains

$$\begin{aligned} P(E) = {} & 1/2\,(\pi pT)^{1/2} \exp(p/4T) \exp -x/T\, \{\mathrm{erf}\,[(2E^0+p)/2(pT)^{1/2}] - \mathrm{erf}\,[(p-2x)/2(pT)^{1/2}] \\ & + 1/2 \exp - [(p-2x)^2/4pT]\, [\exp[(p-2x-\alpha pT)^2/4pT]\, \{\mathrm{erf}\,[(p-2x-\alpha pT)/2(pT)^{1/2}] + 1\} \\ & - \exp[(p-2x+\alpha pT)^2/4pT]\, \{\mathrm{erf}\,[(2E^0+p+\alpha pT)/2(pT)^{1/2}] - \mathrm{erf}\,[(p-2x+\alpha pT)/2(pT)^{1/2}]\}]\} \end{aligned} \qquad (23)$$

$$= K \exp -x/T\, (M-N+1/2(L-J)) \qquad (24)$$

For the second form (20) one obtains:

$$P(E) = K \exp -x/T \, [1/2\,(2x-p)\,(M-N)+1/2\,(2x-p+1/2\alpha pT)\,L\, -$$

$$1/2\,(2x-p-1/2\alpha pT)\,J - 1/2\,(pT/\pi)^{1/2}\,[2-\exp -\alpha(x+E^0)]\,\exp -(2E^0+p)^2/4pT] \quad (25)$$

Presentation of the results

In fig.(2) the spectra corresponding to expressions (21) are shown for a fixed temperature T=2 MeV and two values of the amplification parameter p. At the same time the form $P(x) \propto xe^{-x/T}$ is plotted. Notice that the variable $x=E-E^0$ is the difference between the actual kinetic energy and the kinetic energy resulting from the Coulomb repulsion at the saddle configuration. Therefore even the standard spectrum is somewhat shifted downward from the Coulomb barrier. The effect of the amplification parameter is that of stretching the spectrum toward lower kinetic energies. Notice that this effect is purely classical, as we have not incorporated barrier penetration as yet.

The effect of barrier penetration is shown in fig (3). The spectra, given by eq.(23) are shown for a small temperature and for increasing penetrability (decreasing α). The "subbarrier" emission, already present in the classical equation is enhanced as the penetrability increases. In fig.(4) the absolute and relative differences between the classical and the quantum mechanical expressions are shown for a given temperature and penetrability. The relative difference shows that the lowest kinetic energies are due mainly to barrier penetration. The negative value of $\Delta P/P$ observed between x=0 and x=2 MeV is due to the reflection of the barrier. Fig. (5) shows the spectra for a fixed barrier penetrability and progressively higher temperature. The rapid extension of the spectrum to ever present subbarrier energies is due to the increasing thermal fluctuations along the amplifying mode.

Conclusion

We have developed a completely consistent formalism to generate evaporation spectr for light particles with inclusion of shape fluctuations and quantum penetration. The resulting analytical formulae portay a substantial subbarrier emission, increasing with temperature and due mainly to shape fluctuations.

Acknowledgements.

One of us (L.G.M.) would like to thank the Alexander von Humboldt Foundation for its kind hospitality and support.

This work was supported by the Director, Office of Energy Research, Division of Nuclear Physics of the Office of High Energy and Nuclear Physics of the U.S. Department of Energy under Contract DE-AC03-76SF00098.

Figure Captions

Fig. 1 Schematic illustration of the three classes of saddle point modes.

Fig. 2 Evaporation spectra for two values of the amplification parameter at fixed temperature. The standard evaporation spectrum is also shown.

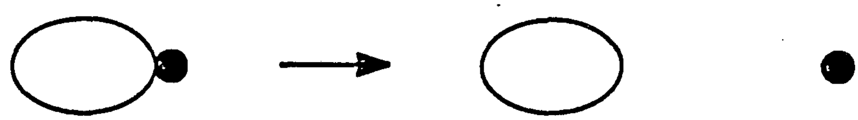
Fig. 3 Effect of barrier penetration on the evaporation spectrum.

Fig. 4 Absolute (left) and relative (right) difference between a quantal and a classical evaporation spectrum, illustrating the contribution of quantum penetration as a function of final particle energy.

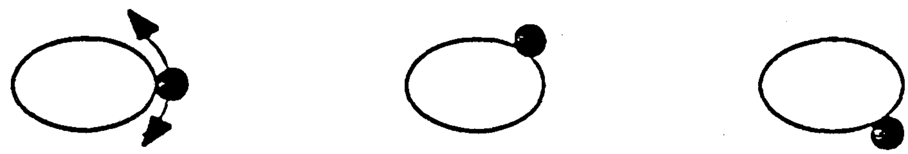
Fig. 5 Evaporation spectra at fixed barrier penetrability for a range of temperatures.

Saddle Point and Normal Modes

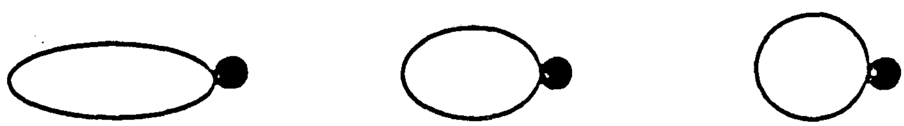
i) decay mode:



ii) non-amplifying mode:



iii) amplifying mode:



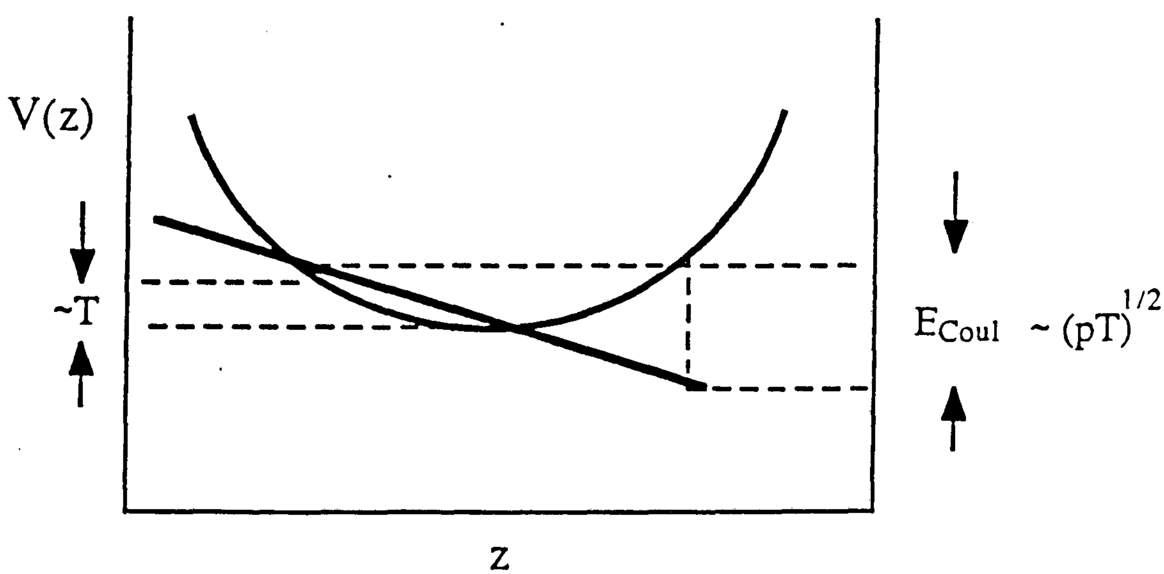


Fig. 1

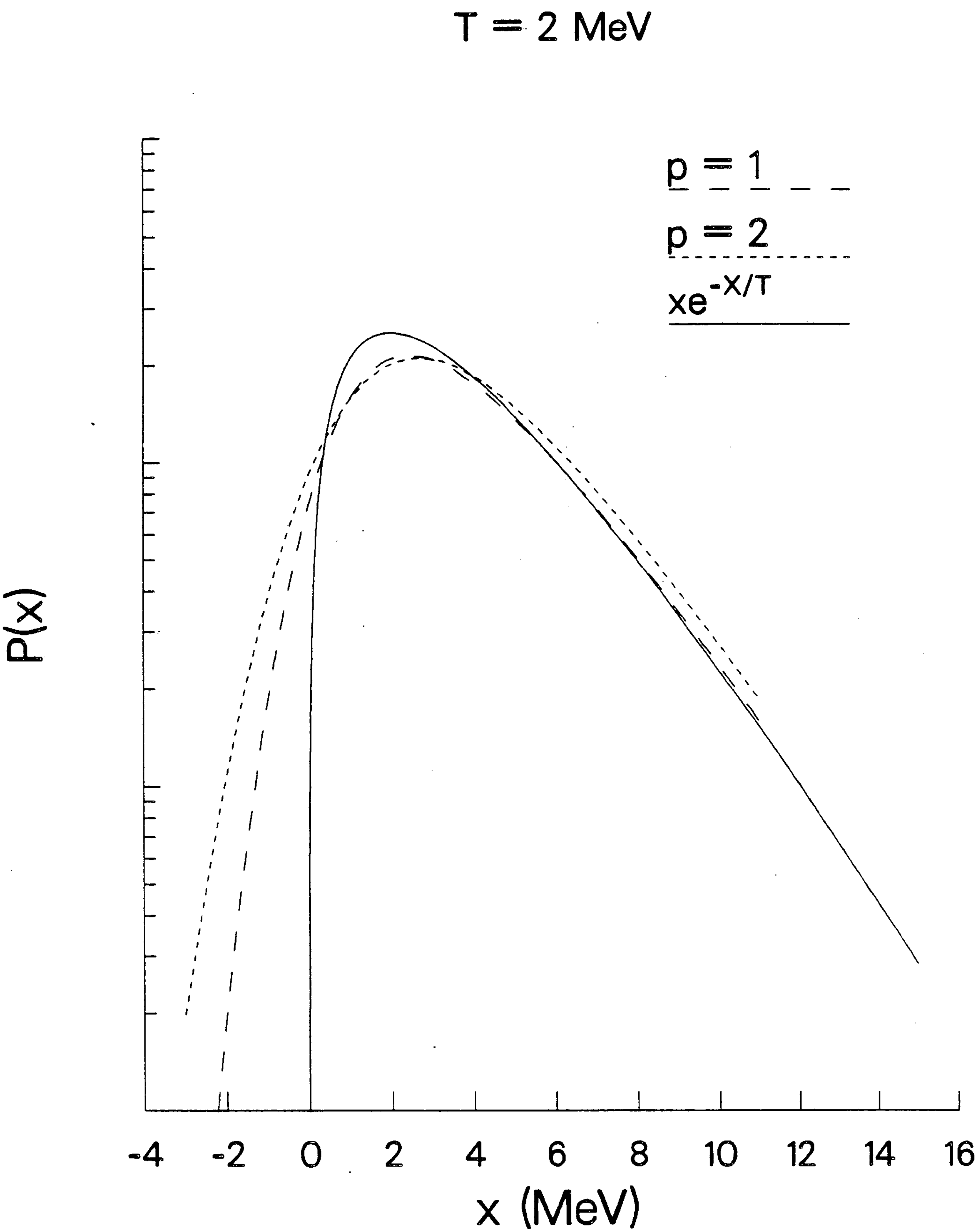


Fig. 2

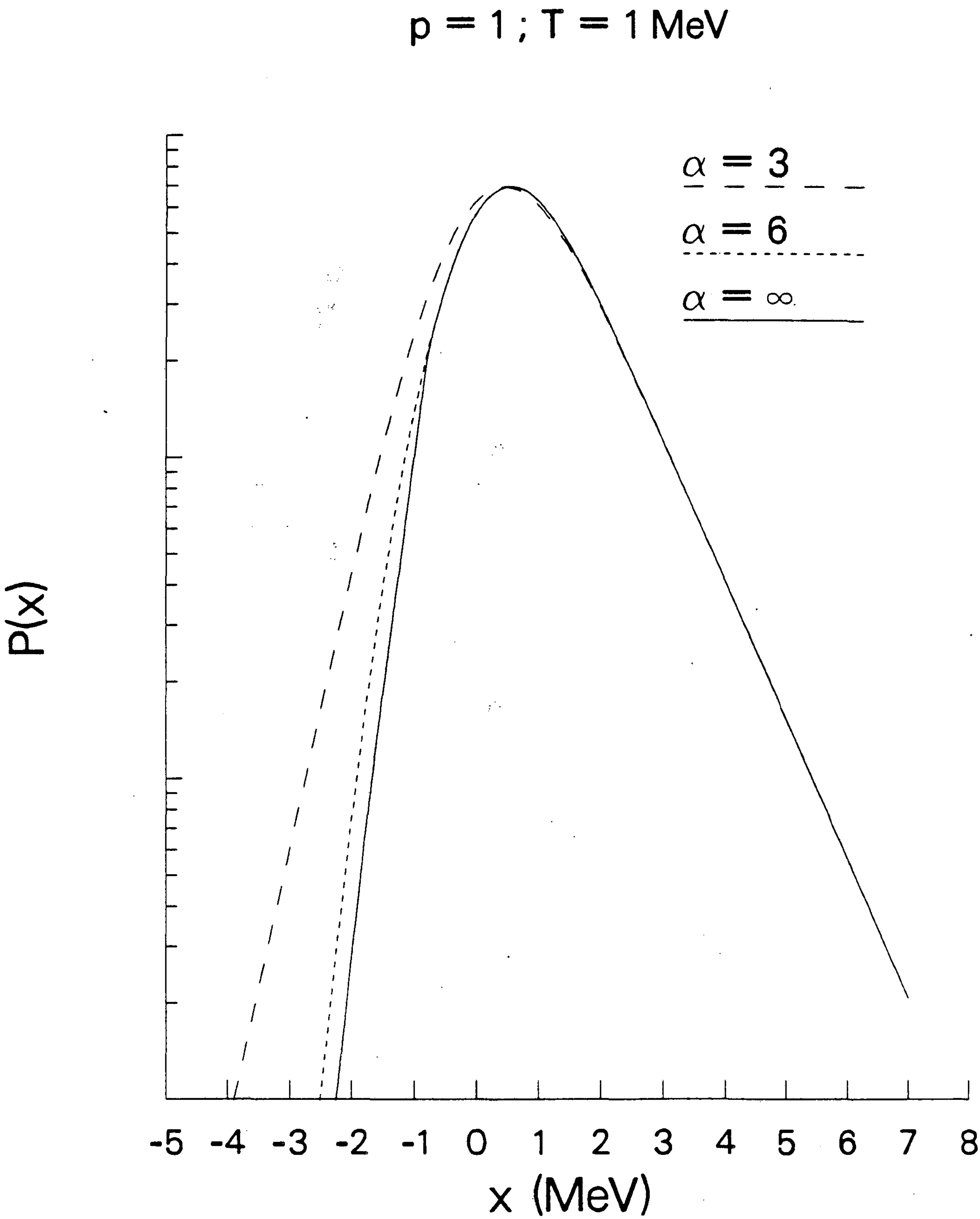


Fig. 3

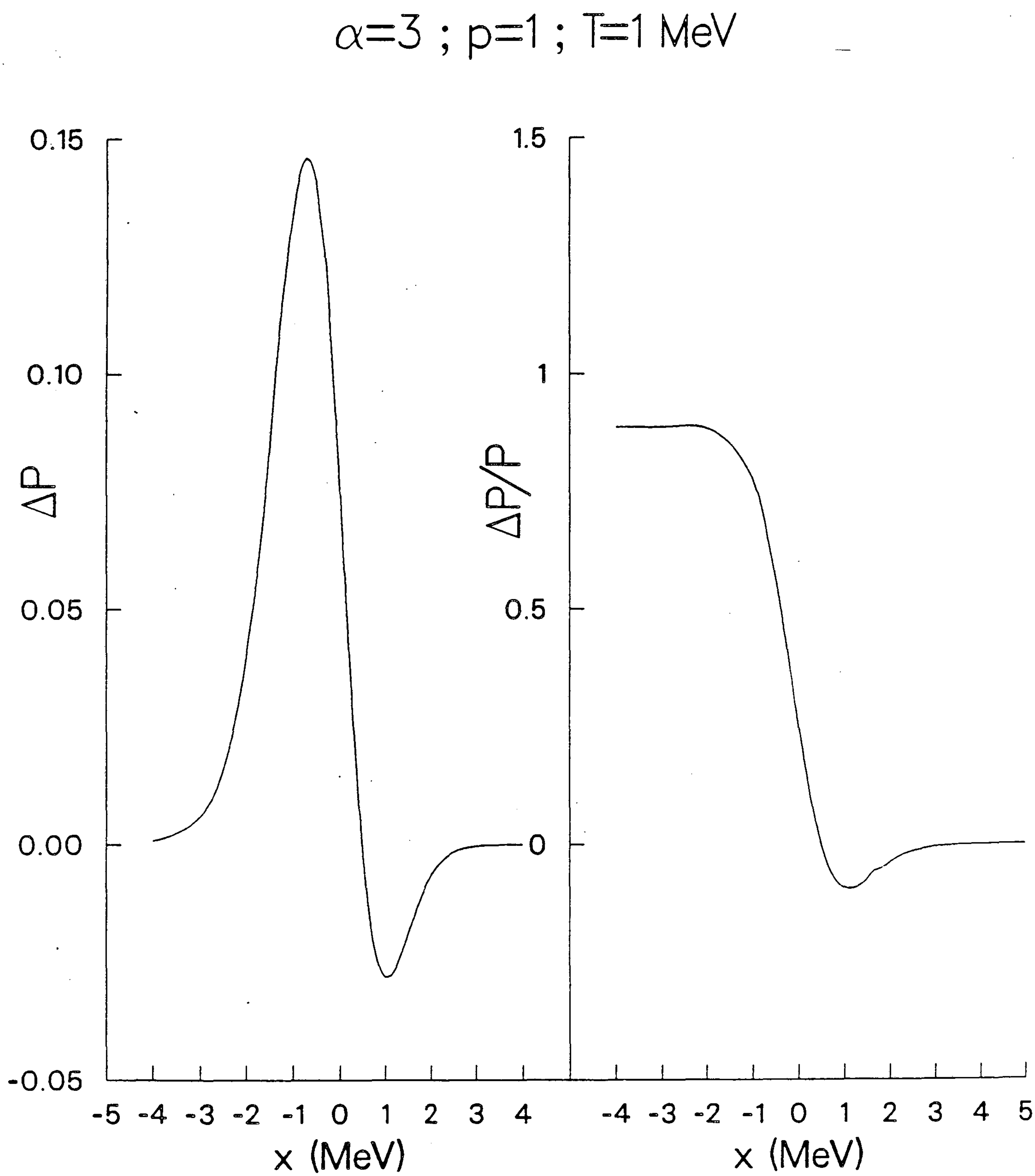

α=3 ; p=1 ; T=1 MeV
0.15
0.10
0.05
0.00
-0.05
ΔP
-5 -4 -3 -2 -1 0 1 2 3 4
x (MeV)
1.5
1
0.5
0
ΔP/P
-4 -3 -2 -1 0 1 2 3 4 5
x (MeV)

Fig. 4

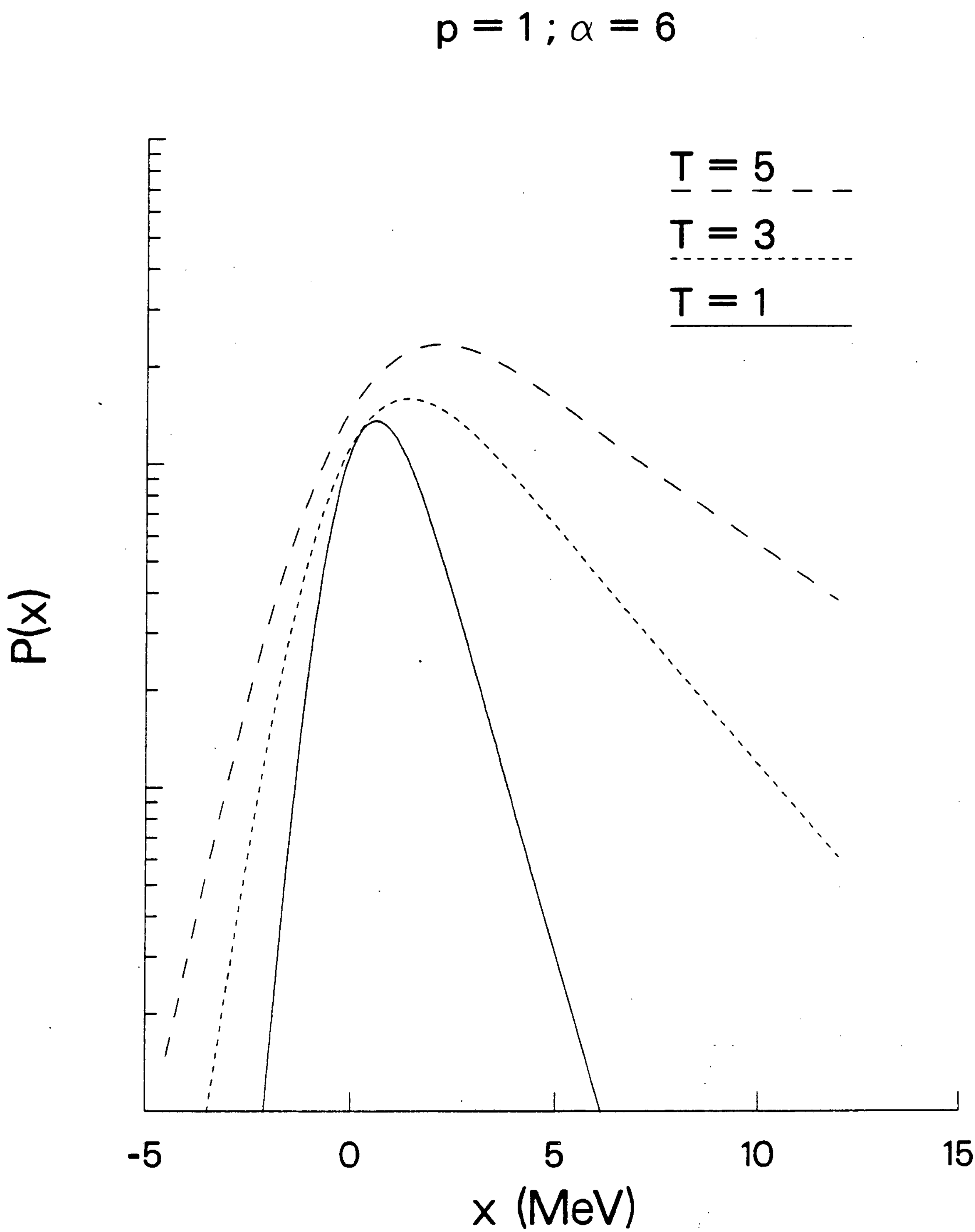


Fig. 5

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