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NOTE ON THE DISAPPEARANCE OF SHELL EFFECTS WITH EXCITATION ENERGY AND THE STRUTINSKI SMOOTHING PROCEDURE†

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The energy dependence of the nuclear entropy at high excitation energy is calculated for non equidistant and shell models. The deviation from a linear dependence in the square of the entropy is shown. The relation between the Strutinski and the statistical averaging of the spectrum is discussed.

- - -

Recently detailed numerical calculations performed on the basis of realistic single particle level spectra [1,2,3] have shown the influence of shell effects on the level densities and their disappearance with excitation energy.

A model calculation by Kahn and Rosenzweig [4] based upon a periodically bunched spectrum has shown that the asymptotic behaviour of the entropy with excitation energy is similar to that of the equidistant model:

$$S = 2\sqrt{aE^*} \qquad (1)$$

where $E^* = E - \Delta E$.

Here E is the excitation energy and ΔE is an energy shift which is strictly related to and has been identified with the ground state shell effect [5]. By analogy, some authors [6,7] have assumed that the asymptotic behaviour of the level density derived from an arbitrary set of single particle levels is also similar to that of the equidistant model.

Plots of the nuclear entropy square versus excitation energy have been

†Work performed under the auspices of the U. S. Atomic Energy Commission.

claimed to become linear at sufficiently large excitation energies, and the intercepts of the straight lines with the excitation energy axis have been identified with the ground state shell effects [5,8]. Such procedure has also been suggested as a possible substitute for the Strutinski method [9].

In the first part of this paper the relevant thermodynamical quantities will be derived for models where the first and second derivatives of the single particle level density are different from zero. It will be shown that the entropy square versus the excitation energy does not become linear at any excitation energy. In the second part the relation between the smoothing due to temperature and that employed in the Strutinski procedure will be discussed. In the third part the results of statistical calculations performed on the basis of the Nilsson diagram will be illustrated and it will be shown that, just as for the non equidistant models, no linear dependence of the entropy square versus energy is obtained and that no clear-cut method can be derived to obtain shell effects from statistical calculations

a) The logarithm of the Grand Partition Function for a system of Fermions is given by the relation:

$$\Omega = \sum_k \ln\left[1 + \exp - \beta(e_k - \mu)\right] \qquad (2)$$

where β is the inverse of the temperature, μ is the chemical potential and e_k are the single particle energy levels.

The summation can be substituted by an integral if one introduces the single particle level density $g(e)$. Expanding $g(e)$ about the chemical potential and retaining terms up to second order one obtains [10]:

$$\Omega = \beta \frac{\mu^2}{2} g(\mu) + \frac{\pi^2}{6\beta} g(\mu) - \beta \frac{\mu^3}{3} g'(\mu) + \beta \frac{\mu^4}{8} g''(\mu) + \frac{7}{360} \frac{\pi^4}{\beta^3} g''(\mu) \ . \qquad (3)$$

The number of particles N, the total energy E and the entropy S can be

immediately obtained:

$$N = \frac{1}{\beta}\frac{\partial\Omega}{\partial\mu} = \mu g(\mu) - \frac{1}{2}\mu^2 g'(\mu) + \frac{1}{6}\mu^3 g''(\mu) + \frac{\pi^2}{6\beta^2} g'(\mu) \tag{4}$$

$$E_t = -\frac{\partial\Omega}{\partial\beta} = \frac{1}{2}\mu^2 g(\mu) - \frac{1}{6}\mu^3 g'(\mu) + \frac{1}{24}\mu^4 g''(\mu) + \frac{\pi^2}{6\beta^2} g(\mu) + \frac{\pi^2}{6\beta^2}\mu g'(\mu) + \frac{7}{120}\frac{\pi^4}{\beta^4} g''(\mu) \tag{5}$$

$$S = \Omega - \beta\mu N + \beta E = \frac{\pi^2}{3\beta} g(\mu)\left(1 + \frac{7}{30\beta^2}\pi^2 \frac{g''(\mu)}{g(\mu)}\right) \tag{6}$$

The statistical properties of the system are defined by the values of β and μ which can be obtained by solving eq. (4) and eq. (5). Alternatively eq. (4) yields the value of μ for a given value of the temperature. It can be seen immediately that only if $g'(\mu) = g''(\mu) = 0$ then μ = constant, $E_t - E_o = E = \frac{\pi^2}{6\beta} g$ and $S = \frac{\pi^2}{3\beta} g = 2at = 2\sqrt{aE}$.

Only in such case a linear dependence of S^2 versus E is obtained. The condition $g'(\mu) = g''(\mu) = 0$ corresponds to a rather unrealistic case. Even the simple Fermi gas model deviates substantially from such conditions. In fig. 1 the intercepts of the tangent to S^2 with the excitation energy axis are presented. In this calculation it is assumed that the single particle level density behaves as in a Fermi gas, namely $g(e) = k\sqrt{e}$

and k is chosen so that the level density at the Fermi surface is equal to $\frac{6}{\pi^2}\frac{A}{10}$ $(a = \frac{A}{10})$. The calculation has been performed for a nucleus with mass number A = 200.

The intercepts ΔE vary from zero at low excitation energy to an ever increasing negative value, thereby simulating a "shell effect" varying with energy. The qualitative reason for such a behaviour can be easily understood. From eq. (4)

it can be noticed that the chemical potential is attracted towards the regions of low single particle level density as the temperature and the excitation energy increase. This is also illustrated in fig. (1). Consequently the entropy is evaluated at regions of decreasing single particle level density. Therefore the slope of S^2 versus E_x decreases continuously and the intercept becomes increasingly negative.

Similar calculations have been performed by assuming a linear and a quadratic energy dependence of the single particle level density with similar results.

b) In actual nuclei the single particle level density can be considered as composed of a smooth component and a rapidly fluctuating component. The former component is expected to be intermediate between a $\sqrt{e}$ dependence typical of a square well potential and a e^2 dependence typical of a harmonic oscillator potential. The latter component is due to the nuclear shell structure. The excitation energy has the effect of averaging over the single particle level density, so that, at sufficiently large excitation energies, the nucleus will be affected only by the smooth, but not constant component of the single particle level density. The smoothing of the single particle level density inherent to the statistical calculation is performed by the smoothing function:

$$f(x) = \frac{4}{\beta} \frac{1}{\cosh^2 \frac{1}{2} \beta x} \tag{7}$$

and the smooth single particle level density is given by:

$$g(e) = \frac{4}{\beta} \sum_k \frac{1}{\cosh^2 \frac{1}{2} \beta (e_k - e)} \tag{8}$$

In the Strutinski procedure, a similar smoothing is performed by means of a Gaussian and the smooth single particle level density is given by:

$$g(e) = \frac{1}{\gamma\sqrt{\pi}} \sum_k F_k \exp - \left(\frac{e_k - e}{\gamma}\right)^2 . \tag{9}$$

The function F_k is a correction function whose purpose is to retain unaltered the low order derivatives in the single particle level density.

It can be seen that the two expressions are very similar indeed: in particular the function (7) is very close to a Gaussian. A simple relation can be derived between γ and t ($t = \frac{1}{\beta}$)

$$\gamma \simeq 2.12\ t \quad . \tag{10}$$

It is known that, in order to smooth-out the shell effects, the Strutinski method requires a value of γ of the order of the major shell spacing (in the Nilsson model, $\hbar\omega o$). In order to obtain the same smoothing, the statistical calculation then requires a temperature much smaller than the major shell spacing.

However the smoothing performed in the Strutinski method differs from the statistical smoothing in two respects. First, the Strutinski smoothing is performed from the bottom of the well up to the Fermi surface, while the statistical smoothing occurs only at the Fermi surface. Second, as can be seen in Eq. (9), the Strutinski method obtains an accurate expression for g(e) as far as the low order derivatives are concerned because of the function F_k, while no equivalent function can be found in the statistical smoothing.

c) In order to illustrate the conclusions reached in the above discussion, numerical calculations have been performed on the basis of the Nilsson diagram. In order to eliminate numerical difficulties associated with a truncated set of Nilsson levels, 600 neutron and proton levels have been used; it has been verified that a variation of 50 in the number of levels produces a variation of less than 0.03 MeV at 500 MeV excitation energy in the S^2 versus E_x intercepts.

The nuclei which were studied are $^{132}_{50}Sn$, $^{124}_{46}Pd$, and $^{144}_{50}Ba$. In Figs. 2, 3, and 4 the intercepts of the tangent to the function S^2 vs E_x are plotted versus excitation energy together with the proton chemical potential. In Fig. 5 the quantity

$$D = \frac{1}{4}\frac{dS^2}{dE_x} \quad , \tag{11}$$

is plotted for the three isotopes. Such a quantity, for the equidistant model is the level density parameter a as it can be verified from equation (1).

This parameter is proportional to the local single particle level density g.

$$a = \frac{\pi^2}{6} g \quad . \tag{12}$$

The behavior of the quantities ΔE, μ, and D is rather complicated, but can be understood on the basis of very simple rules. 1) The chemical potential μ always moves towards regions of low single particle level density. 2) The effective single particle level density, or the quantity D which is proportional to it, depends upon the actual position of the chemical potential and it is obtained by smoothing the single particle spectrum over a width proportional to the temperature. 3) The intercept ΔE follows closely the behavior of D which is proportional to the local level density and to the slope of S^2 versus E_x.

In the case of the doubly magic ^{132}Sn the chemical potential starts in the middle of the shell gap where the density is very low. An increase in energy increases the local density because the averaging is performed over a

larger width. Therefore both D and ΔE increase until a maximum is achieved when the shell is completely washed out. This occurs at a rather large excitation energy ($\sim$ 150 MeV). Meanwhile the chemical potential drifts deeper into the well, attracted by the lower smooth level density. For this reason both D and ΔE must decrease indefinitely with increasing energy.

In the case of $^{124}_{46}Pd$ and $^{144}_{56}Ba$ the initial level density is rather high because the chemical potentials are very close to partially filled degenerate levels. With increasing excitation energy, the chemical potentials are driven into the shells: they come down in the case of ^{144}Ba, and go up in the case of ^{124}Pd. This produces a rapid decrease of the effective single particle level densities and of D. A further increase in temperature allows a broader average and both D and ΔE increase. Again, once the excitation energy is well above 100 MeV and the shell structure is washed out, the chemical potentials move deeper into the well, the level density and D decrease indefinitely and so does the intercept ΔE.

Therefore the quantity ΔE when considered as a function of excitation energy can be used together with the chemical potentials and the quantity D, to illustrate the rather complex phenomena associated with the warming up of a nucleus. However, in general, the entropy square never becomes linear with excitation energy and ΔE never becomes a constant. If the excitation energy is suitably chosen, a correlation between the local value of ΔE and the shell effect determined from the Strutinski procedure is to be expected but there is no unique way of identifying ΔE with the shell effect or reasons to prefer it to the value calculated by means of the Strutinski method.

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Figure Captions

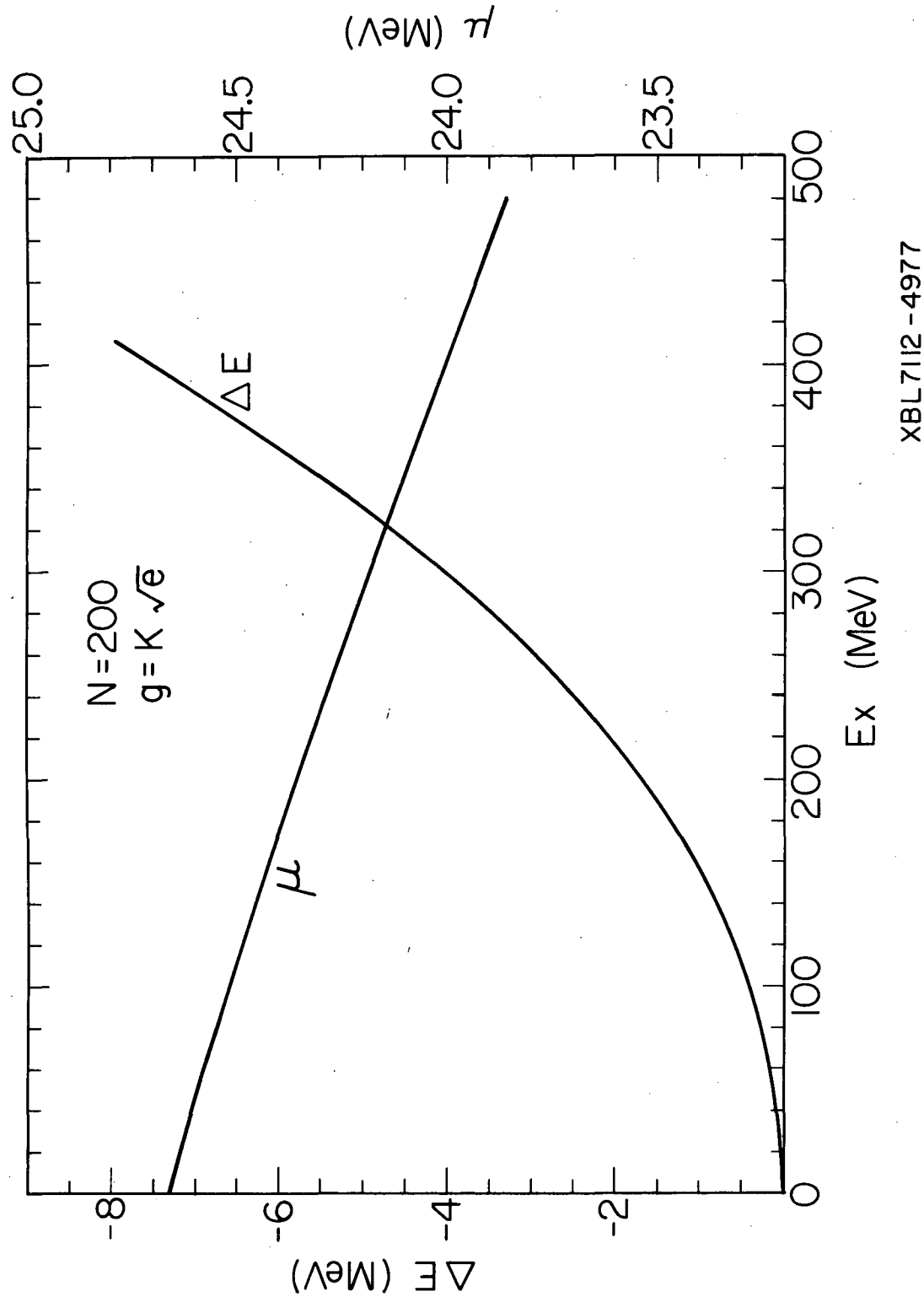
Fig. 1. Intercept ΔE and chemical potential μ versus excitation energy for a Fermi gas ($g = \kappa \sqrt{e}$) of 200 particles.

Fig. 2. Intercept ΔE and proton chemical potential μp versus excitation energy for ^{132}Sn.

Fig. 3. Same as in Fig. 2 for ^{124}Pd.

Fig. 4. Same as in Fig. 2 for ^{144}Ba.

Fig. 5. The quantity $D = \frac{1}{4} \frac{dS^2}{dE_x}$ plotted versus excitation energy for ^{132}Sn, ^{124}Pd, and ^{144}Ba.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g=K √e
ΔE
μ
ΔE (MeV)
μ (MeV)
Ex (MeV)
-8
-6
-4
-2
25.0
24.5
24.0
23.5
0
100
200
300
400
500
XBL7112-4977

Fig. 1

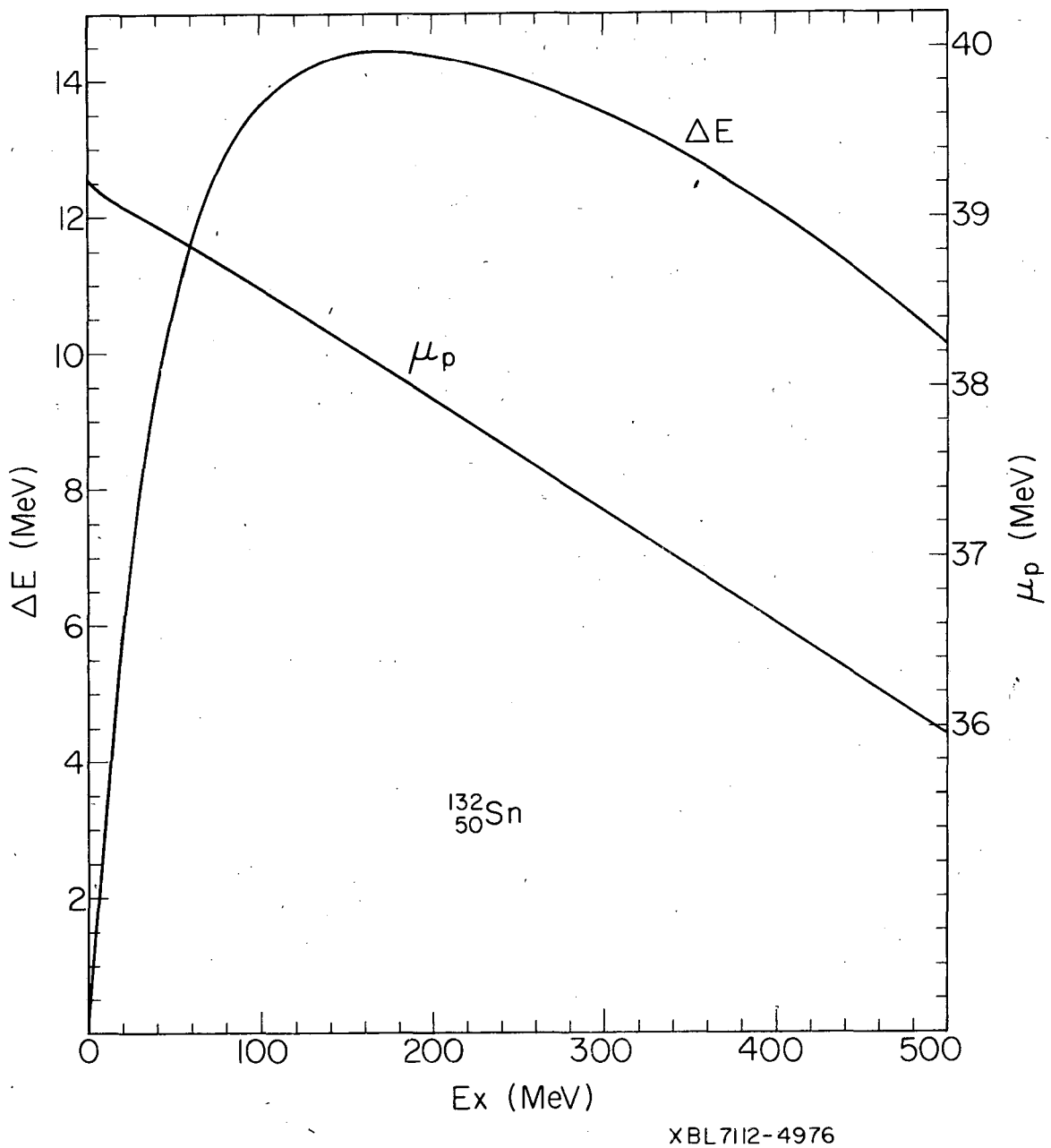
ΔE
μp
$^{132}_{50}$Sn
ΔE (MeV)
μp (MeV)
Ex (MeV)
0
100
200
300
400
500
2
4
6
8
10
12
14
36
37
38
39
40
XBL7112-4976

Fig. 2

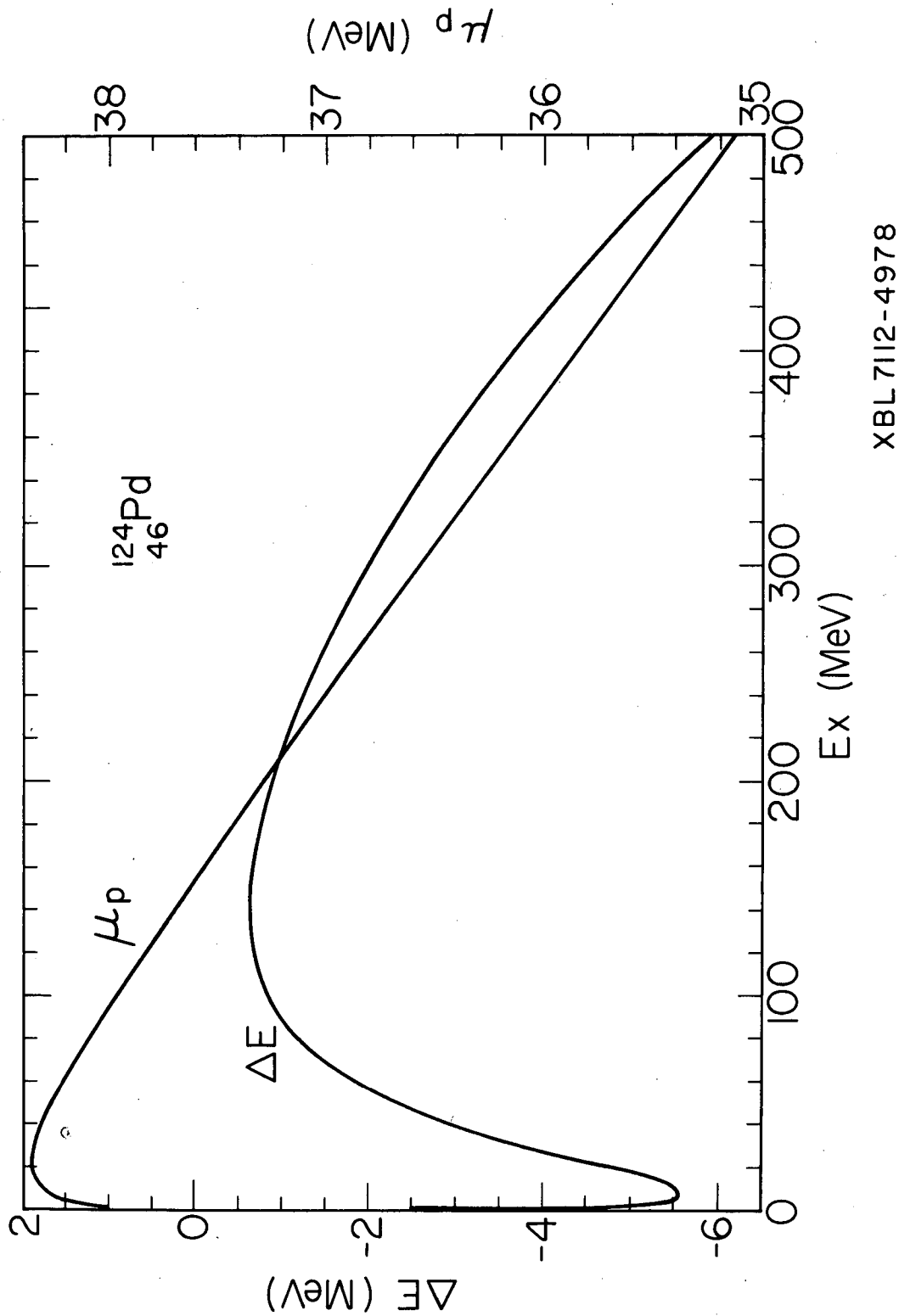
μ_p (MeV)
38
37
36
35
$^{124}_{46}$Pd
μ_p
ΔE
ΔE (MeV)
2
0
-2
-4
-6
0
100
200
300
400
500
Ex (MeV)
XBL 7112-4978

Fig. 3

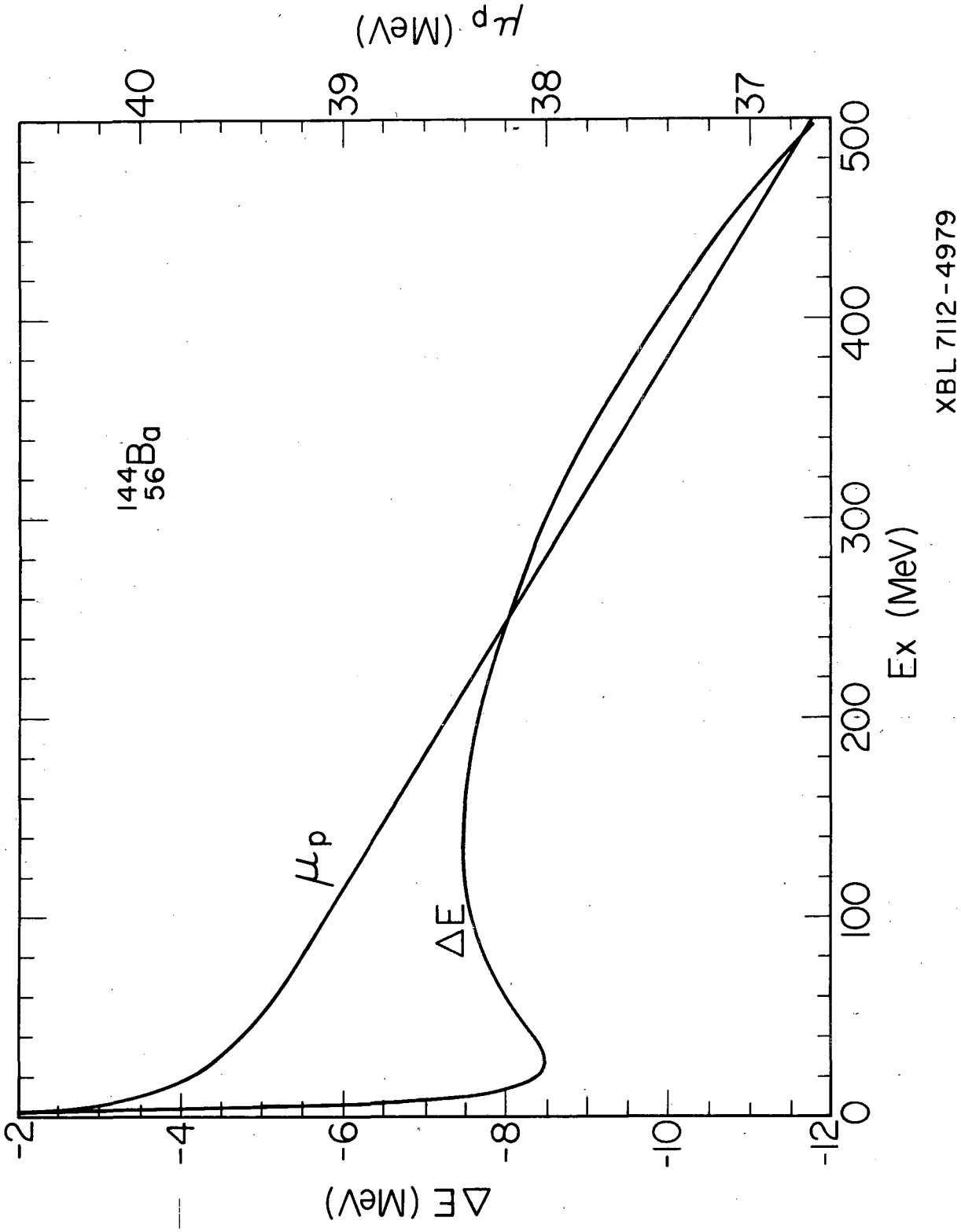
$^{144}_{56}Ba$
μ_p
ΔE
ΔE (MeV)
μ_p (MeV)
Ex (MeV)
-2
-4
-6
-8
-10
-12
40
39
38
37
0
100
200
300
400
500
XBL 7112-4979

Fig. 4

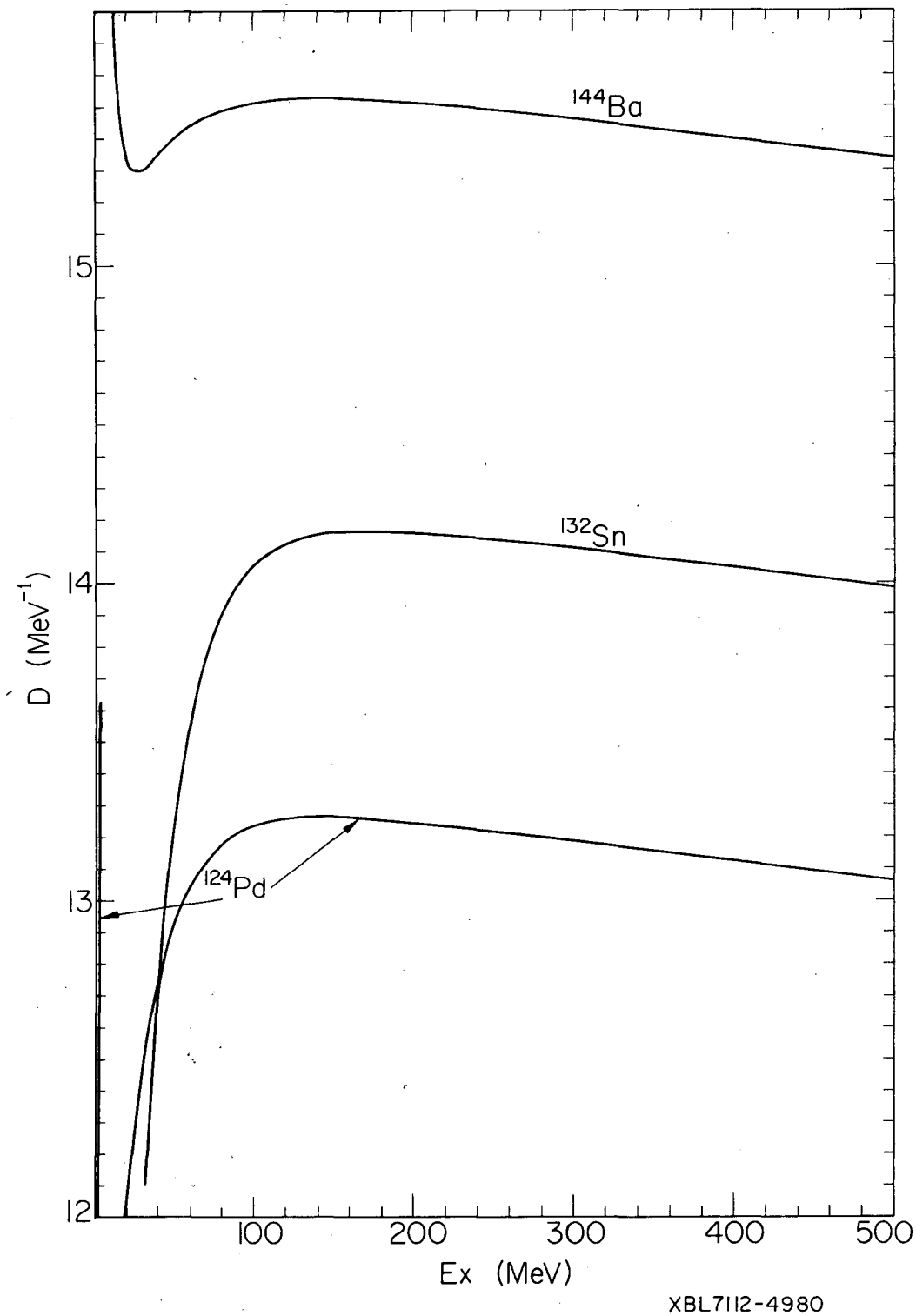
144Ba
132Sn
124Pd
15
14
13
12
D (MeV-1)
100
200
300
400
500
Ex (MeV)
XBL7112-4980

Fig. 5

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