# STATISTICAL TREATMENT OF NUCLEAR ENERGY LEVELS

# STATISTICAL TREATMENT OF NUCLEAR ENERGY LEVELS

by

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Low-lying nuclear energy levels are analyzed in terms of certain parameters of the correlation between the level spacing and the excitation energy. The statistical properties of the estimates for the parameters arising from a constant nuclear temperature model are examined. Estimates are made for the parameters for the levels of $Mn^{56}$ inferred from capture gamma spectra.

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# CHAPTER I

# INTRODUCTION

The energy of nuclear levels can be inferred by two general methods. The first is the study of $\alpha$, $\beta$ and $\gamma$-spectra of radioactive nuclides. The transitions involved are subject to selection rules so that only certain levels are populated. Furthermore the Q - values associated with such transitions place an upper limit of a few MeV on levels which can be observed by these methods. The second method is the study of reactions such as (p, p'), (d, p) and (n, $\gamma$ ) by which level structures can be observed up to higher excitations.

For a set of energy levels of a nucleus $\{E_i\}$ , where i = 1 to n, let us define the level spacing to be

$$D(E) = E_{i+1} - E_i ,$$

where $E = \frac{E_{i+1} + E_i}{2}$ . It is of interest to investigate the correlation between the spacing D and the average excitation energy E. For this reason it is convenient to introduce a level density, defined as $\rho(E) = \frac{dN(E)}{dE}$ , where dN(E) is the number of levels between E and E + dE. For a set of discrete levels, the density can be represented as a sum of Dirac delta-functions:

$$\rho(E) = \sum_{i=1}^{n} \delta(E - E_i).$$

We shall, however, consider the density to be a smooth function of excitation energy given by the reciprocal of the spacing: $\rho(E) = 1/D(E)$. Energies will be handled in units of keV, so the density will be given in units of $keV^{-1}$.

It is difficult to obtain from experimental data the exact form of the function D(E) because the spacing D is a random variable. Functional forms of D(E) can be derived containing certain parameters for nuclear models of various degrees of sophistication. Then assuming some distribution in the spacings, one can form estimates for these parameters from data and assign accuracies to the estimates. It is desireable also to have statistical criteria to measure the "goodness of fit" of the suggested spacing functions to actual data.

This thesis will be concerned with fitting spacing functions to data. Functional forms of the spacing - excitation correlation will be examined and a useful form chosen. The distributions of the spacings will be considered, and then the treatment of data to form estimates of the parameters involved. The statistical properties of the estimates are investigated. The level structure of $Mn^{56}$ is used as an example to illustrate the treatment of data and its application to resolution losses in capture gamma spectra.

# CHAPTER II

# THEORY

## 2.1 Level Densities

The basic experimental facts are the following: The first excited states of medium and heavy nuclei typically occur in the order of hundreds of kilovolts about the ground state. This is equivalent to a level density, the reciprocal of level spacing, of the order of .01 per keV. The spacings of neutron resonances observed at excitations of 6 - 8 MeV are much smaller than those near the ground state, and indicate densities of the order of hundreds per keV in spite of the fact that only certain levels are excited because of angular momentum and parity selection rules. The density of levels is seen to change four orders of magnitude over a few MeV of excitation energy, and so is anticipated to be an exponential function of energy.

It has been observed that log N(E), where $N(E) = \int_0^E \rho(E')dE'$, the number of levels up to energy E, when plotted against E, is quite linear over several MeV. As the level density increases with energy, one finds that log N(E) falls below the straight line initially observed. This effect can be attributed to missed levels and arises because of the finite experimental resolution. A pairing effect is also evident in these plots, for the straight lines are displaced from each other for neighboring odd and even nuclei (3).

Level density is known to be dependent on shell structure. The density of neutron resonances of magic or nearly magic nuclei is orders of magnitude smaller than between the shells at the same excitation (5). To be successful, a theory of nuclear level densities should explain and predict the features mentioned above.

It has often been fruitful to make analogies between different physical systems in spite of an apparent dissimilarity. A good example is Bethe's conception (1, 2) of the nucleus as a mixture of two Fermi gases, one of protons and one of neutrons, constrained within a box. Much of the theoretical work done on nuclear level densities is based on this original idea.

It is useful to consider a simple model as a first approach in order to get some general results - specifically the exponential increase of level density with energy which is observed in experiments. Consider then a nucleus, when A is not too small, as an ensemble of free protons and neutrons which behave as a perfect gas of fermions enclosed in a box in a state of degeneracy.

The gas "heats up" when it is excited, and the energy of excitation E, can be related to a "temperature" T' by the following (4):

$$E = a\,(kT')^2, \qquad (2.1.1)$$

where k is Boltzmann's constant, and a is a constant which depends on A and Z, the atomic weight and number respectively. The density of nuclear states $\rho(E)$ is related to the nuclear entropy S by the approximate relation:

$$S = k \log \left( \frac{\rho(E)}{\rho_o} \right)$$

where $\rho_o = \rho(0)$ . The density is then

$$\rho(E) = \rho_o\, e^{S/k} \qquad (2.1.2)$$

The thermodynamical definition of entropy is:

$$S\,(E) = \int_0^E \frac{dE}{T'} \qquad (2.1.3)$$

Substituting from (2.1.1), we get:

$$S\,(T') = 2\,a\,k^2 \int_0^{T'} T'dT' = 2\,a\,k^2\,T'$$

$$S\,(E) = 2\,k\,\sqrt{aE}$$

Putting this result in equation (2.1.2) we get the density:

$$\rho(E) = \rho_o\, e^{2\sqrt{aE}}$$

Experimental data has been used to find values of the constants $\rho_o$ and a. For example, at A = 63, the values of $\rho_o$ and a are 0.3 MeV and 2 MeV (6) respectively.

There is some experimental evidence from N (E) - E curves (3) and reactions (7) that the nuclear temperature T, which has units of energy and is related to temperature* T' of the nucleon gas by T = kT', is constant below about 10 MeV. This suggests that the nucleus is undergoing a first order phase change or a "melting". The excitation energy added to the system does not raise the temperature but goes into disrupting ordered pairs which arise as in a superconductor due to large pairing forces (3). Then, according to equation (2.1.3) the entropy is:

$$S = \int_0^E \frac{dE}{T'} = \frac{E}{T'}$$

From equation (2.1.2) we get the level density:

$$\rho(E) = \rho_0 \, e^{E/T} \qquad (2.1.4)$$

where T is the temperature in the energy units of E, keV.

These two densities, one proportional to $e^{2\sqrt{aE}}$, and the other to $e^{E/T}$, are likely the two extremes. Gilbert et al (8, 9) have devised a method of analyzing densities in terms of both forms. The constant temperature representation is used at low energies, and the Fermi gas is used at higher excitations.

Exact theories of level densities which predict actual numbers of states per energy interval require sophisticated models including shell effects and pairing energies, and are reviewed in reference 5. This thesis is concerned, however, with the process of estimating parameters of density functions from experimental data.

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* "Nuclear Temperature" is defined as: $T = \left[ \frac{d}{dE} \ln(\rho(E)) \right]^{-1}$

We restrict ourselves further to level spacings below the neutron binding energy, so that the constant temperature density $\sim e^{E/T}$ will be employed rather than the Fermi gas form which is more reasonable at higher excitations.

Level densities are functions of spin and parity as well as energy. Experimental level densities include levels of only certain spin and parity values. For a given angular momentum J of the nucleus, the density of states of spin J is given approximately by (3):

$$\rho_J(E) = (2J + 1) \quad e^{-J(J + 1)/2\sigma^2} \rho(E)$$

where $\sigma^2$ is related to the nuclear moment of inertia I by $\sigma^2 = IT/\hbar^2$, and $\rho(E)$ is the density given by equation (2.1.4). This theory associates a rotation energy $\hbar^2 J(J + 1)/2I$ with the spinning nucleus. Assuming either parity is equally probable, we get an observed density:

$$\rho_{obs}(E) = \frac{\rho(E)}{2} \sum (2J + 1) \quad e^{-J(J + 1)/2\sigma^2}$$

where the summation occurs over all observable spin-parity combinations. For example in an (n, $\gamma$ ) reaction, the summation would be from $J_c - 1$ to $J_c + 1$, where $J_c$ is the spin of the capture state. Since mainly E1 transitions are involved only one parity need by considered in the summation.

The constant temperature form of the spacing function D (E) is given by the reciprocal of equation (2.1.4):

$$D(E) = D_o\, e^{-E/T} \qquad (2.1.5)$$

where $D_o = 1/\rho_o$. The spacing as a function of excitation and spin will then be

$$D_{obs}(E) = \frac{D_o\, e^{-E/T}}{\sum(2J + 1)\, e^{-J(J + 1)/2\sigma^2}}$$

## 2.2 Distributions of Level Spacings

When a projectile nucleon impinges upon a target nucleus, it may simply be deflected by the nuclear potential in a process called direct elastic scattering, or may collide with a target nucleon. It the energy of the projectile or the struck nucleon exceeds its separation energy, we have a direct reaction. If, however, these nucleons undergo further collisions spreading their energy over the whole nucleus until a statistical equilibrium is reached, then a "compound nucleus" is formed. It can de-excite by ejection of one or more particles or by gamma emission. Reactions may also occur before equilibrium is established and direct reactions and the compound nucleus are the limiting cases of the mechanism involved.

Slow neutron resonances in a heavy element like uranium have widths $\Gamma$ from hundredths to several eV (10), which correspond to lifetimes, $\Gamma/\hbar$, of $10^{-14}$ to $10^{-16}$ sec. These states are long-lived on a nuclear scale, and indicate the formation of a compound nucleus. By comparison, the time for a 25 MeV nucleon to cross the nucleus is around $10^{-22}$ sec., which we can associate with direct reactions. The compound nucleus at excitations around the neutron separation energy lives long enough for electro-magnetic transitions to compete with particle emission.

The compound nucleus reaction mechanism is the basis for statistical models of the nucleus. The compound states can be represented by the elements of a random matrix. The eigenvalues of this matrix (which correspond to energy levels) are consequently randomly distributed. The distribution of the spacing between adjacent energy levels of the same spin and parity is given approximately by the Wigner distribution (10):

$$f(S) = \frac{\pi S}{2D^2} \exp \left(\frac{-\pi S^2}{4D^2}\right)$$

where S is the spacing between levels, and D is the mean spacing or expectation of S, E(S):

$$D = \int_0^\infty f(S) S dS = E(S)$$

For a set of energy levels comprising all spins and parities, the effects of the Wigner distribution become much less pronounced. Each subset of levels having common spin and parity belong to a Wigner distribution. As many such subsets are superimposed, the totality of energy levels can be described as random, and the spacings between them belong to a distribution which is essentially exponential:

$$f(S) = \frac{1}{D} \quad e^{-S/D} \qquad 0 \leq S < \infty$$

$$= 0 \qquad\qquad -\infty < S < 0 \,.$$

where D is the mean spacing, E(S). The distribution is normalized, so that

$$\int_0^\infty f(S)dS = 1.$$

Evans (11) derives the analogous distribution of the time intervals between successive random decays of the nuclei of a radioactive source. The probability of an interval of duration between t and t + dt is shown to be:

$$f(t)\ dt = ae^{-at}\ dt,$$

where a is the mean rate of events, or 1/a is the mean time between successive events.

## 2.3 Maximum Likelihood Estimation for Spacing Parameters

We have seen that a spacing S between consecutive energy levels is a randomly distributed variable, whose mean D is assumed to be an exponential function of energy $\sim D_o\ e^{-E/T}$, where $D_o = 1/\rho_o$. In order to fit this function to data, the constants $D_o$ and T are considered parameters which can be evaluated by the statistical theory of estimation.

The general problem is to find "good" estimates for the parameters $\alpha_i$ in a given correlation $y = f\ (x, \alpha_i)$. Observations consist of a set of statistically independent samples ($x_j$ , $y_j'$), j = 1 to n. The $x_j$ are known exactly, and the $y_j'$ are sampled from distributions p ($y_j'$) such that the mean E ($y_j'$) satisfies: E ($y_j'$) = $y_j$ = $f(x_j , \alpha_i)$. For each sampled $y_j'$, the distribution p ($y_j'$) is a function of the parameters $\alpha_i$ and will be written p ($y_j'$ , $\alpha_i$). Since the observations are independent, the probability density function for sample is:

$$L\ (\alpha_i) = \prod_{j=1}^{n} p\ (y_j' , \alpha_i),$$

where L ($\alpha_i$) is the likelihood function.

When L ($\alpha_i$) is maximized according to the equations

$$\frac{\partial L(\alpha_i)}{\partial \alpha_i} = 0,$$

then the solutions $\alpha_i'$ are maximum likelihood (M. L.) estimates of the parameters $\alpha_i$. This method (12) gives estimates with certain desireable properties to be discussed later. For example, if p ($y_j'$) is the normal distribution $\frac{1}{\sqrt{2\pi}\,\sigma} \exp\left[-\frac{1}{2\sigma}(y_j' - y_j)^2\right]$, whose mean $y_j$ is assumed a function of x linear in the parameters $y_j = a\,x_j + b$, the likelihood function for a sample $\{x_j , y_j'\}$ (j = 1 to n) is:

$$L\ (a,b) = \left(\frac{1}{\sqrt{2\pi}\,\sigma}\right)^n \exp\left[-\frac{1}{2\sigma}\sum_{j=1}^{n}(y_j' - ax_j - b)^2\right].$$

Partial derivatives of L (a, b) lead to the normal equations of least squares methods in this case.

The spacings between consecutive energy levels with corresponding mean energies form a sample $(E_i\ ,\ S_i)$, $i = 1$ to $n$, where each $S_i$ belongs to a distribution $p\ (S_i) = \frac{1}{D_i}\ e^{-S_i/D_i}$, whose mean $D_i$ satisfies the equation: $D_i = D_o\ e^{-E_i/T}$. The likelihood function is:

$$L\ (D_o\ ,\ T) = \prod_{i=1}^{n} p\ (S_i)$$

$$= \prod_{i=1}^{n} \frac{e^{E_i/T}}{D_o} \exp\left( - \frac{S_i e^{E_i/T}}{D_o}\right)$$

$$= \frac{1}{D_o{}^n}\ e^{\frac{1}{T} \sum_{i=1}^{n} E_i} \exp\left( - \frac{1}{D_o} \sum_{i=1}^{n} S_i\ e^{E_i/T}\right)$$

The parameters $D_o$ and $T$ are the zero energy spacing and the nuclear temperature, respectively, in keV. Since L is a maximum if log L is a maximum, we can write the M. L. equations more conveniently as:

$$\frac{\partial \ln L(D_o\ ,\ T)}{\partial D_o} = 0$$

$$\frac{\partial \ln L(D_o\ ,\ T)}{\partial T} = 0$$

where $\ln L(D_o\ ,\ T) = \frac{1}{T} \sum_{i=1}^{n} E_i - n \ln D_o - \frac{1}{D_o} \sum_{i=1}^{n} S_i\ e^{E_i/T}$

Then we get:

$$\frac{\partial \ln L}{\partial D_o} = \frac{-n}{D_o} + \frac{1}{D_o{}^2} \sum S_i\ e^{E_i/T} = 0$$

$$\frac{\partial \ln L}{\partial T} = - \frac{1}{T^2} \sum E_i + \frac{1}{D_o T^2} \sum S_i E_i\ e^{E_i/T} = 0$$

Simultaneous solutions to these equations give the estimates $D_o'$ and $T'$ for the parameters $D_o$ and $T$:

$$D_o' = \frac{1}{n} \sum S_i \ e^{E_i/T'} \tag{2.3.1}$$

$$D_o' \sum E_i = \sum S_i E_i \ e^{E_i/T'} \tag{2.3.2}$$

It is seen that an analytic solution is not possible, for on eliminating $D_o'$, we get

$$\frac{1}{n} \left(\sum S_i \ e^{E_i/T'}\right) \left(\sum E_i\right) = \sum S_i E_i \ e^{E_i/T'} \tag{2.3.3}$$

Consequently, the properties of the joint estimates $D_o'$ and $T'$ are indeterminable. Three different cases will be investigated. As a first approach, we will assume that the true temperature T is known. On a semi-log plot, the spacing function (2.1.5) is a straight line of slope $-1/T$ and intercept $\ln D_o$. We are then estimating the intercept of a line of known slope from a series of measurements of D as a function of E. An explicit theory of the properties of the estimate $D_o'$ is then possible which serves to test Monte Carlo methods used in less simple approaches.

The second approach is to eliminate the temperature as a parameter. If the spacing is known accurately at some energy, then we can get a relation $T = T(D_o)$, and the likelihood function is a function of only $D_o$. The straight line mentioned above is being forced to go through one known point. Monte Carlo methods are used to investigate the properties of the single estimate $D_o'$.

The third approach is the joint estimation of the slope and intercept of the function D(E). A Monte Carlo calculation gives some indication of the properties of the estimates $D_o'$ and T'.

## 2.4 Properties of the Estimates

Since values for any estimates of parameters depend on the sample, it is clear that $D_o'$ and T' will generally be different for different samples, and belong to some distribution themselves. An estimator $D_o'$ is unbiased if its expectation E $(D_o')$ is equal to the true value $D_o$, and this is obviously a desireable property since it means there is no "systematic" error or bias in our estimates.

The question then arises as to what exactly are the distributions of our estimates $D_o'$ and T' and their variances, for these indicate the accuracy of our estimates. There is a theorem (12) which states that the variance of unbiased estimators is bounded from below for a given sample size. In the case of a likelihood function L with one parameter $\alpha$ the minimum variance is given by:

$$\sigma^2_{min} = \frac{1}{E\left(\frac{d^2 \ln L(\alpha)}{d\alpha^2}\right)}$$

An estimate with this mi..imum ..riance is said to be efficient. If the variance is a minimum as the sample size goes to infinity, the estimate is said to be asymtotically efficient. Efficiency is clearly desireable in an estimator because it implies that maximum accuracy is attained.

Most maximum likelihood estimators have the following property (12). As the sample size $n \to \infty$, the likelihood equation $\frac{d \ln L}{d\alpha} = o$ has the solution $\alpha'$ with probability tending to one, and the probability that $|\alpha' - \alpha| > \epsilon > 0$ for a given $\epsilon$ tends to zero. The solution $\alpha'$ is also asymtotically normal with mean $\alpha$, and is an asymtotically efficient estimate of $\alpha$, i.e. with a variance equal to the lower bound given above.

(i) Estimation of $D_o$ for Known Temperature

If we consider estimating only the parameter $D_o$, then the M. L. conditions reduce to equation (2.3.1) in which T' is replaced with the known temperature T:

$$D_o' = \frac{1}{n} \sum_{i=1}^{n} S_i \quad e^{E_i/T} \qquad (2.4.1)$$

The expectation is

$$E\ (D_o') = E\left(\frac{1}{n} \sum S_i \quad e^{E_i/T}\right)$$

$$= \frac{1}{n} \sum e^{E_i/T}\ E(S_i)$$

$$= \frac{1}{n} \sum e^{E_i/T}\ D_i$$

$$= D_o,$$

since $D_i = D_o \; e^{-E_i/T}$. The estimate $D_o'$ is therefore unbiased independently of n.

The distribution of $D_o'$ can be derived by writing equation (2.4.1) as:

$$D_o' = \frac{D_o}{n} \sum_{i=1}^{n} x_i, \qquad (2.4.2)$$

where $x_i = S_i/D_i$. Since the probability density function of $S_i$ is $p\,(S_i) = \frac{1}{D_i} \; e^{-S_i/D_i}$, then the probability density of $x_i$ is $f_i(x_i) = p\,(x_i D_i) \; \frac{dS_i}{dx_i}$

$$= e^{-x_i} \qquad (2.4.3)$$

Consider the sum $z_n = \sum_{i=1}^{n} x_i$ in equation (2.4.2). If n = 1, then the probability density function (abbreviated p.d.f.) of $z_1$ is simply $e^{-z_1}$. For n = 2 the sum $z_2 = x_1 + x_2$, where the p.d.f. of $x_1$ and $x_2$ are given by equation (2.4.3), has the p.d.f. (13):

$$p_2\,(z_2\,) = \int_0^{z_2} f_1\,(x_1)\; f_2\,(z_2 - x_1)\; dx_1$$

$$= \int e^{-x_1} \; e^{-z_2 + \; x_1} \; dx_1$$

$$p_2\,(z_2) \; = \; z_2\, e^{-z_2} \; .$$

For n = 3, we consider the sum $z_3 = z_2 + x_3$ and get $p_3\,(z_3) = \frac{1}{2} \; z_3^{\,2} \; e^{-z_3}$. Inspection suggests the general p.d.f.

$$p_n\,(z_n) = \frac{1}{(n-1)!} \; z_n^{\,n-1} \; e^{-z_n} \; . \qquad (2.4.4)$$

For $z_{n+1} = z_n + x_{n+1}$, with the assumption that $p_n(z_n)$ is given by equation (2.4.4), we can write

$$p_{n+1}(z_{n+1}) = \int_0^{z_{n+1}} p_n(z_n)\, f_{n+1}(z_{n+1} - z_n)\, dz_n$$

$$= \frac{1}{(n-1)!} \int z_n^{n-1} e^{-z_n} e^{-(z_{n+1}-z_n)} dz_n$$

$$= \frac{1}{(n-1)!} e^{-z_{n+1}} \frac{z_{n+1}^{n}}{n}$$

$$= \frac{1}{((n+1)-1)!} z_{n+1}^{(n+1)-1} e^{-z_{n+1}}$$

This is precisely the equation for $p_n(z_n)$ with n + 1 in place of n, so that the general p.d.f. for the sum $z_n$ given by (2.4.4) has been proven by induction for all $n \geqslant 1$. Since $D_o' = \frac{D_o}{n} z_n$, then $D_o'$ has the p.d.f.:

$$p(D_o') = \frac{n}{D_o} \frac{1}{(n-1)!} \left(\frac{nD_o'}{D_o}\right)^{n-1} e^{-n\frac{D_o'}{D_o}}$$

$$= \left(\frac{n}{D_o}\right)^{n} \frac{1}{(n-1)!} (D_o')^{n-1} e^{-\frac{n}{D_o} D_o'} \tag{2.4.5}$$

This is called a gamma distribution, which is identical in form to the generalized n - fold interval distribution (11). It is normalized because

$$\int_0^{\infty} p(D_o')dD_o' = \frac{1}{(n-1)!} \int_0^{\infty} \left(\frac{nD_o'}{D_o}\right)^{n-1} e^{-\frac{nD_o'}{D_o}} d\left(\frac{nD_o'}{D_o}\right)$$

$$= \frac{\Gamma(n)}{(n-1)!}$$

$$= 1$$

The variance of this distribution is given by

$$\sigma^2 = E\left[D_o' - E(D_o')\right]^2$$

$$\sigma^2 = \int_0^{\infty} (D_o' - D_o)^2 \; p(D_o') \, dD_o'$$

$$\sigma^2 = \frac{D_o^2}{n} \qquad (2.4.6)$$

The likelihood function can be written in terms of the estimate $D_o'$:

$$L = \frac{1}{D_o^n} \; e^{\frac{1}{T}\sum E_i} \; e^{-\frac{1}{D_o}\sum S_i \, e^{E_i/T}}$$

$$L = e^{\ln(D_o^{-n})} \; e^{\frac{1}{T}\sum E_i} \; e^{-n\frac{D_o'}{D_o}}$$

$$L = e^{\frac{1}{T}\sum E_i} \; e^{-\frac{nD_o'}{D_o} + \ln(D_o^{-n})}$$

There is a theorem (14) which states that if the likelihood function can be written in this form,* then the M. L. estimate $D_o'$ is efficient, so that the variance given by equation (2.4.6) is the minimum for all unbiased estimates of $D_o$.

Thus we have shown that $D_o'$ as given by equation (2.4.1) is an unbiased efficient estimate of $D_o$ and have given expressions for the p.d.f. and variance of $D_o'$.

(ii) Elimination of T

The second case to be considered in solving the M. L. equations is the case in which the nuclear temperature

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* *The general form required in the theorem is:* $L = H(E_i) \exp\left[A(D_o) D_o' + B(D_o)\right]$

can be considered a function of $D_o$. Suppose that at the neutron separation energy, $E_n$, the level spacing, $D_n$, is accurately known. Typical values would be 70 eV spacing at 8 MeV. From $D_n = D_o\, e^{-E_n/T}$, we get

$T = E_n/\ln(D_o/D_n)$. The likelihood function can then be written as a function of $D_o$ only:

$$L\,(D_o\,,\,T) = \frac{1}{D_o{}^n}\; e^{\frac{1}{T}\sum E_i}\; \exp\left(-\frac{1}{D_o}\sum S_i\, e^{E_i/T}\right)$$

$$L\,(D_o) = \frac{1}{D_o{}^n}\; \exp\left\{\frac{1}{E_n}\ln(D_o/D_n)\sum E_i - \frac{1}{D_o}\sum S_i\, e^{(E_i/E_n)\ln(D_o/D_n)}\right\} \qquad (2.4.7)$$

Then $\dfrac{\partial \ln L}{\partial D_o} = \dfrac{d \ln L}{dD} = 0$ gives the maximum likelihood estimate $D_o'$. This equation cannot be solved explicitly, so numerical methods must be used.

It is not possible to investigate directly as in case (i) the bias, efficiency, variance or distribution of the estimate $D_o'$. A Monte Carlo type of calculation was therefore performed. For each of many samples of spacings $\{S_i\}$, an estimate $D_o'_j$ was found. The set of such estimates $\{D_o'_j\}$ constitute a sample which illustrates in histogram form the distribution of $D_o'$. A sample mean and variance can be calculated and a bias detected if it is appreciable. Such a Monte Carlo calculation does not give general results, but does give an indication of the distibutions involved for certain initial values of $D_o$ and T.

(iii) Joint Estimation of $D_o$ and T

The third case in that in which estimates of both $D_o$ and T are to be made. The conditions for maximum likelihood (2.3.1) and (2.3.2) lead to the transcendental equation (2.3.3) for the estimate T'. This equation is solved numerically. The estimate $D_o'$ is then given by equation (2.3.1). The estimates belong to a two-dimensional distribution f ($D_o'$ , T') which can be represented by a surface. The intersection of this surface with the plane T' = T will form a curve which is the gamma distribution of equation (2.4.5). This is all that is known of the surface f ($D_o'$ , T') because of the absence of explicit solutions of the M. L. equations. The gross features of the joint distribution were illuminated by a Monte Carlo calculation. A histogram was generated from a large number of joint estimates, each pair of which was obtained from a different sample of spacings.

CHAPTER III

# MONTE CARLO CALCULATIONS

## 3.1 The Generation of Level Spacings

In order to get many estimates for $D_o$ (and T) from a Monte Carlo calculation, it is necessary to be able to generate many sets of level spacings which are exponentially distributed. In this section a method for doing this is given starting from a set of pseudo-random numbers which were generated in a computer subroutine. A particular set of 69 such numbers taken as an example is followed through their transformation to a set of spacings in order to show the algorithm.

Let us originally choose some reasonable values for $\rho_o = 1/D_o$ and T. Then if there are N energy levels between zero and $E_o$ keV, the probability of a level of energy between E and E + dE if E is less than $E_o$ and greater than zero is:

$$\phi(E)dE = \frac{\rho(E)dE}{N}$$

The level density $\rho(E)$ is the exponential function given by equation (2.1.4) for low excitations. For consistency, we must have

$$N = \int_o^{E_o} \rho(E)dE$$

It is easy to generate pseudo-random numbers y between zero and 1.0 by the multiplication of large integers followed by suitable truncations. The probability of such a number being between y and y + dy is

$$\psi(y)\, dy = dy \qquad 0 \leq y \leq 1$$

Equating these two probabilities we get

$$\rho_o e^{E/T} dE = dy$$

Integration gives the solution:

$$E = T \ln\left(\frac{Ny}{\rho_o T} + 1\right) \qquad (3.1.1)$$

From a set of numbers $\{y_i\}$ drawn from the uniform distribution $\psi(y)$, it is therefore possible to form a set of numbers $\{E_i\}$ which are exponentially distributed. This latter set represents a set of energy levels with the exponential density $\rho(E)$. Then by definition we can form a set of spacings $\{S_i\}$ where $S_i = E_{i+1} - E_i$, and $S_i$ is considered a function of the average energy $(E_{i+1}+E_i)/2$. For a sample of n spacings, N levels were generated from a set of N values of y, and N itself was sampled from a normal distribution with a mean of approximately $n + 3\sigma$ and a variance $\sigma^2 = n + 3\sigma$. This insured an initial sample $\{y_i\}$ of a size which was always bigger than the number of spacings desired but never large enough to waste much computational time. For example, for the generation of forty spacings, N was sampled from the normal distribution of mean 81 and variance 81, so the probability that

$N \geq 40$ was almost one. One such sample had $N = 69$, and the frequency histogram for the uniformly distributed numbers $\{y_i\}$ $(i=1, 2, \ldots 69)$ is shown in Figure 1. The distribution $\psi(y)$ is also shown suitably normalized to the area under the histogram. The irregularities of such a small sample are somewhat smoothed in the cumulative distribution $\Psi(y)$ in Figure 2, where

$$\Psi(y) = \int_0^y \psi(y')dy' \qquad o \leq y \leq 1$$

$$= y$$

The pseudo-random numbers $\{y_i\}$ appear uniformly distributed from zero to one.

Each $y_i$ is now transformed by equation (3.1.1) to an energy level $E_i$ which belongs to an exponentially distributed set. The initial values of $\rho_o$ and T were 0.005 $keV^{-1}$ and 1000 keV respectively. In Figure 3 is shown the histogram of the levels obtained from the pseudo-random numbers of Figure 1. The exponential level density $\rho(E) \sim e^{E/T}$ is also shown with suitable normalization. In Figure 4 the total number of levels up to some energy E is plotted and can be compared to the integral of level density given by

$$N(E) = \int_0^E \rho(E')dE'$$

$$= \rho_o \int_0^E e^{E'/T} dE'$$

$$= \rho_o T \, (e^{E/T} - 1)$$

It is seen from Figures 3 and 4 that the random sample of energy levels $\{E_i\}$ $(i = 1, 2, \ldots 69)$ does exhibit an exponential density. No statistical criteria are given here to test how well the histograms fit the smooth curves of theory. In making comparisons, it must be remembered that the number of levels in each energy interval is quite small and it is not unreasonable to assign an uncertainty of the order of the square root of the number of levels counted in each energy interval in Figure 3. The number of levels counted up to some energy E in Figure 4 can also be given this uncertainty. The curves $\rho(E)$ and $N(E)$ then fall within the limits of uncertainty of the plotted points in most cases.

From this typical set of energy levels $\{E_i\}$ $(i = 1, 2, \ldots 69)$ was formed the set of level spacings $\{S_i\}$ according to $S_i = E_{i+1} - E_i$. Each spacing $S_i$ is a random variable whose mean $D_i$ can be calculated from the average excitation $(E_{i+1} + E_i)/2$ by equation (2.1.5). We can now form the set of ratios $\{x_i\}$ $(i = 1, 2, \ldots 69)$ where $x_i = S_i/D_i$. In section (2.4) it was shown that such ratios should be distributed as $e^{-x}$, and Figure 5 shows that the frequency histogram of the set $x_i$ does resemble an exponential probability density. In Figure 6 it is shown the set $\{x_i\}$ has the cumulative distribution given by

$$F(x) = \int_0^x e^{-x'}\, dx' \qquad 0 \leq x < \infty$$

$$= 1 - e^{-x}$$

We therefore have a method of generating random exponentially distributed level spacings $S_i$ whose means $D_i$ are an exponential function of energy. In Figure 7 is plotted the set of spacings used in our example. The straight line is the spacing function corresponding to the initial values of the parameters $D_o$ and T from which the spacings were generated. From this set of "data points", estimates $D_o'$ and T' can be made which won't usually be the same as the true values $D_o$ and T. By generating many different such sets of spacings and forming estimates from each set, the statistical properties of the estimates are studied.

## 3.2 Monte Carlo Calculation for Known Temperature

When only $D_o$ is estimated by maximum likelihood, and the temperature T is considered known, the estimate $D_o'$ has been shown to have an explicit solution which is unbiased and efficient according to section (2.4). The estimate also belongs to a gamma distribution given by equation (2.4.5). A Monte Carlo calculation was done because in this case there is an explicit theory to which results can be compared. Validity of Monte Carlo methods in this instance warrants its use in two further cases in which the properties of the estimates are not explicitly available.

According to the method of section (3.1), N pseudo-random numbers were generated m times. For each set, N was sampled for a normal distribution of mean 121 and variance 121. The pseudo-random numbers were transformed by equation (3.1.1) into N energy levels, so that on the average 121 levels were available to form n spacings. For each set of levels, four estimates $D_o'$ were made: the first from the first ten spacings (n = 10); the second with the first twenty spacings (n = 20); the third with the first forty (n = 40); and the fourth and last with the first eighty (n = 80). One hundred (m = 100) sets of levels were generated, so that one hundred estimates $D_o'$ were found for each of four values of n. The initial values of the parameters were 200 keV for $D_o$ and 1000 keV for the temperature T. The estimates are shown in histograms as a function of n in Figure 8 to 11. The smooth curves in these figures are the gamma distributions f $(D_o')$ given by equation (2.4.5) which have been normalized so that the integral of f $(D_o')$ from zero to infinity is equal to the area under each histogram. The numbers of estimates falling in each interval of $D_o'$ are quite small, and within an uncertainty given by the root of these numbers, the histograms agree with the gamma distributions. The only exception is in Figure 11, where the histogram seems unusually high.

Let the set of m estimates be represented by $\{D_o'_j\}$, (j = 1, 2, ... m). This set constitutes a sample from the distribution f $(D_o')$, whose expectation E $(D_o')$ is $D_o$. It is easy to show that the sample mean $\overline{D_o'}$ is an unbiased estimate of the true mean $D_o$. The sample mean is by definition:

$$\overline{D_o'} = \frac{1}{m} \sum_{j=1}^{m} D_o'_j .$$

The sample variance $s^2$ is also an unbiased estimate of the variance $\sigma^2$ of the distribution f $(D_o')$, and is given by

$$s^2 = \frac{1}{m-1} \sum_{j=1}^{m} (D_o'_j - \overline{D_o'})^2$$

The results of the sets of one hundred estimates are shown in Table I for different values of n. The sample means do not show a bias, since $D_o'$ is an unbiased estimate of $D_o$. The sample variances vary almost as 1/n as shown in Figure 12. This is in agreement with the variance $\sigma^2$ found in equation (2.4.6).

Figures 8 to 11 demonstrate how increasing the number of level spacings affects the accuracy of the estimate $D_o'$. They also demonstrate the theorem mentioned in section (2.3) that maximum likelihood estimates have asymtotically normal distributions. It is seen that f $(D_o')$ becomes less skewed as n increases until at n = 80, it appears nearly Gaussian in shape.

The conclusion to be drawn from these Monte Carlo calculations is that they furnish a means to generate the approximate form of the distributions of the estimates $D_o'$. In the next two sections this is the only means available.

TABLE I

Monte Carlo Results for T Known

| Expectation Value $E(D_o') = D_o$ | Number of Spacings $n$ | Sample Mean $\overline{D_o'}$ | Sample Variance $s^2$ | Standard Deviation $s$ |
|---|---|---|---|---|
| 200 keV | 10 | 192.2 keV | 3144 $keV^2$ | 56 keV |
| 200 | 20 | 198.6 | 1347 | 37 |
| 200 | 40 | 201.0 | 638 | 25 |
| 200 | 80 | 200.0 | 208 | 14 |

## 3.3 Monte Carlo Results for Elimination of T

A spacing of $D_n = 70$ eV was assumed at an excitation $E_n = 8$ MeV in order to make the temperature T a function of $D_o$. Then the likelihood function given by (2.4.7) is a function of only $D_o$ but no explicit solution is possible. The maximum likelihood estimator was found by forming the derivative $\frac{d \ln L}{d D_o}$ and evaluating it at a series of test values $D_o$ which converged on the point $D_o'$ at which the derivative is zero. The function $\ln L\ (D_o)$

if plotted as a function of ln $D_o$ appears almost parabolic. The simple method of solution by test evaluations was possible because of the speed of the McMaster IBM 7040 with which all calculations were made.

For each of one hundred sets of pseudo-random numbers $\{y_i\}$ (i = 1, 2, ... N), a set of energy levels $\{E_i\}$ (i = 1, 2, ... N) and $n \leq N$ spacings $\{S_i\}$ were formed and an estimate $D_o'$ found for $D_o$. The histograms of estimates are plotted in Figures 13 to 16 for the number of spacings n equal to 10, 20, 40 and 80. The sample means $\overline{D_o'}$ and sample variances $s^2$ were calculated as per Table II. The comparison of the assumed value of $D_o$ and the sample mean show that the M. L. estimates $D_o'$ are essentially unbiased. The variances $s^2$ are plotted against 1/n in Figure 17 and show the same linear behaviour as in section (3.2). The estimates in a sense become more precise as the distribution f $(D_o')$ becomes narrower with increasing n.

It is important to recall the motivation for these Monte Carlo calculations. The likelihood function is a statistic, that is, a function of the "observations" $\{S_i\}$, and gives an estimator at its maximum value. It further contains the lower limit of accuracy of any unbiased estimator, maximum likelihood or otherwise, as given by the minimum variance in section (2.3). The quantity $E\left(-\frac{\partial^2 \ln L}{\partial \alpha^2}\right)$, where $\alpha$ is the parameter, is called Fisher's amount of information (12). There is a temptation to draw more than this amount of information from the likelihood function. Muradyan and Adamchuk (15) for example assert that the probability density function of an estimate is proportional to the likelihood function, and use its full width half maximum as a variance. This has been disputed by Slavinskas and Kennett (16). Monte Carlo methods can give some insight into the distributions of estimates without over-interpreting the significance of the likelihood function.

TABLE II

Results of 100 Estimates

$D_o'$ for Different Sample Sizes

| Assumed Value of $D_o$ | n = Sample Size of Spacings $S_i$ | Sample Mean $\overline{D_o'}$ | Sample Variance $s^2$ | Standard Deviation |
|---|---|---|---|---|
| 208.7 keV | 10 | 198.1 keV | 3228.2 $keV^2$ | 56.8 keV |
| 208.7 | 20 | 201.6 | 1615.5 | 40.2 |
| 208.7 | 40 | 201.9 | 865.4 | 29.4 |
| 208.7 | 80 | 205.5 | 340.0 | 18.4 |

## 3.4 Monte Carlo Results for Estimation of $D_o$ and T

The estimates belong to some probability density function f ($D_o'$, T') whose form is not known except for the cross-section through T' = T. Since a surface and not merely a curve is to be built up by the Monte Carlo method, a very great number of joint estimates must be calculated. By the method of section (3.1), four thousand and five hundred sets of forty spacings were generated from sets of pseudo-random numbers and estimates $D_o'$ and $T'$ were made for each set. The parameters $D_o$ and $T$ were given values of 200 keV and 1000 keV respectively. The transcendental equation (2.3.3) whose solution is $T'$ was solved by test evaluations in an interval which converged on $T'$. The set of estimates $\{D_o'_i , T_i'\}$ (i = 1, 2, ... 4500) was sorted into a thirty-two by thirty-two matrix formed by dividing the $D_o' - T'$ plane into intervals of 10 keV along the $D_o'$ axis and of 50 keV along the $T'$ axis. A scatter-plot is shown in Figure 18. The points given by the coordinates $(D_o', T')$ were plotted uniformly over the areas into which they fell. The height of the histogram is then proportional to the density of points. Figure 19 shows a series of cross-sections of the scatter plot with constant intervals on the $D_o'$ axis indicated by the arrows. Figure 20 shows a series of cross-sections of constant interval on the $T'$ axis. For each $D_o'$, a sample variance could be calculated for $T'$ and vice versa. The scatter plot shows that the regression of $D_o'$ on $T'$ or of $T'$ on $D_o'$ is not linear. The points falling between $T'$ = 950 and 1050 keV are shown in a separate histogram in Figure 21 in order to compare it with the gamma distribution which it should and does resemble.

These calculations were done only for forty spacings because this is a reasonable number of spacings which are observed by (n, $\gamma$ ) studies. Consider the regression of T' on $D_o$'. For any value of $D_o$', the mean temperature is

$$E\ (T') = \int_0^\infty f\ (D_o', T')\ T'\ dT' = g\ (D_o')$$

The function g is not linear. In order to calculate a correlation coefficient, a transformation must be effected to make g a linear function. The choice of such a transformation is, however, difficult to make. An exponential $\sim e^{\text{constant} \times D_o'}$ was tried, and the scatter plot is re-drawn in Figure 22 in a semi-log representation which is still non-linear. Dalby (17) gives a quick method for choosing a transformation. His method suggests a function of the general form a + b $(c + D_o')^p$, where a, b, c are constants and from our data, p is about 3.

# CHAPTER IV

## APPLICATION TO $Mn^{56}$

The gamma radiation from the $^{55}Mn(n,\gamma)^{56}Mn$ reaction has been studied using a Ge (Li) spectrometer and a Ge (Li) - NaI coincidence spectrometer (18). The number of levels N(E) is shown as a function of the excitation E in Figure 23. The decreasing slope of the curve is characteristic of levels undetected because of finite resolution. The constant temperature spacing function $D_o\ e^{-E/T}$ was assumed and maximum likelihood estimates were made for the parameters $D_o$ and T. The estimates were 268 keV and 1080 keV respectively. Contours of constant likelihhod are shown in relative units in Figure 24.

The estimates provide a useful measure of resolution losses in gamma spectra. Consider transitions from the capture state at the neutron separation energy $S_n$ to adjacent levels at an average energy E. If the spacing at this energy is less than the detector resolution, 15 keV, the gamma rays are not resolved. The probability of a spectral multiplet is therefore

$$P(E_\gamma) = \frac{1}{D}\int_0^{15} e^{-S/D}\, dS,$$

where $E_\gamma$ is the energy of the gamma ray, and $D = D_o\ e^{-(S_n-E_\gamma)/T}$. For the $Mn^{56}$ spectrum, this probability is 0.17 for a 6 MeV gamma ray, and is 0.69 for a 4 MeV gamma ray. The fraction of unresolved gamma rays therefore becomes quite appreciable as the gamma ray energy decreases.

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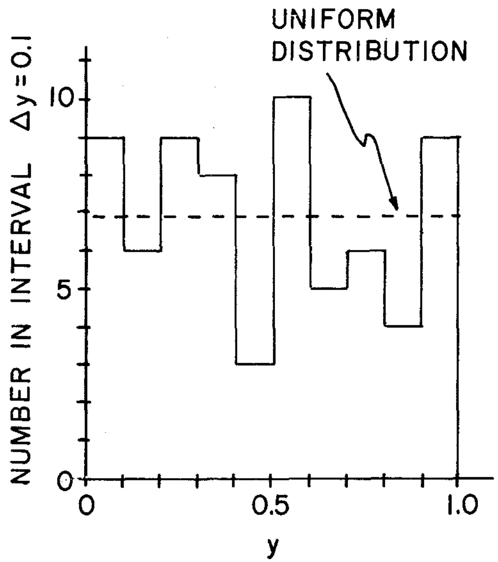


FIGURE 1.

DISTRIBUTION OF RANDOM NUMBERS

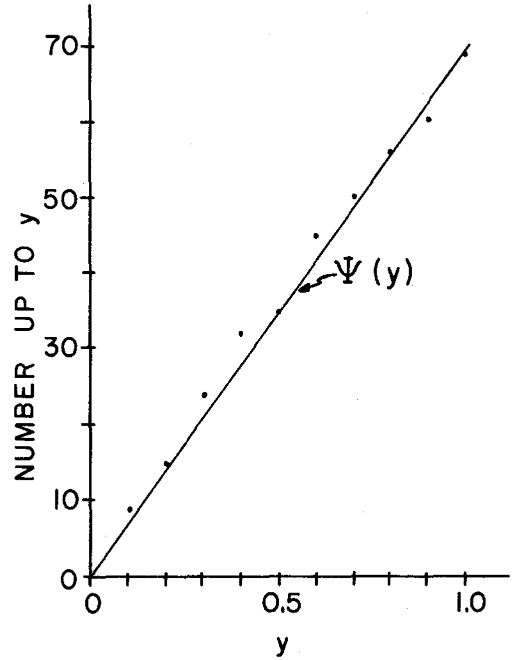


FIGURE 2.

CUMULATIVE DISTRIBUTION OF RANDOM NUMBERS

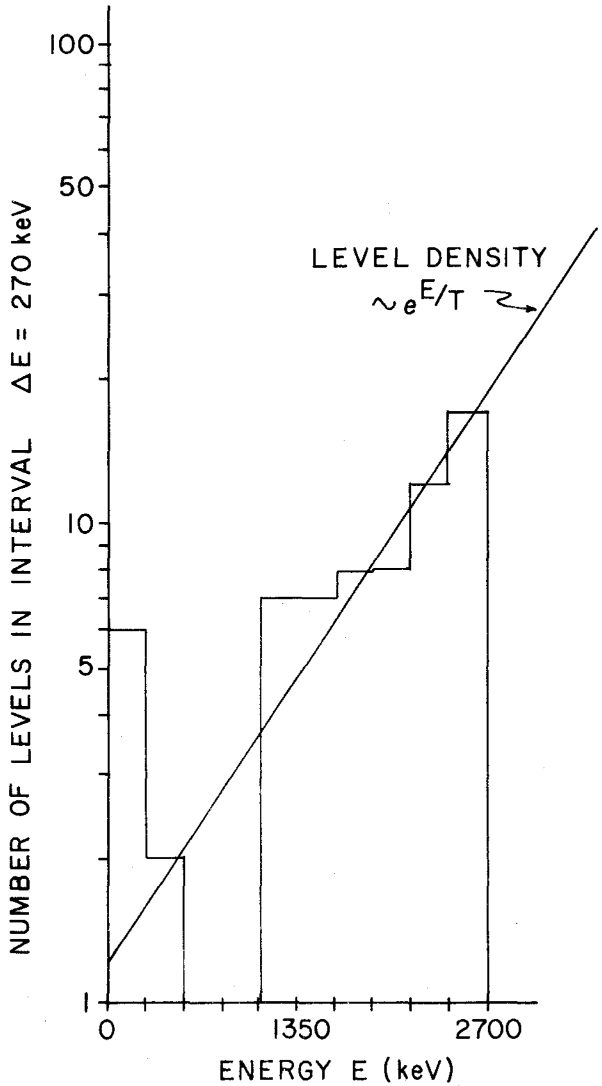


FIGURE 3
DISTRIBUTION OF ENERGY LEVELS

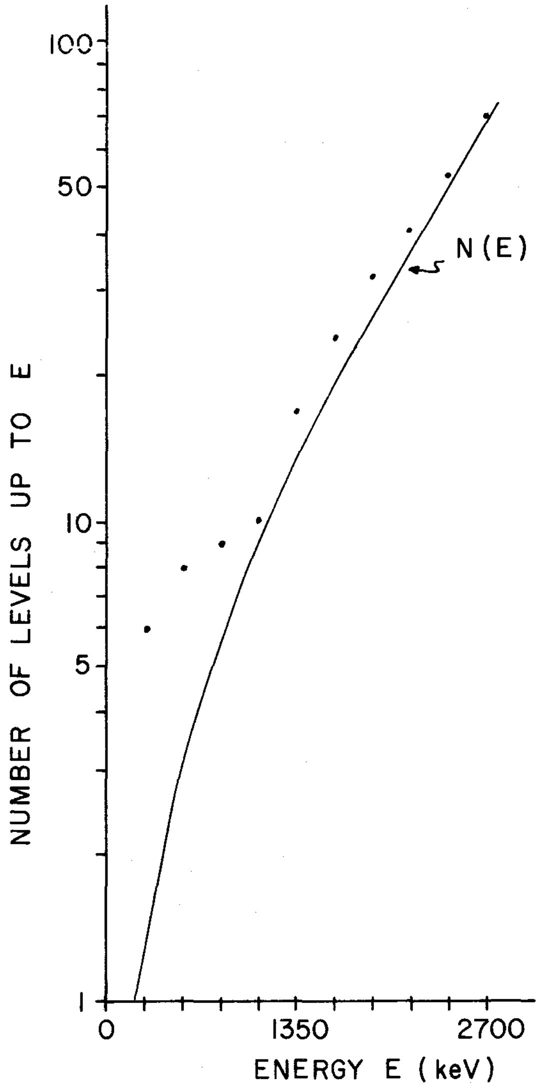


FIGURE 4
CUMULATIVE DISTRIBUTION OF ENERGY LEVELS

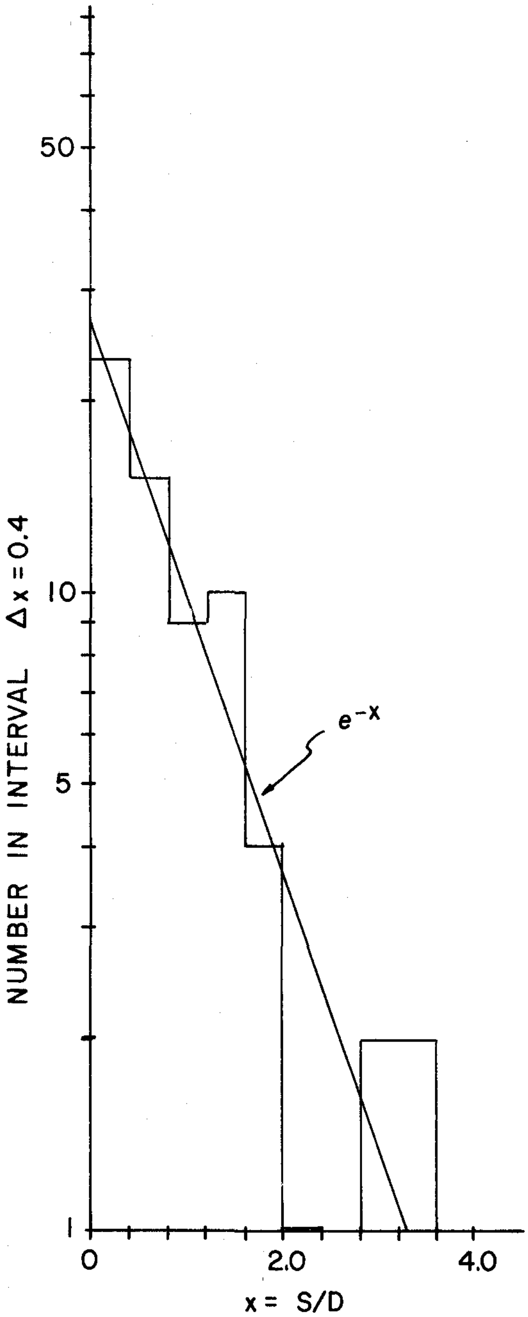


FIGURE 5

DISTRIBUTION OF THE RATIOS x

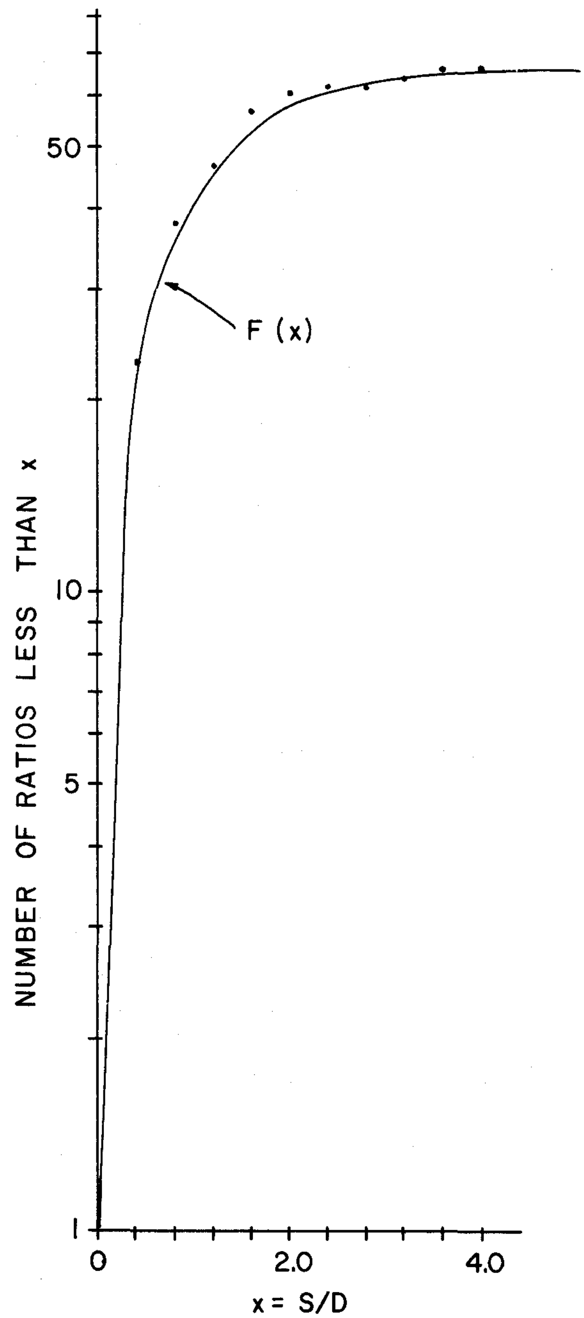


FIGURE 6

CUMULATIVE DISTRIBUTION OF RATIOS

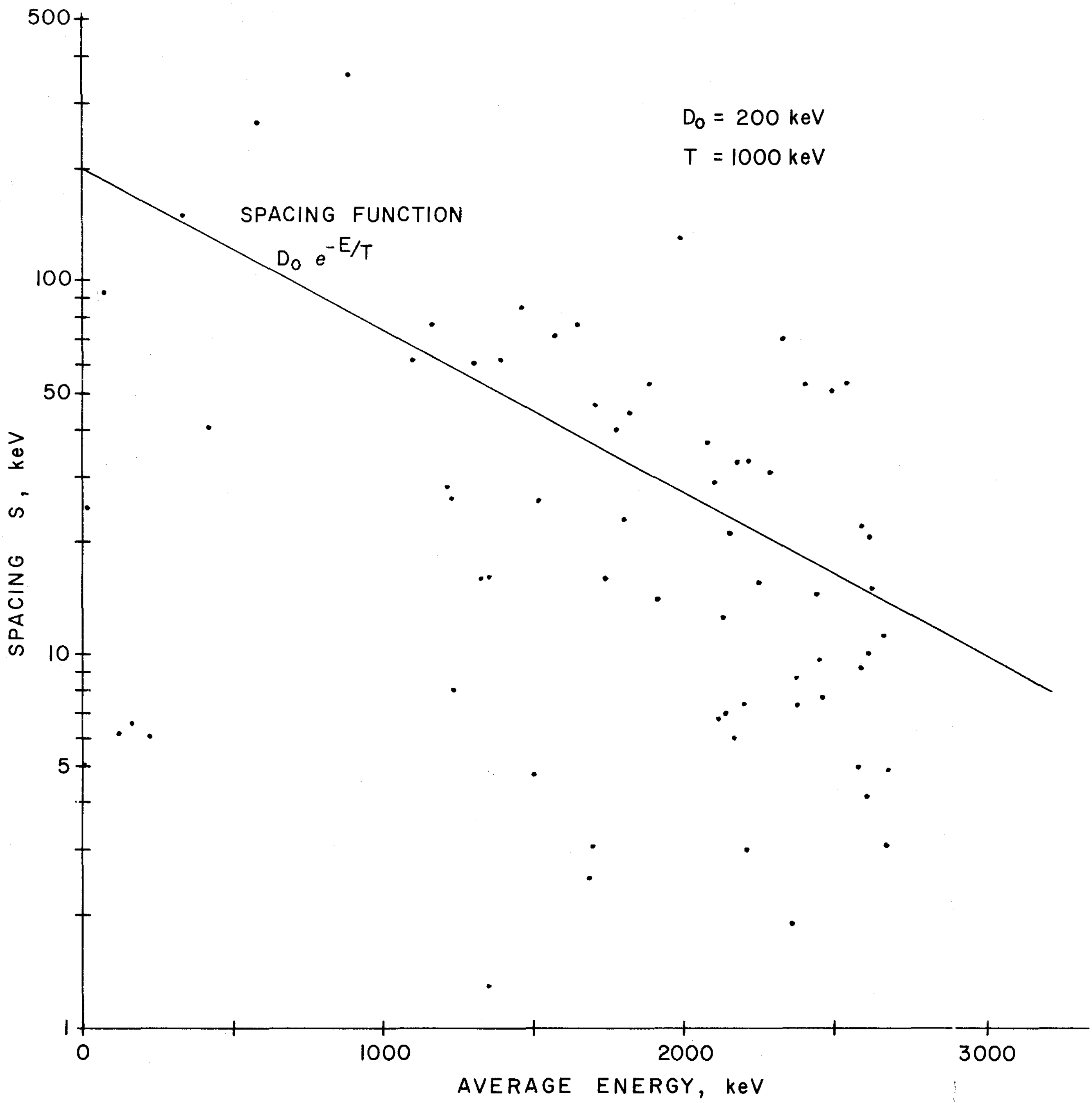


FIGURE 7
A SET OF GENERATED LEVEL SPACINGS

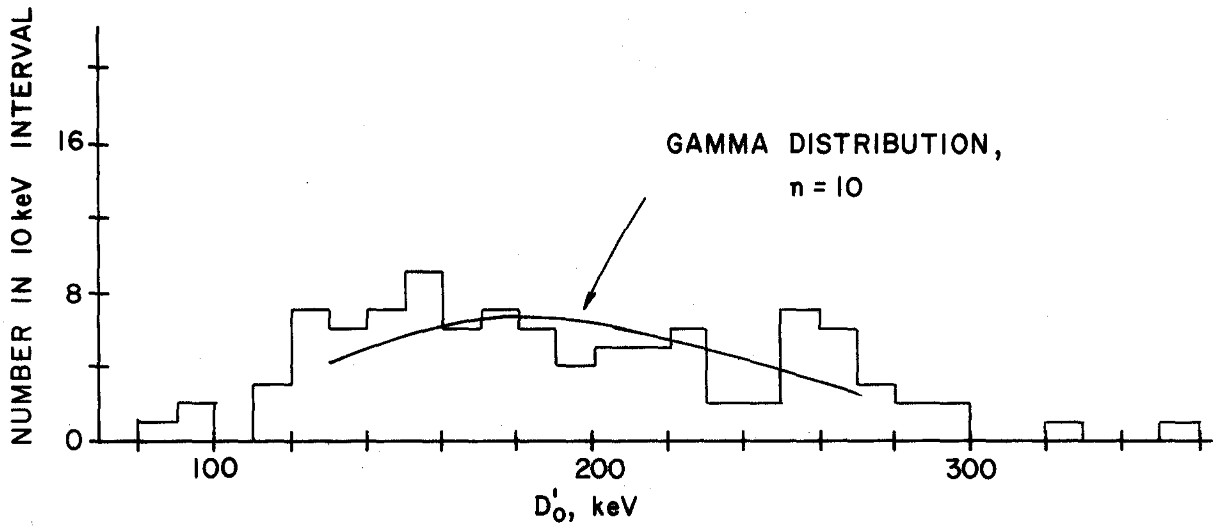


FIGURE 8
DISTRIBUTION OF $D_0'$ FOR 10 SPACINGS

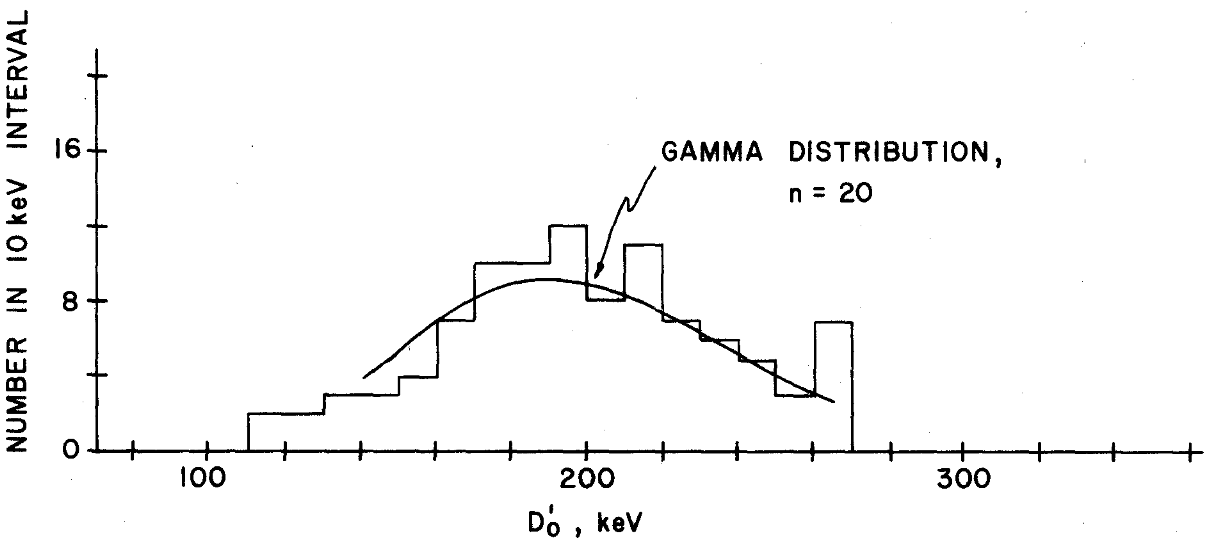


FIGURE 9
DISTRIBUTION OF $D_0'$ FOR 20 SPACINGS

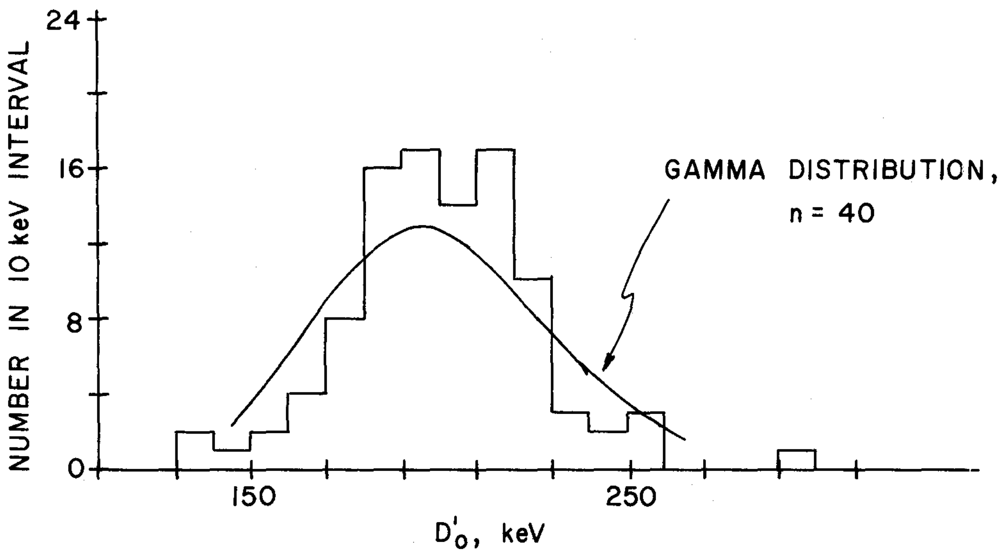


FIGURE 10
DISTRIBUTION OF $D'_0$ FOR 40 SPACINGS

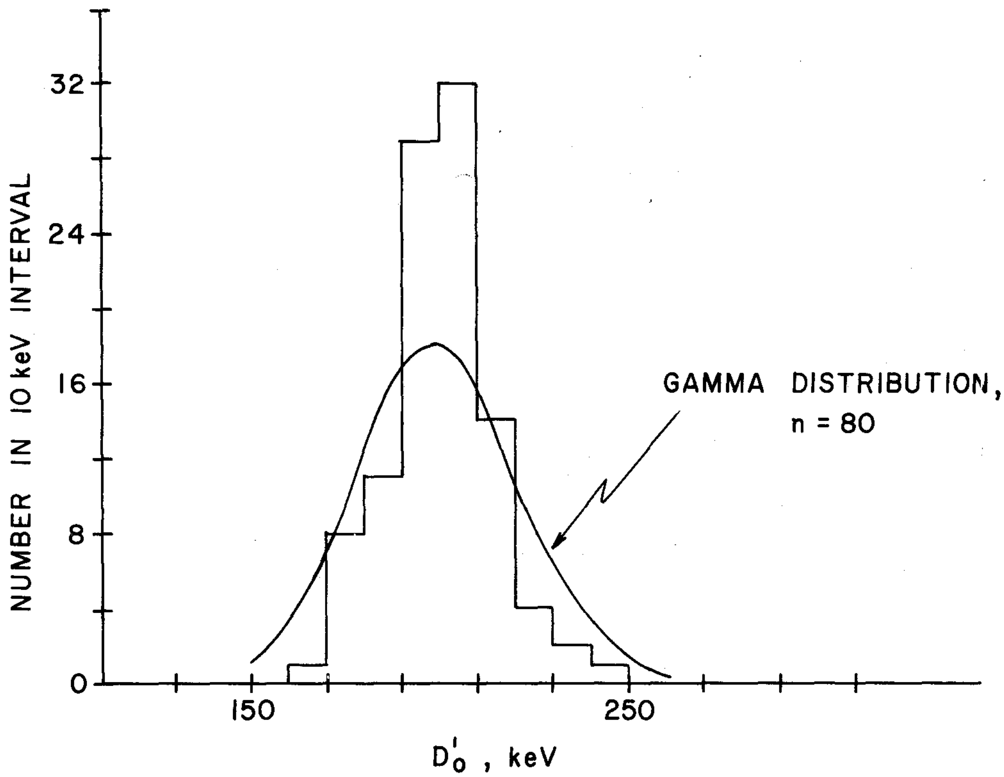


FIGURE 11
DISTRIBUTION OF $D'_0$ FOR 80 SPACINGS

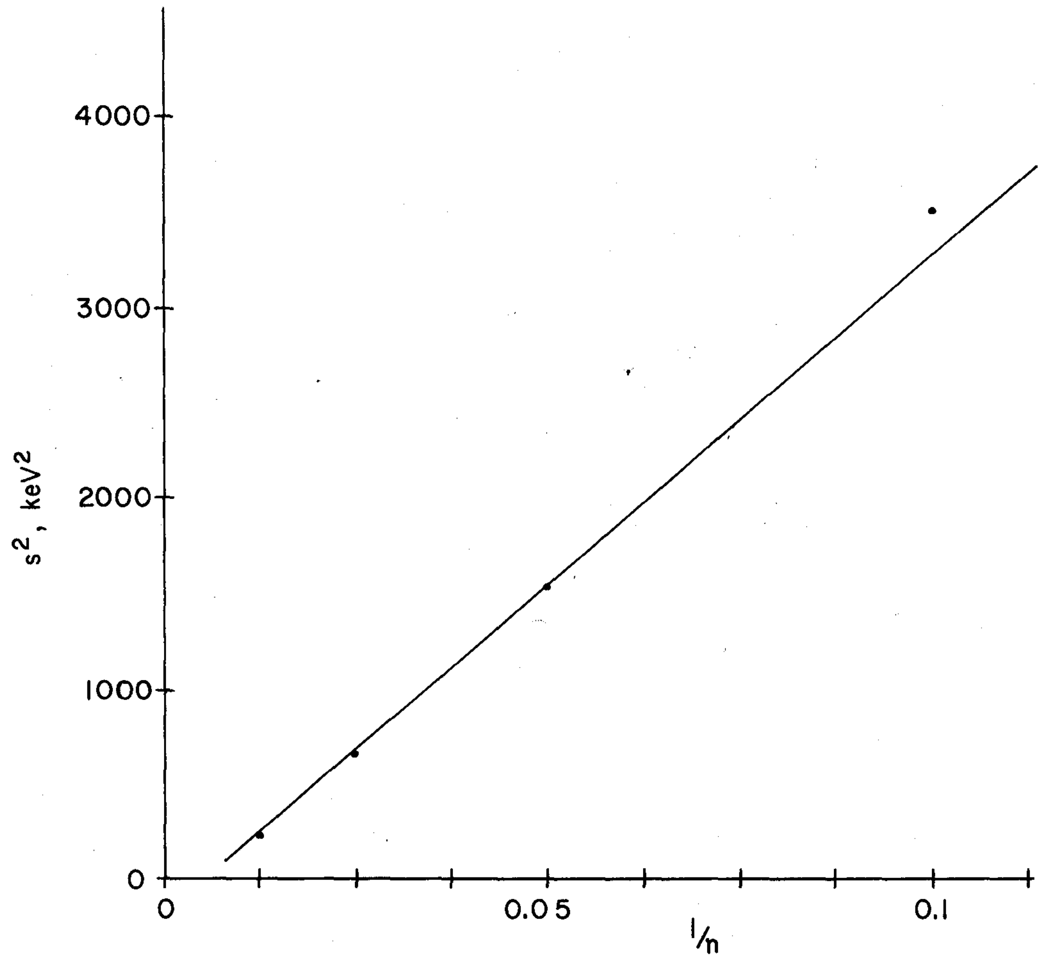


FIGURE 12

SAMPLE VARIANCE FOR DIFFERENT n

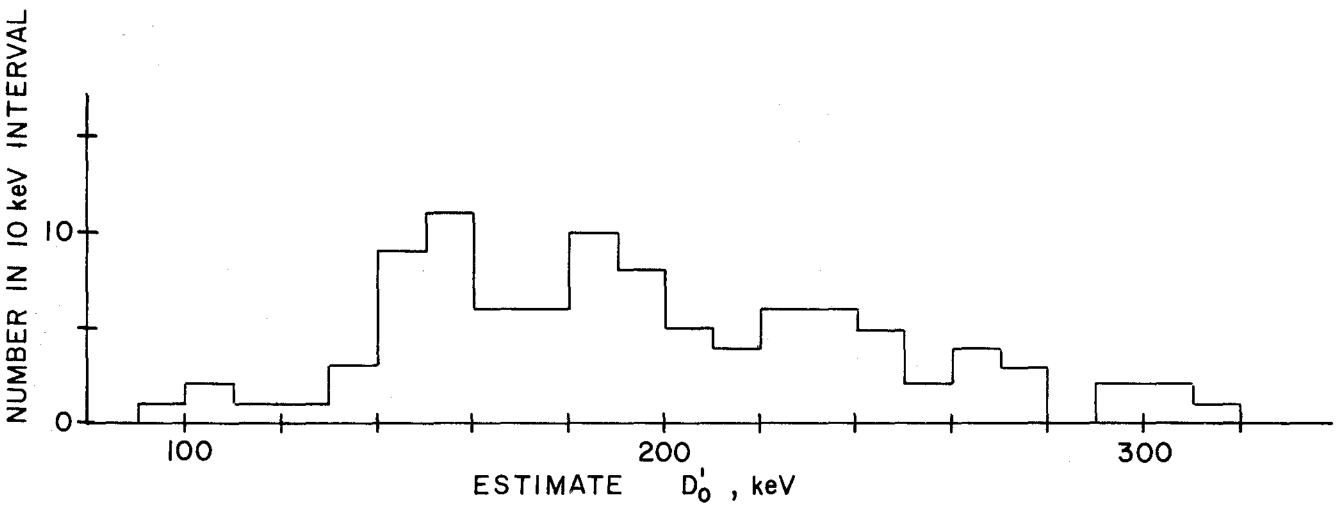


FIGURE 13
HISTOGRAM OF ESTIMATES FOR 10 SPACINGS

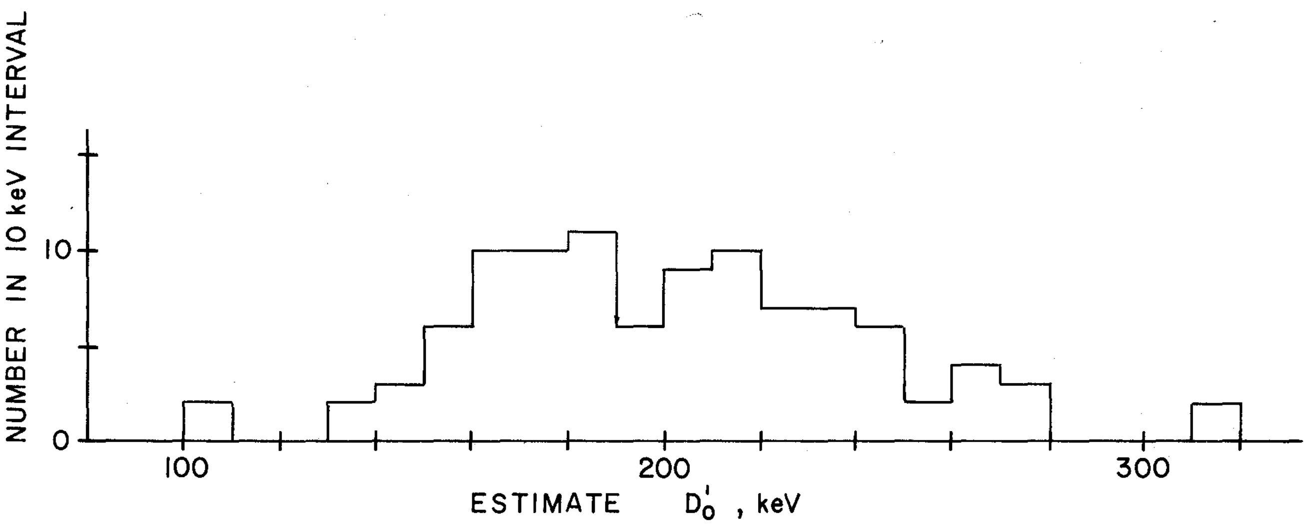


FIGURE 14
HISTOGRAM OF ESTIMATES FOR 20 SPACINGS

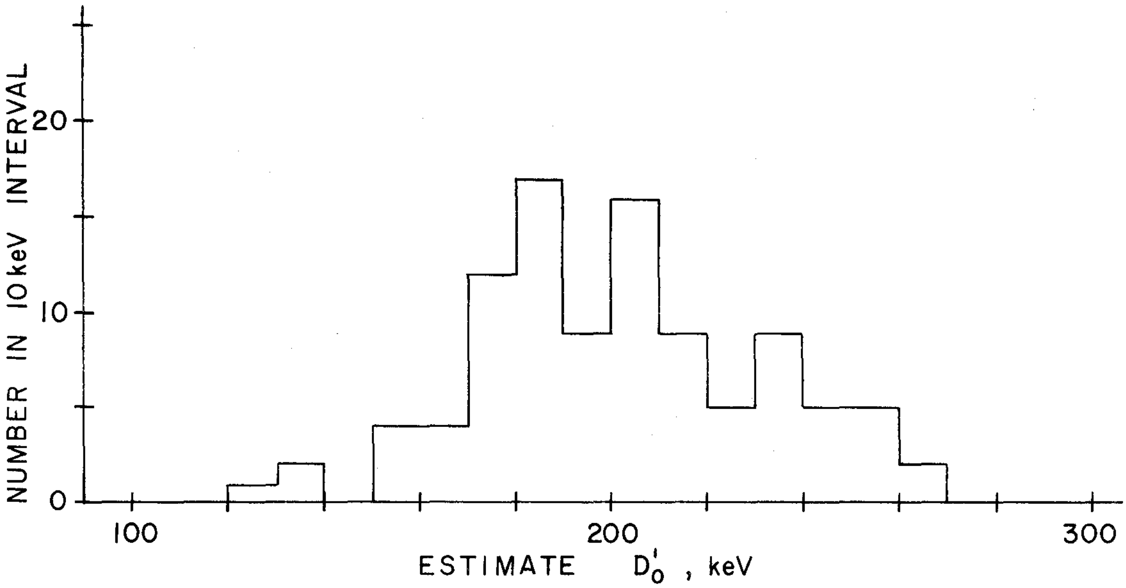


FIGURE 15
HISTOGRAM OF ESTIMATES FOR 40 SPACINGS

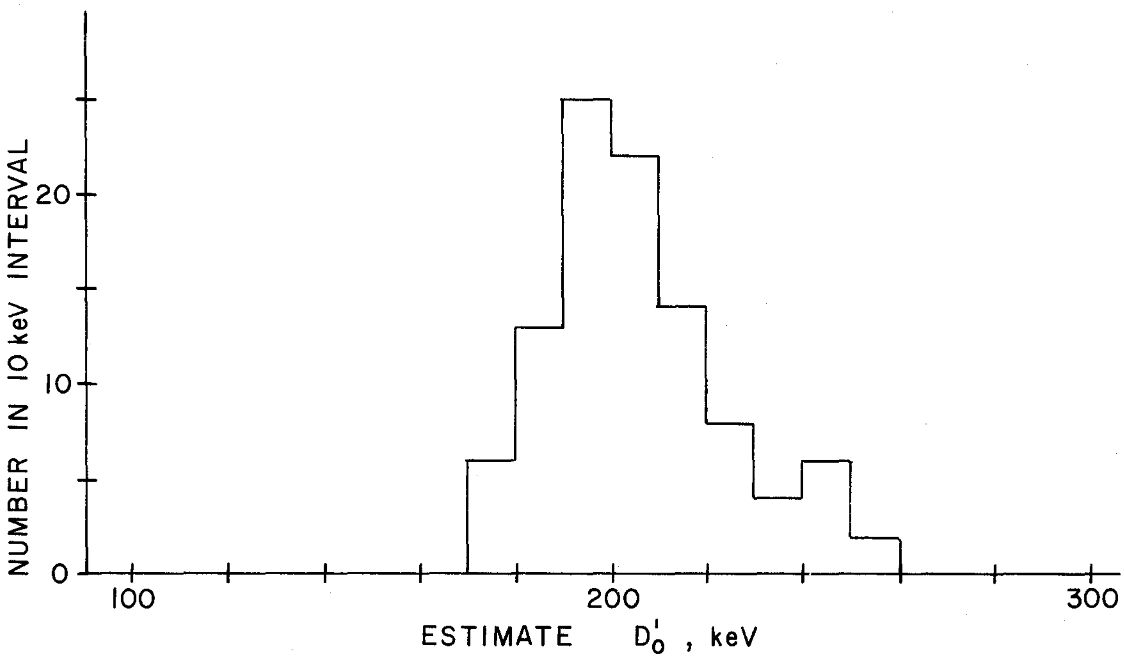


FIGURE 16
HISTOGRAM OF ESTIMATES FOR 80 SPACINGS

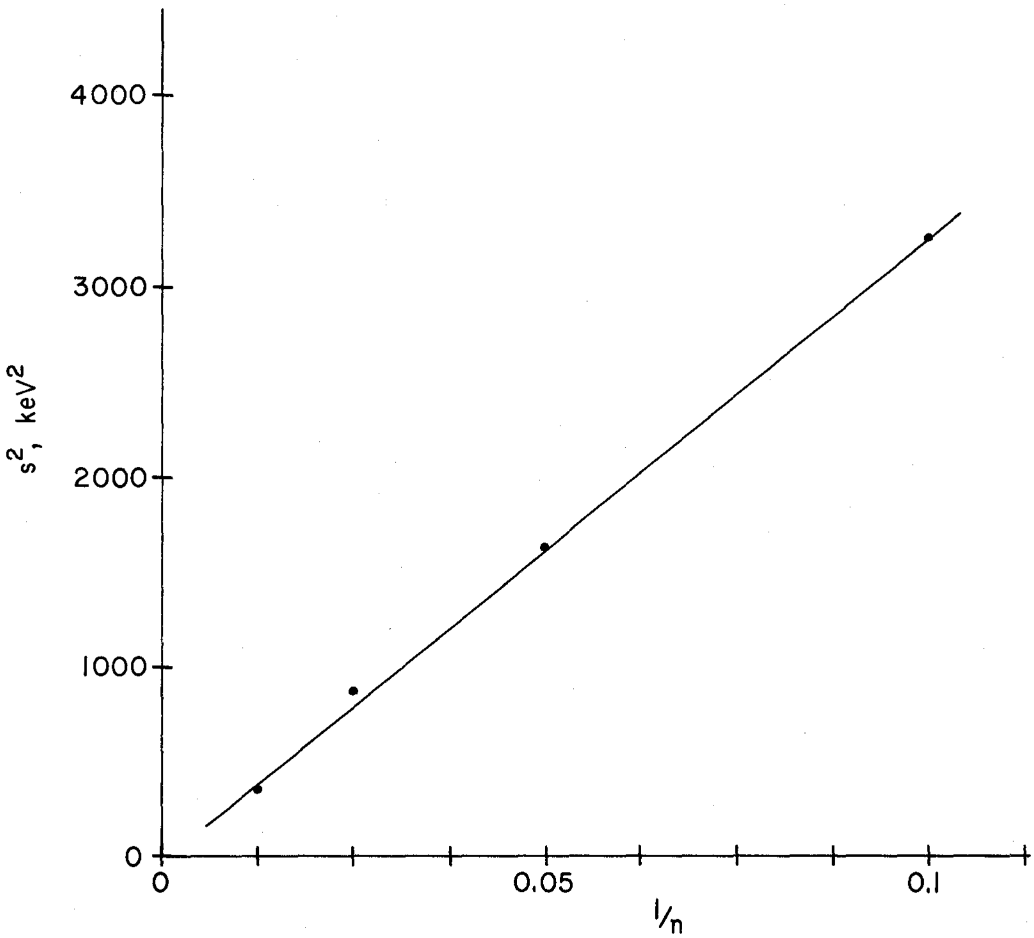


FIGURE 17
SAMPLE VARIANCE FOR DIFFERENT n

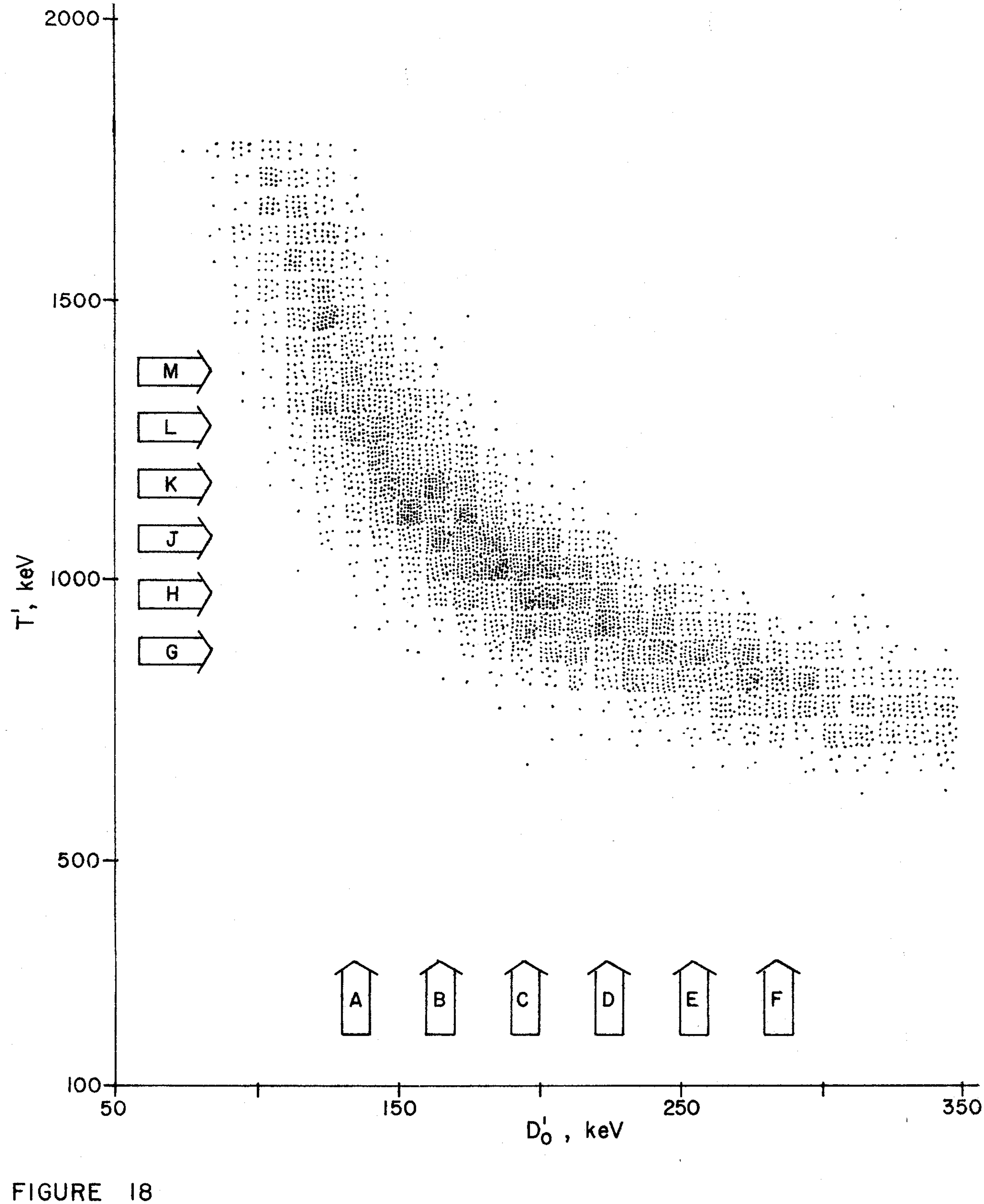


FIGURE 18
SCATTER PLOT FOR JOINT ESTIMATES $D'_0$ AND T'

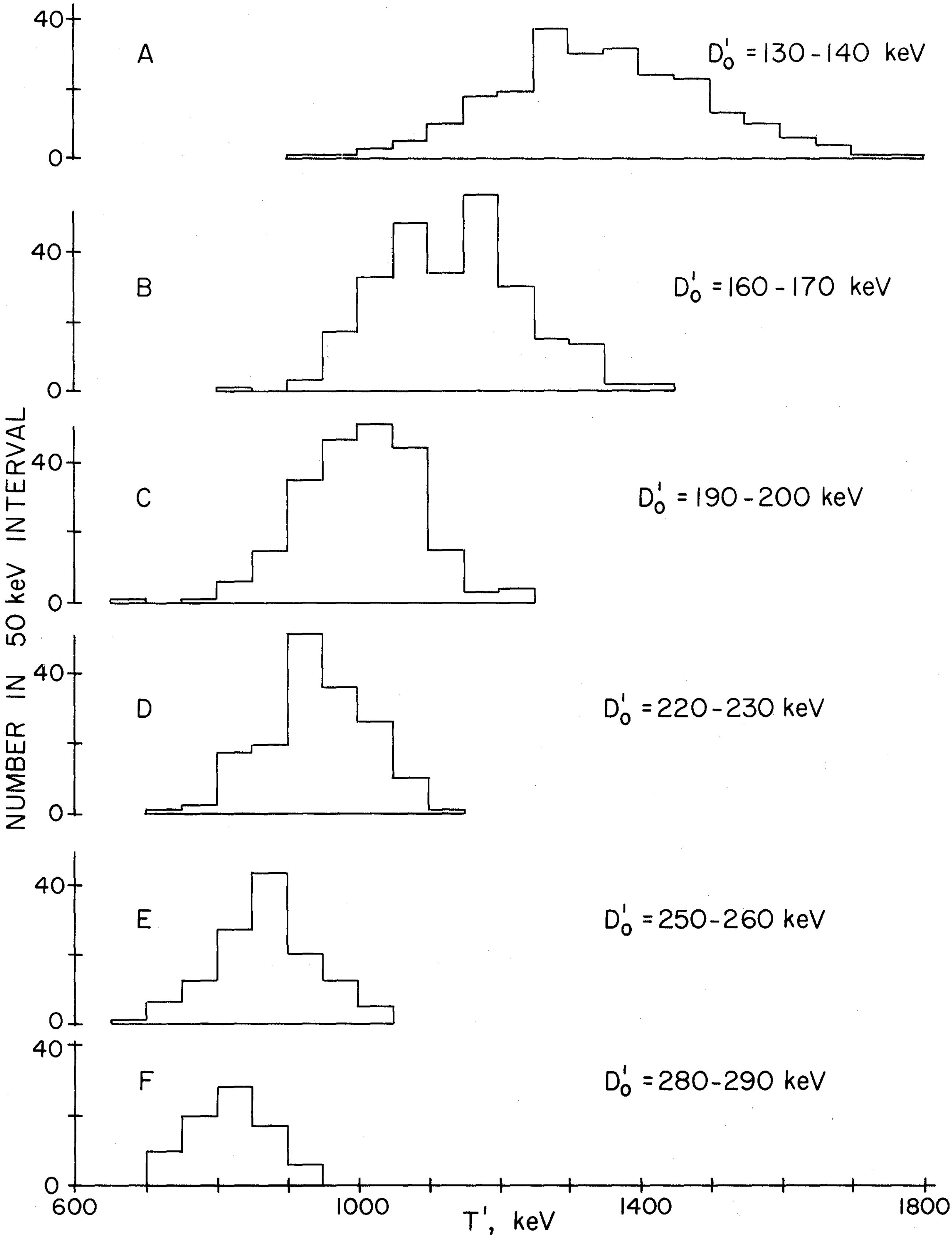


FIGURE 19. CROSS SECTIONS OF FIGURE 18

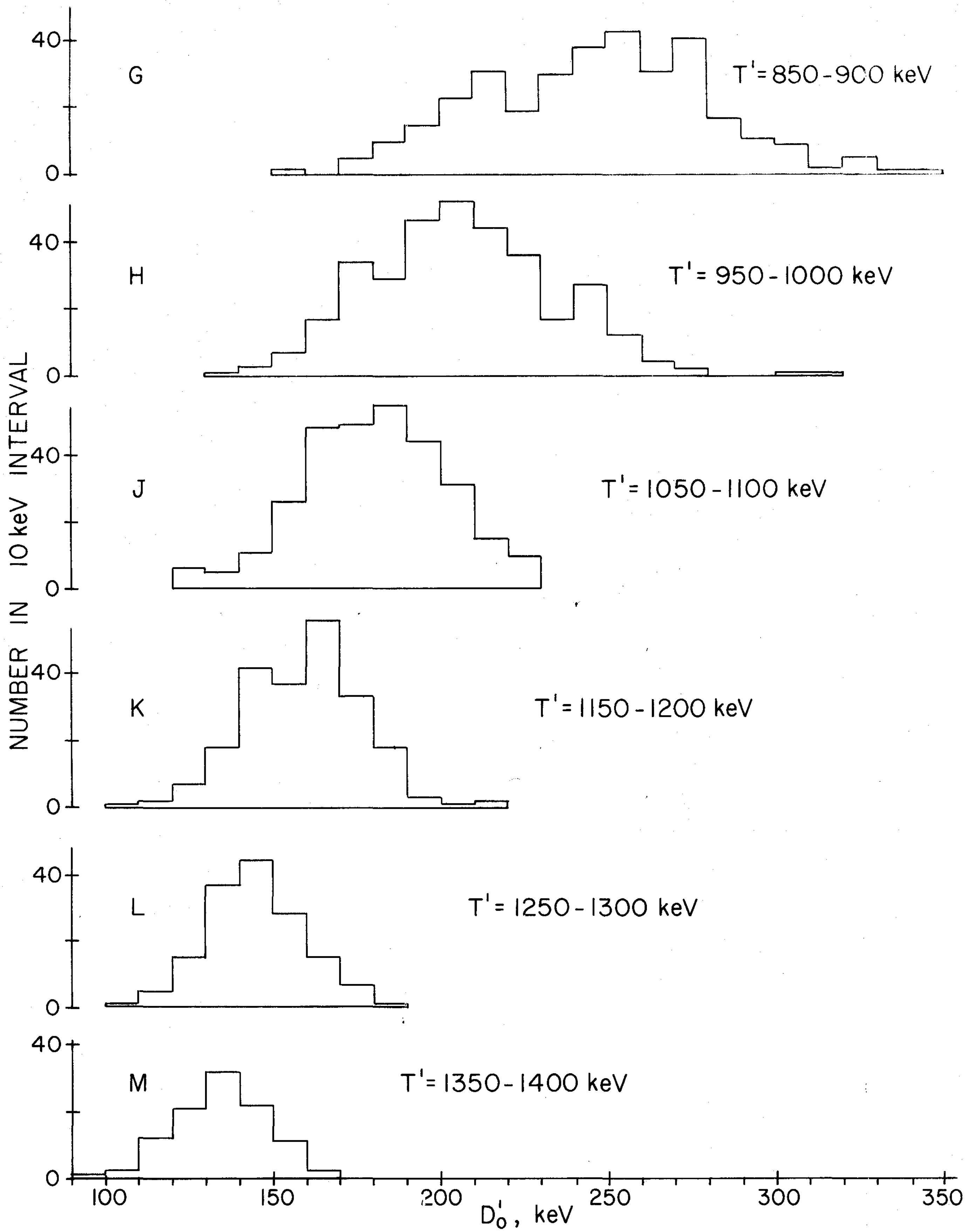


FIGURE 20. CROSS SECTIONS OF FIGURE 18

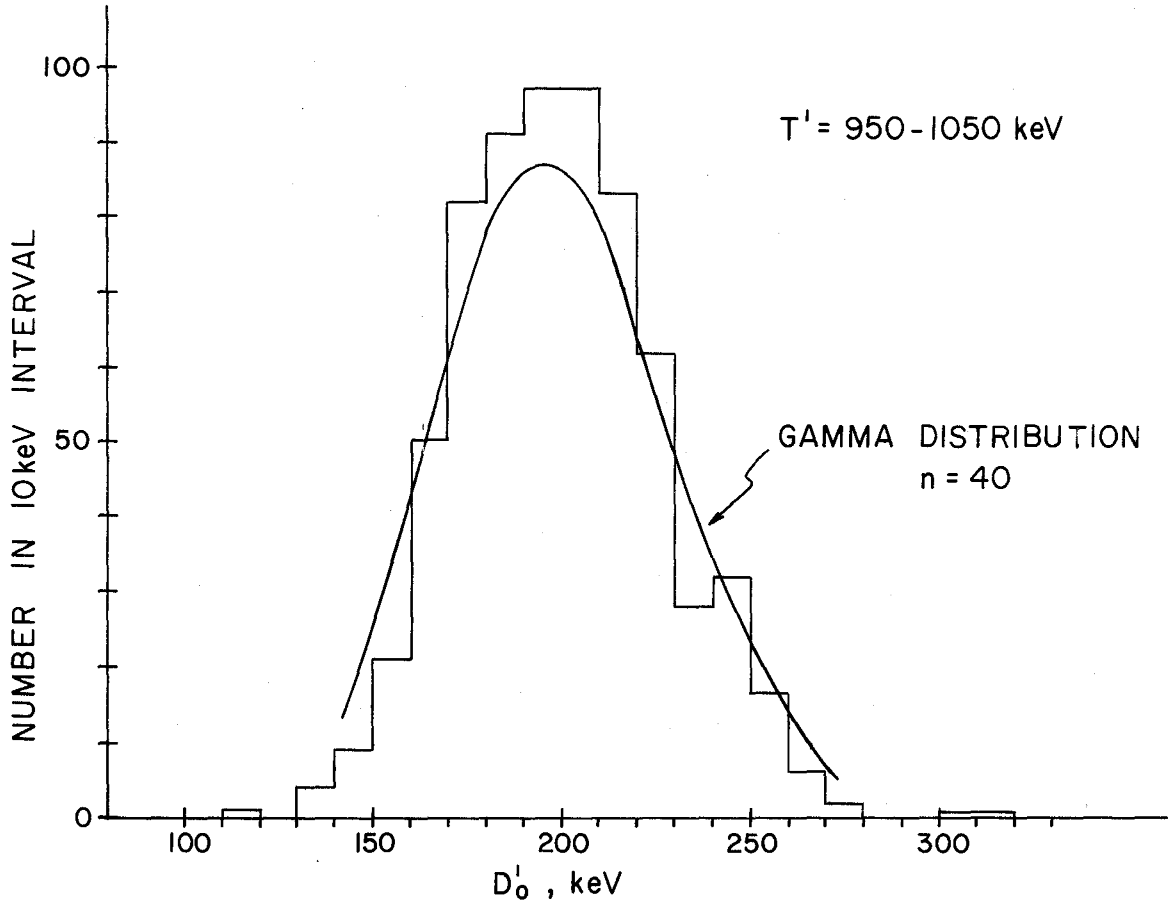


FIGURE 21
HISTOGRAM OF ESTIMATES $D_o'$ (SEE FIGURE 18)

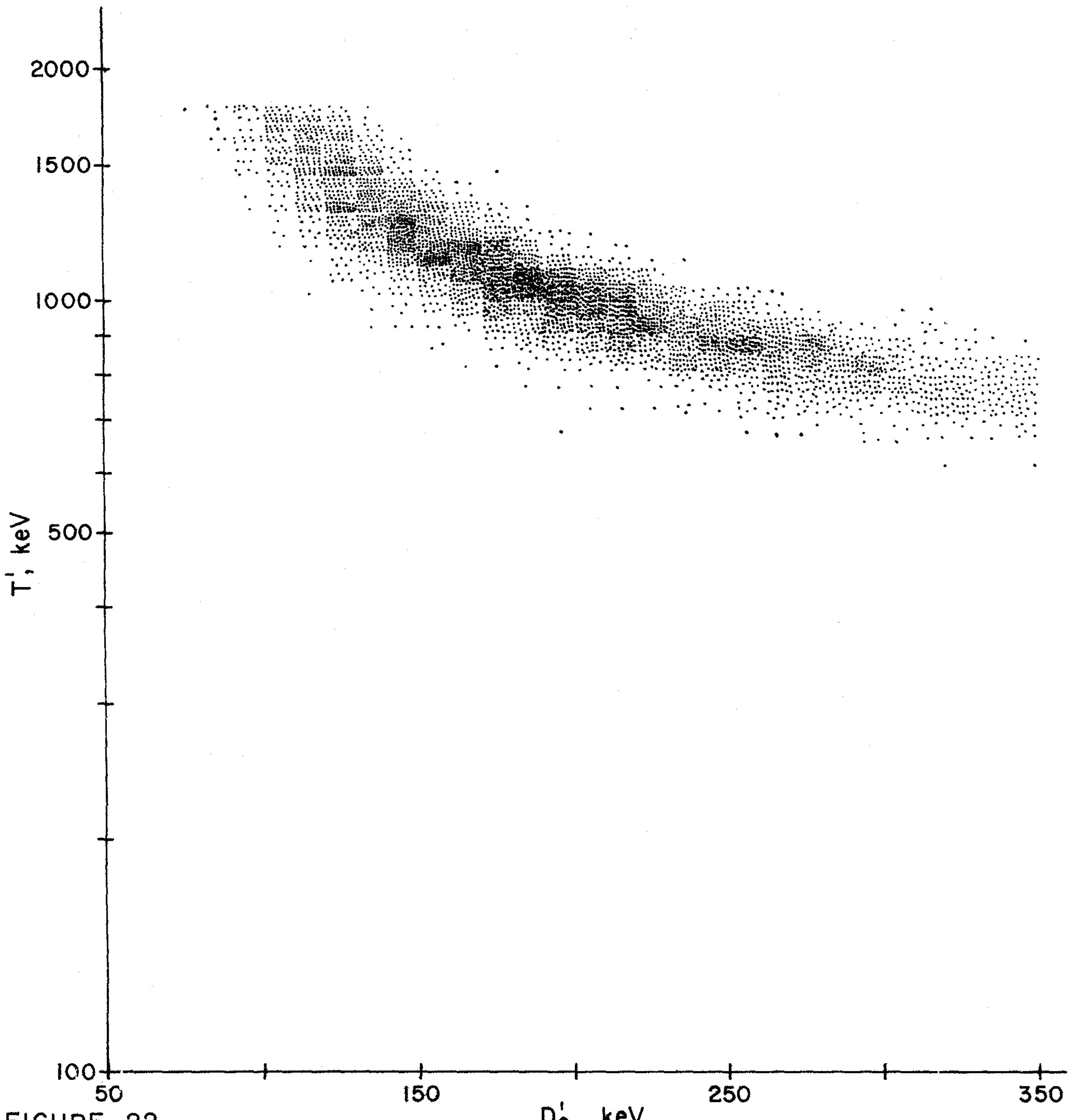


FIGURE 22
SCATTER PLOT FOR JOINT ESTIMATES $D_0'$ AND $T'$

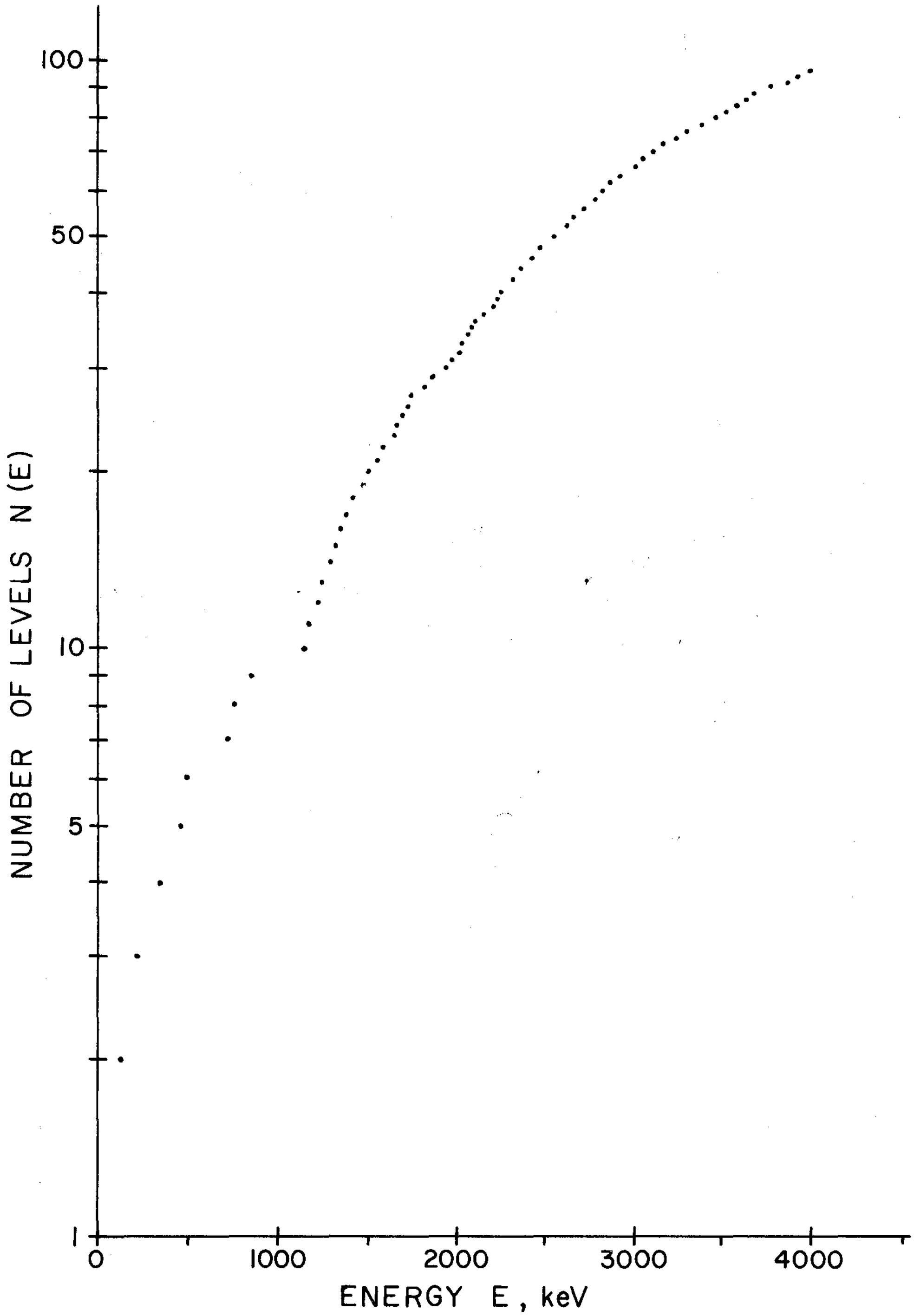


FIGURE 23
N(E) - E CURVE FOR $Mn^{56}$

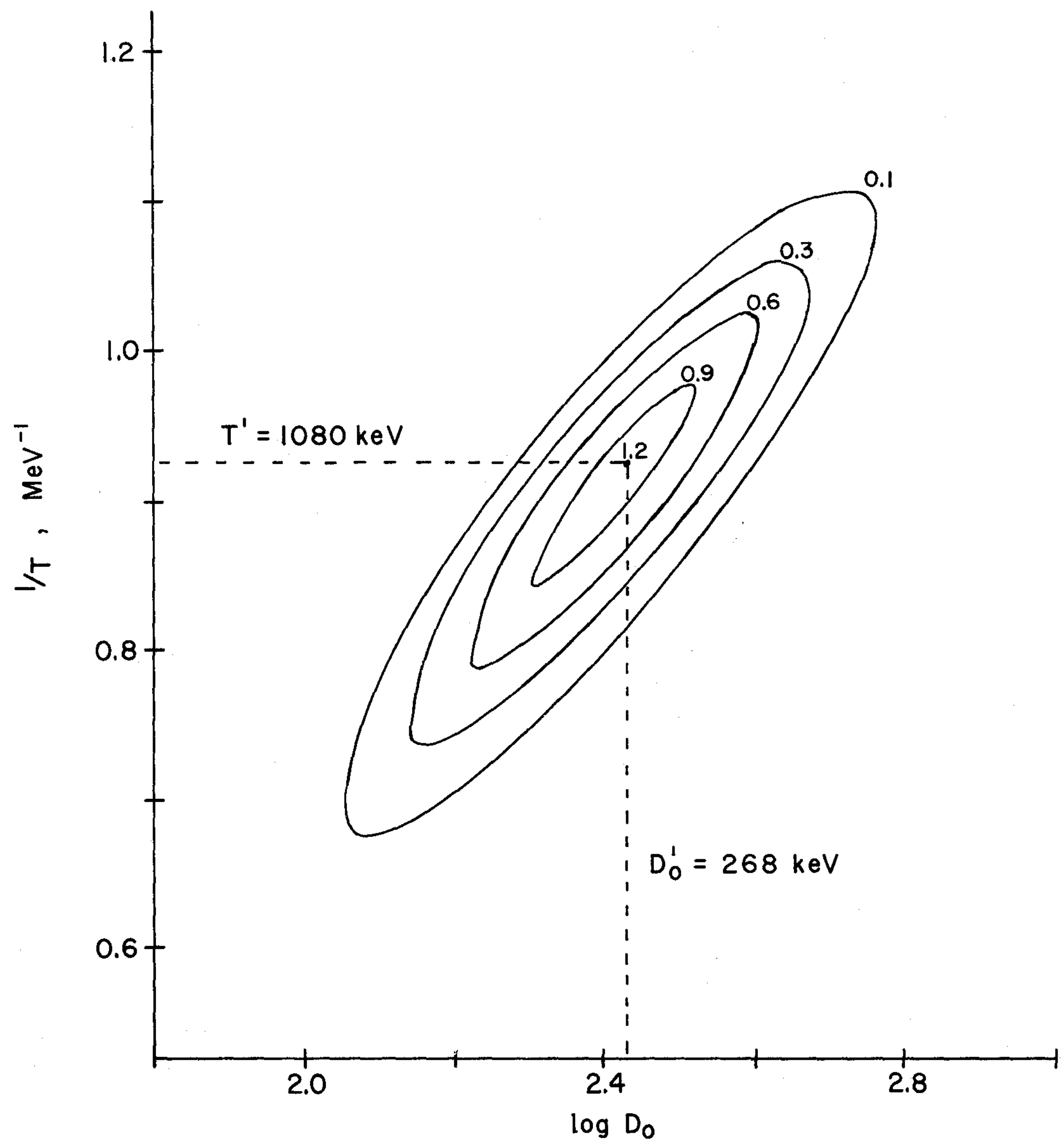


FIGURE 24
CONTOURS OF CONSTANT LIKELIHOOD FOR $Mn^{56}$