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SESSION I

Chairman : Mr ROSSI

OPENING OF THE SYMPOSIUM

- |               |  |    |
|---------------|--|----|
| Miss T. ALPER | Mechanisms of lethal radiation damage to cells.  | 5  |
| G.J. NEARY    | The interpretation of survival curves in relation to radiation quality and cellular repair mechanisms. | 51 |

SESSION II

Chairman : Mr ALLISY

- |                                 |   |     |
|---------------------------------|---|-----|
| G.W. BARENDSEN                  | Local energy density requirements for biological radiation damage and their modification by environmental conditions. | 83  |
| A.M. KELLERER                   | Analysis of patterns of energy deposition.  | 107 |
| K.S.J. WILSON and<br>S.B. FIELD | Further measurements of LET spectra with a 10 cm spherical Rossi counter.   | 137 |

SESSION III

Chairman : Mr POLVANI

- |                                   |   |     |
|-----------------------------------|---|-----|
| S. SRDOČ                          | Dose distribution in small tissue equivalent volumes.   | 153 |
| B. HOGEWEG and<br>G.W. BARENDSEN  | Distribution of energy deposition by gamma-rays and 15 MeV neutrons in cylindrical volumes.   | 171 |
| A. ALLISY and<br>Mrs M. BOUTILLON | Distribution de l'énergie déposée par des neutrons à l'intérieur d'ellipsoïdes de révolution. | 183 |

SESSION IV

Chairman : Mr BARENSEN

J.F. FOWLER	Variation of RBE values and OER for complex heavy particle spectra.	
E.W. EMERY	Wall-less counters and the lines of their future development.	219
K.S.J. WILSON	Preliminary measurements with a cylindrical wall-less counter.	235

SESSION V

Chairman : Mr JACOBI

W. GROSS	Microdosimetry of directly ionizing particles with wall-less proportional counters.	249
U. OLDENBURG and J. BOOZ	Wall effects of spherical proportional counters.	269
R. KATZ	Randomness.	283

SESSION VI

Chairman : Mr HARDER

H.H. ROSSI	Experimental limitations of microdosimetry.	303
B. DAY	Development of a lightweight robust LET spectrometer.	327
I.J. WILSON	A recombination ionization chamber system as a sensitive three channel LET indicator for stratospheric use.	343

SESSION VII

Chairman : Mr NEARY

J. HANDL and W. KÜHN	Development of a coincidence-counter to measure the absorbed energy inside the cell for beta-emitters deposited in the cellmembrane.	363
J.E. TURNER, R.D. BIRKHOFF, V.E. ANDERSON, H.A. WRIGHT, E.B. WAGNER and W.H. SHINPAUGH	Monte Carlo method of determining LET spectra from pulse-height measurements.	373
L.G. BENGTSSON	Assessment of dose equivalent from fluctuations of energy deposition.	375

SESSION VIII

Chairman : Mr BERGER

J.P. PATAU, D. BLANC, J. MATHIEU and G. MASON	Transport simulé d'électrons de 2 MeV dans divers matériaux.	401
J. MATHIEU, D. BLANC, J. CASANOVAS, Mrs A. DUTREIX, A. WAMBERSIE and Miss M. PRIGNOT	Mesure de la répartition de la dose déposée en profondeur dans un fantôme de plexiglas irradié par un faisceau d'électrons monocinétiques de 10, 15, 20 ou 30 MeV.	437
T.E. BURLIN and R.J. SNELLING	The application of general cavity ionization theory to the dosimetry of electron fields.	455

SESSION IX

Chairman : Mr BLANC

D. FRANKENBERG	Determination of the energy loss for an inelastic collision of fast electrons in water.	479
J.A. DENNIS	The variation of W with the energy of heavy ions.	493

SESSION X

Chairman : Mrs PARMENTIER

H. BICHSEL	Quantum mechanical bound state corrections to the $1/E^2$ collision spectrum.	511
M. MARSHALL, J.A.B. GIBSON and P.D. HOLT	The stopping power of low energy electrons in biological materials.	529
M.J. BERGER	Spectrum of energy deposited by electrons in spherical regions.	541

SESSION XI

Chairman : Mr KELLERER

D. HARDER	Some general results from the transport theory of electron absorption.	567
H.J. SCHULZ and D. HARDER	Aufbau des Sekundärelektronenspektrums bei energiereicher Elektronenstrahlung.	595
H. PARETZKE und G. BURGER	Spatial distribution of deposited energy along the path of heavy charged particles.	631

SESSION XII

Chairman : Mr BOOZ

R. KATZ	Particle tracks in emulsion.	615
J.W. BAUM	Comparison of distance- and energy-restricted linear energy transfer for heavy particles with 0.25 to 1000 MeV/AMU.	653

SESSION XIII

Chairman : Mr CASNATI

- Mrs N.C. PARMENTIER,  
M. CHEMTOB,  
D. CHMELEVSKY and  
J.C. CHIANELLI
- Essais de quelques techniques applicables à la microdosimétrie de particules chargées. 667
- P.R.J. BURCH
- Track structure in relation to target structure. 685
- W. JACOBI and  
J. HACKE
- Mikrodosimetrische Folgerungen aus Leitfähigkeitsmessungen in gamma-bestrahlten dielektrischen Flüssigkeiten. 715

SESSION XIV

Chairman : Miss ALPER

- J. BOOZ
- Interpretation of radiobiological effects with microdosimetry. 737
- J.J. BROERSE,  
L.M. VAN PUTTEN and  
G.W. BARENSEN
- The relation between mouse lethality and energy deposition by secondary particles from neutrons and X-rays. 761
- J. KIEFER
- Some theoretical considerations concerning ultra-high dose rate survival experiments. 779

SESSION XV

Chairman : Mr FOWLER

- H.H. ERTL and  
L.E. FEINENDEGEN
- Microdosimetry of iodine-125 with reference to the Auger effect. 787
- B. MARKUS
- Electron degradation and biological effects. 801
- H. KRÜGER
- Tiefenabhängigkeit der LET-Spektren für schnelle Neutronen in einem menschlichen Rumpfphantom. 813
- J.F. FOWLER
- CONCLUSIONS AND CLOSING OF THE SYMPOSIUM. 835

ANNEX I

A.M. KELLERER and  
H.H. ROSSI

Summary of quantities and functions  
employed in microdosimetry.

841

ANNEX II

List of participants.

855

## ANALYSIS OF PATTERNS OF ENERGY DEPOSITION

### A Survey of Theoretical Relations in Microdosimetry

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and Rad. Res. Lab. Columbia University, New York.*

*Abstract: The microscopic patterns of energy deposition by ionizing radiation are described by ROSSIs probability distributions of specific energy,  $z$ . Theoretical derivation and analysis of the microdosimetric functions is based on the concepts of probability theory. These concepts are outlined, some theoretical relations of practical import are listed, and existing computational techniques are referred to.*

## I N T R O D U C T I O N

Historically microdosimetry has originated from the attempt to determine LET distributions or fluence distributions of charged particles from pulse height spectra observed in proportional counters. While this attempt has been only partly successful, it was soon realized that the experimental spectra are of interest in themselves, and of direct applicability to radiobiology. It has been for this reason that H.H.ROSSI and his coworkers started to inquire the distributions of energy imparted to microscopic volumes. The present paper compiles some of the more important properties of these probability distributions. The survey is based on the definitions and terminology presented in the proceedings of this conference<sup>1</sup>. It is intended to provide an easy orientation, and no claim for completeness is made. For brevity some of the material is presented without detailed explanations, and proofs for some of the theoretical statements have to be omitted.

Probability theory is the tool of theoretical microdosimetry. The monographs by FISZ<sup>2</sup>, FELLER<sup>3</sup>, or GNEDENKO<sup>4</sup> as well as any other standard textbook on probability may be used for reference to the concepts of distributions, their moments, their characteristic functions, and their semi-invariants.

There is every reason to assume that radiation fields which produce the same spatial patterns of energy deposition also

produce the same biological effects. It further appears that there is essentially a one-to-one relation between the spatial patterns of energy deposition and the set of probability distributions  $f_1(z)$  for a region of given shape but varying size. Theoretically it should therefore be possible to reconstruct spatial patterns of energy deposition from a set of distributions  $f_1(z)$ . One may, conceptually, subdivide a block of tissue into infinitesimal elements each small enough to contain at most one ionization. The number of possible permutations of a given number of ionizations into these cells is finite. For each assumed permutation one can calculate the set of functions  $f_1(z)$ . Consequently one can select the permutations with minimal difference of these functions to a given set of distributions. Due to the enormous number of possible permutations the method is, of course, entirely impracticable. It indicates, however, that there is, at least in principle, a way back from the microdosimetric functions to the actual patterns of energy deposition. The question whether an operational method can be found to reconstruct the spatial patterns of energy deposition from the distributions  $f_1(z)$  is one of the interesting open problems of microdosimetry. If such a method existed it would strongly support the present system of microdosimetric functions. If it did not, one may have to look for more appropriate ways to describe the microscopic patterns of energy distribution.

As yet there is no technique to extract all information contained in the distributions  $f_1(z)$ . Consequently it is also not possible to calculate the distributions for a non-spherical region from those determined in spheres. Neither is it possible to calculate the joint distributions for adjacent regions if the distributions are known for the individual regions. Knowledge of the mechanisms of radiation action and of the sensitive sites in the cell is still too spurious to warrant extensive model building involving hypothetical critical regions and their z-distribution. There are, however, certain experimental findings which even now require the application of z-distributions other than those belonging to individual spherical regions<sup>5</sup>. Experimental determination of the distributions for all cases of possible interest would lead to an unmanageable pile-up of data. It is for this reason that one has to go back to the fluence distribution of charged particles associated with a radiation field. Knowing the collision cross sections one can in principle calculate all distributions of imparted energy which may be needed. Accordingly the following survey will first deal with the general properties of specific energy,  $z$ , and its distributions. Then the derivation of the distributions for a given radiation field is discussed. Finally some of the methods will be mentioned which have to be employed if LET distributions or fluence distributions are to be derived from observed z-distributions.

## A. GENERAL PROPERTIES OF MICRODOSIMETRIC QUANTITIES

### 1. The random variable, specific energy, $z$ .

The specific energy,  $z$ , is defined as the energy imparted to a specified region by ionizing particles divided by the mass of that region. There is no statement about the precise energy value above which a charged particle is called ionizing. Consequently the cut-off energy below which further degradation of energy is not considered is left open; it may lie somewhere between 1eV and 30eV. In addition there is some question whether a portion of the imparted energy should be altogether excluded from the bookkeeping<sup>6</sup>. Fortunately the freedom in the definition of  $z$  does not affect the distributions of  $z$  too strongly except for extremely small volumes. Electrons up to 30eV have a range short as compared to the dimension of volumes for which microdosimetric functions are presently available. The choice of the exact cut-off level below which a further spatial degradation of energy is neglected is therefore irrelevant. The second ambiguity is more serious. If one derives  $z$ -distributions by looking only at a fraction of the absorbed energy, the distributions may appreciably change. The change is, however, small if one deals with energies much larger than the  $w$ -value of the events which are taken into account. If, for example, one counts ionizations in gas, one should (with appropriate correction for the multiplication statistics) obtain dependable spectra at  $z$ -values which correspond to more than 100eV. For lower energies the definition of  $z$  is indeed critical.

### 2. Distributions of specific energy

$f(z;D)$  is the probability density (differential distribution) of  $z$ . The corresponding sumdistribution is  $F(z;D)$ . The value of  $F(z;D)$  is equal to the probability that the specific energy is not larger than  $z$  at dose  $D$ ; it is also equal to the probability that a dose larger than  $D$  is needed to reach the value  $z$  of specific energy:

$$F(z;D) = P(\underline{z} \leq z; D) = P(\underline{D} > D; z) \quad (1)$$

Thus  $F(z;D)$  is a distribution with regard to both  $z$  and  $D$ . One must note, however, that  $f(z;D)$  does not have this double property; it is not the probability density for the dose  $D$  needed to reach the value  $z$ . For a discussion of the latter function and its application to radiobiology data see<sup>7</sup>. The distributions  $f(z;D)$  or  $F(z;D)$  need not be derived experimentally, they can be calculated from the single event distribution  $f_1(z)$  as discussed in section C and E.

The single event distribution  $f_1(z)$  and the corresponding sum distribution  $F_1(z)$  are commonly derived from pulse height spectra observed in proportional counters. The pulse height spectra are broadened due to the fluctuations in the number of ion pairs produced by a certain energy and in addition by the multiplication statistics of the counter. These two stochastic factors can, however, to a first approximation be neglected in comparison to the genuine fluctuations of energy deposition (see section D). Moreover the resolution error can be eliminated from the spectra (see section E).

Theoretical derivation of  $f_1(z)$  involves LET distribution, cord length distribution in the volume of interest, and straggling distributions. In general the interplay of these statistical factors is complicated, and there is no unified approach. A special case is that of heavy charged particles and large mean energy losses. There the particle tracks may be treated as straight continuous lines of energy deposition, and straggling may be neglected (see CASWELL<sup>8</sup>). Another special case is that of a region small as compared to the range of the charged particles which are considered, but not much smaller than  $1\mu\text{m}$  in diameter so that delta-ray effects are not prominent. Then the particle segments can be treated as straight lines of constant LET (see<sup>7,9</sup>). Straggling is then the central problem. With very small volumes the delta-ray

problem becomes exceedingly complicated. Monte Carlo calculations of delta-ray tracks and experiments with wall-less proportional counters must then be used.

### 3. Related quantities

The distributions of specific energy are the basic microdosimetric functions. The random variable  $y$  and its distributions are useful for certain comparisons to LET theory. They are, however, so closely connected to  $z$  and its distributions, that they need not be separately discussed here. The same is true for the distributions of energy in  $z$  or  $y$  (see<sup>1</sup>). The moments of the  $z$ -distributions, however, are additional quantities of great practical importance, and must therefore be mentioned here.

Absorbed dose,  $D$ , is equal to the mean value,  $\bar{z}$ , of specific energy. In a radiation field or in a material with significant gradients on a microscopic scale  $D$  is defined as the limit of  $\bar{z}$  as the volume surrounding the point of interest shrinks to zero.

The frequency mean,  $\bar{z}_F$ , of  $f_1(z)$  determines the mean number,  $D/\bar{z}_F$ , of absorption events at dose  $D$ . The probability for exactly  $\nu$  events is:

$$p(\nu) = e^{-D/\bar{z}_F} \cdot (D/\bar{z}_F)^\nu / \nu! \quad \text{with } \bar{z}_F = \int_0^\infty z \cdot f_1(z) dz \quad (2)$$

The 'energy mean',  $\bar{z}_D$ , of  $f_1(z)$  determines the mean square deviation,  $\sigma^2$ , of specific energy from its mean value, the absorbed dose,  $D$ :

$$\sigma^2 = \bar{z}_D \cdot D \quad \text{with } \bar{z}_D = \int_0^\infty z^2 f_1(z) dz / \bar{z}_F \quad (3)$$

The relative variance of  $z$  (or of imparted energy) is therefore equal to  $\bar{z}_D/D$ . These relations are special cases of the formulae derived in section C.

If one approximates the energy absorption process by equal and statistically independent energy absorption events (pure Poisson process, i.e.  $f_1(z)$  is assumed to be a Dirac delta function) and if one wants to obtain the correct mean square fluctuations of energy deposition then one must choose the event size  $\bar{z}_D$ . If on the other hand one wants the right frequency of absorption events one must choose the event size  $\bar{z}_F$ . Both quantities may differ by an order of magnitude,  $\bar{z}_D$  being always larger. This indicates the inadequacy of any model assuming pure Poissonian statistics.

## B. AUXILIARY RELATIONS

### 1. Moments

In this and the following paragraphs relations are given for continuous random variables. For discrete type variables the integration has to be substituted by summation over all jump points. Integration or summation is understood to extend over the full range of the random variable whenever the limits 0 to  $\infty$  are given. The random variable is denoted by  $x$ , its distribution by  $f(x)$ .

The moment of order  $\kappa$  is the expectation value of  $x^\kappa$ :

$$m_\kappa = \overline{x^\kappa} = \int_0^\infty x^\kappa \cdot f(x) dx \quad (4)$$

The moments with respect to the mean are called central moments:

$$\mu_\kappa = \overline{(x-\bar{x})^\kappa} \quad (5)$$

The second central moment is also called variance,  $\sigma^2 = m_2 - m_1^2$ . The third central moment is equal to  $m_3 - 3m_1 \cdot m_2 + 2m_1^3$ .

## 2. Characteristic functions

The characteristic function of a random variable,  $x$ , is the expectation value of  $e^{itx}$ . Except for a constant factor it is equal to the Fourier transform of the distribution  $f(x)$ . The characteristic function will be designated by the Greek letter corresponding to the Roman letter used for the distribution:

$$\phi(t) = \overline{e^{itx}} = \int_0^{\infty} e^{itx} \cdot f(x) dx \quad (6)$$

Expanding  $e^{itx}$  into a power series:

$$e^{itx} = \sum_{v=0}^{\infty} \frac{(itx)^v}{v!}, \quad (7)$$

one can express  $\phi(t)$  in terms of the moments:

$$\phi(t) = \sum_{v=0}^{\infty} \frac{m_v}{v!} \cdot (it)^v \quad (8)$$

## 3. Convolution

If a random variable is the sum of two statistically independent random variables distributed according to  $f(x)$  and  $g(x)$  then the distribution of this sum is the result of the convolution operation:

$$h(x) = \int_0^x f(x-x') g(x') dx' \quad (9)$$

This operation is commonly abbreviated by  $f(x) * g(x)$ . The characteristic function (the same holds true for related transformations as for example the Laplace transform) is of great practical significance because it reduces the convolution to a mere multiplication. If  $\eta(t)$ ,  $\phi(t)$ , and  $\gamma(t)$  are the characteristic functions belonging to  $h(x)$ ,  $f(x)$ , and  $g(x)$  one has:

$$\eta(t) = \phi(t) \cdot \gamma(t) \quad (10)$$

If one considers the logarithm of the characteristic function:

$$\ln \eta(t) = \ln \phi(t) + \ln \gamma(t) \quad (11)$$

One may expand  $\ln \phi(t)$  into a power series:

$$\ln \phi(t) = \sum_{v=1}^{\infty} \frac{\kappa_v}{v!} (it)^v \quad (\phi(0)=1 \text{ therefore } \kappa_0=0) \quad (12)$$

The coefficients,  $\kappa_v$ , are called semi-invariants. They are important because they are simple combinations of the moments, and according to equ.(11) they add in a convolution.

#### 4. Relations between the moments, the central moments, and the semi-invariants.

Comparison of the coefficients in equ.(8) and (12) leads to the following relations between the moments and the semi-invariants:

$$\begin{aligned} \kappa_1 &= m_1 \\ \kappa_2 &= m_2 - m_1^2 = \sigma^2 \\ \kappa_3 &= m_3 - m_1 \cdot m_2 + 2m_1^2 = \mu_3 \\ \kappa_4 &= m_4 - 3m_2^2 - 4m_1 \cdot m_3 + 12m_1^2 \cdot m_2 - 6m_1^4 = \mu_4 - 3\mu_2^2 \end{aligned} \quad (13)$$

The inverse relations are:

$$\begin{aligned} m_2 &= \kappa_2 + \kappa_1^2 \\ m_3 &= \kappa_3 + 3\kappa_1 \cdot \kappa_2 + \kappa_1^3 \\ m_4 &= \kappa_4 + 3\kappa_2^2 + 4\kappa_1 \cdot \kappa_3 + 6\kappa_1^2 \cdot \kappa_2 + \kappa_1^4 \end{aligned} \quad (14)$$

In practical cases one may use the mean and three dimensionless parameters to characterise a distribution. The parameters are the relative variance,  $V$ ; the skewness,  $SK$ ; and the kurtosis,  $K$  (sometimes called peakedness):

$$\begin{aligned}
 V &= \sigma^2 / \bar{X}^2 = \kappa_2 / \kappa_1^2 = m_2 / m_1^2 - 1 \\
 SK &= \mu_3 / \sigma^3 = \kappa_3 / \kappa_2^{1.5} \\
 K &= \mu_4 / \sigma^4 = \kappa_4 / \kappa_2^2 + 3
 \end{aligned}
 \tag{15}$$

For normal distributions the so-called resolution, R, is often used. It is defined as fractional width at half of the maximum value, and it is related to V by:

$$R = 2.77 \cdot \sqrt{V} \tag{16}$$

### C. THE DOSE DEPENDANT z-DISTRIBUTIONS AS FUNCTIONS OF THE SINGLE EVENT SPECTRUM

The central mathematical problem in microdosimetry is the compound Poisson process. The term Poisson process implies that a random variable is the sum of statistically independent increments. The word compound (or mixed) signifies that the size of the increments is not constant but is itself a random variable. The distribution of event size is called spectrum of the Poisson process.

The distributions  $f(z;D)$  are a result of a Poisson process with the spectrum  $f_1(z)$ :

$$f(z;D) = \sum_{v=0}^{\infty} e^{-n} \frac{n^v}{v!} \cdot f_1^{*v}(z) \tag{17}$$

where  $n=D/\bar{z}_F$  is the mean event number at dose D, and  $f_1^{*v}(z)$  is the v-fold convolution product of  $f_1(z)$ . The term  $e^{-n} \cdot n^v / v!$  is the Poissonian probability for the occurrence of exactly v events, and  $f_1^{*v}(z)$  is the distribution of z under the condition that exactly v events have occurred.

In section C.3 it will be shown that the straggling distributions are also solutions of a compound Poisson process. The following considerations are therefore also to be applied to the straggling problem.

Transforming the distributions  $f(z;D)$  and  $f_1(z)$  into their characteristic functions  $\phi(t;D)$  and  $\phi_1(t)$  one obtains the transformed equ. (17):

$$\phi(t;D) = \sum_{v=0}^{\infty} e^{-n} \frac{n^v}{v!} \cdot \phi_1^v(t) = e^{-n} \cdot e^{n\phi_1(t)} = e^{n(\phi_1(t)-1)} \quad (18)$$

and hence:

$$\ln \phi(t;D) = n(\phi_1(t)-1) \quad (19)$$

If  $\kappa_v(D)$  are the semi-invariants of  $f(z;D)$  and if  $m_v$  are the moments of  $f_1(z)$  then according to equ.(8), (12), and (19):

$$\sum_{v=1}^{\infty} \frac{\kappa_v(D)}{v!} (it)^v = n \cdot \sum_{v=1}^{\infty} \frac{m_v}{v!} (it)^v \quad (20)$$

and since this relation holds identical in  $t$ , one has:

$$\kappa_v(D) = n \cdot m_v \quad (21)$$

This important relation says that in a compound Poisson process the semi-invariants of the solutions are equal to the product of the mean event number times the moments of the spectrum of the Poisson process:

If one substitutes the mean event number by  $D$ :

$$n = D/m_1 = D/\bar{z}_F \quad (22)$$

one obtains the following relations for the variance, relative variance, skewness, and kurtosis of the distribution  $f(z;D)$ :

$$\sigma^2 = D \cdot m_2 / m_1 = \overline{z_D} \cdot D \quad (23)$$

$$V = \sigma^2 / D^2 = \overline{z_D} \cdot D^{-1}$$

$$SK = m_1^{0.5} \cdot m_2^{-1.5} \cdot m_3 \cdot D^{-0.5}$$

$$K = m_1 \cdot m_2^{-2} \cdot m_4 \cdot D^{-1} + 3$$

For a given distribution  $f_1(z)$  the dose dependant distributions  $f(z;D)$  are derived numerically. The relations between the characteristics  $V$ ,  $SK$ , and  $K$  of  $f(z;D)$  and the moments of  $f_1(z)$  provide an easy check of accuracy for the numerical calculations. The computational techniques for the solution of the compound Poisson process are referred to in section E.

#### D. FACTORS RELEVANT TO THE SINGLE EVENT SPECTRUM $f_1(z)$

As mentioned in section 2.1 the single event spectrum reflects various stochastic factors. Accordingly there is no general formula for  $f_1(z)$  as a function of the charged particle fluence spectrum and the shape of the volume of interest. The problem has to be treated with analytic or numerical techniques appropriate to each individual case.

In the derivation or in the analysis of the spectrum  $f_1(z)$  one can often start with simplified assumptions, and then account for the deviations from the idealized model by corrections. The most important idealized cases are:

a) One deals with heavy charged particles, and the mean diameter,  $\bar{l}$ , of the volume of interest is large as compared to the maximal range of delta-rays. In this case straggling can be neglected and the tracks of the heavy charged particles can be considered as straight lines. The derivation of  $f_1(z)$  is reduced to the calculation of the distribution of initial energies of heavy charged particles, and to the geometrical problem of intersecting the resulting straight tracks with

the region of interest. For further details one may refer to the detailed treatment given by CASWELL<sup>8</sup>.

b) The mean diameter,  $\bar{\lambda}$ , of the volume of interest is large as compared to the maximal range of delta-rays, but small as compared to the ranges of the primary charged particles. Though this case is hardly ever realized it has been taken as the principal model for the derivation of LET-spectra from measured pulse height distributions. The case is also of interest because it reflects one aspect of the more general treatment mentioned in the next paragraph.

In the following the sum distribution  $F_1(E)$  and the density  $f_1(E)$  of energy,  $E$ , imparted in single absorption events will be used instead of the distributions  $F_1(z)$  and  $f_1(z)$  of specific energy,  $z$ . This is merely done to avoid trivial conversion factors. The LET sum distribution in tracklength is called  $T(L)$ , the corresponding density is called  $t(L)$ . The sumdistribution of cord-length,  $\lambda$ , is  $C(\lambda)$ , the corresponding density  $c(\lambda)$ . Then the sumdistribution of energy deposition in single absorption events is:

$$F_1(E) = \int_0^{\infty} t(L) \cdot C(E/L) dL \quad (24)$$

and therefore:

$$f_1(E) = \frac{d F_1(E)}{d E} = \frac{d}{dE} \int_0^{\infty} t(L) \cdot C(E/L) dL = \int_0^{\infty} t(L) \cdot c(E/L) \frac{dL}{L} \quad (25)$$

or:

$$f_1(E) \cdot E = \int_{-\infty}^{\infty} t(L) \cdot L \cdot c(E/L) \cdot E/L \cdot d \ln L \quad (26)$$

If one considers the logarithms of the variables  $E, L$ , and  $\lambda$  and designates the probability densities of these logarithms by italics, one has:

$$f_1(\ln E) = \frac{d F_1(E)}{d \ln E} = E \cdot f_1(E)$$

$$t(\ln E) = \frac{dT(L)}{d \ln L} = L \cdot t(L) \quad \text{and} \quad (27)$$

$$c(\ln \lambda) = \frac{d C(\lambda)}{d \ln \lambda} = \lambda \cdot c(\lambda)$$

Thus from equ. (26) one obtains:

$$f_1(\ln E) = \int_{-\infty}^{+\infty} t(\ln L) \cdot c(\ln E - \ln L) d \ln L \quad (28)$$

Thus the distribution of  $\ln E$  is the result of a convolution of the distributions of  $\ln L$  and of  $\ln \lambda$ . This is quite obvious even without formal derivation. The random variable  $E$  is the product of the two statistically independent random variables linear transfer,  $L$ , and cord length,  $\lambda$ . Accordingly the logarithm of  $E$  is the sum of the random variables  $\ln L$  and  $\ln \lambda$ ; hence the convolution integral. From equ. (28) it follows that the non-central moments of  $f_1(E)$  are equal to the product of the non-central moments of  $c(\lambda)$  and  $t(L)$ . Specifically:

$$\bar{E} = \bar{\lambda} \cdot \bar{L}_T \quad \text{and} \quad (29)$$

$$\overline{E^2} = \overline{\lambda^2} \cdot \overline{L^2} \quad \text{or} \quad \bar{E}_D = \bar{\lambda} \cdot \bar{L}_D \quad (30)$$

where  $\bar{E}_D = \overline{E^2} / \bar{E}$  is the dose mean of the event spectrum,  $\bar{L}_D$  the dose mean of LET (see<sup>1</sup>), and  $\bar{\lambda} = \overline{\lambda^2} / \bar{\lambda}$  the analogon of a dose mean for the cord length distribution.

From equ.(21) and (30) one can easily derive the relation between the relative variance of  $f_1(E)$ ,  $t(L)$ , and  $c(\lambda)$ :

$$V_E = V_\lambda \cdot V_{LET} + V_\lambda + V_{LET} \quad (31)$$

This is a relation useful for a rough estimate of the shape of the pulse height spectra. For a sphere one has  $V_{\lambda}=0.125$  (see section D.2). Thus whenever the LET-distribution is not extremely narrow, the relative variance of the single event spectrum in a spherical counter is mainly determined by the relative variance of LET:

$$V_E = 1.125 \cdot V_{LET} + 0.125 \quad (32)$$

For the frequency and the dose mean of the single event spectrum one obtains in this case:

$$\bar{E}_F = \frac{2}{3} \cdot d \cdot \bar{L}_T \quad \text{and} \quad \bar{E}_D = \frac{3}{4} \cdot d \cdot \bar{L}_D \quad (d: \text{ sphere diameter}) \quad (33)$$

Energy straggling which is neglected here can strongly increase the value of  $V_E$  and  $\bar{E}_D$ ; this is discussed in D.3.

Equation (28) can be used to derive the LET-distribution from an observed pulse height spectrum  $f_1(E)$  and a known cord length distribution. The method which is based on the use of characteristic functions is mentioned in section E.

c) The mean diameter of the critical volume is small as compared to the range of the primary charged particles. The track segments are considered as straight, but straggling is taken into account.

For very small volumes the problem of delta-ray efflux and influx is too complicated to be discussed here (for details see<sup>9</sup>). For volumes of a diameter of the order of magnitude of a micrometer one may assume a suitable cut-off energy below which the primary collisions are considered as local and above which they are excluded. The cut-off should actually depend on the position of the trajectory and on the velocity of the charged particle. Especially for electrons it is however a reasonable approximation to assume a constant collision spectrum with cut-off energy corresponding to a delta-ray range

equal to half the mean diameter of the volume. This approximation can always serve as a starting point for more refined calculations.

Under this assumption of a constant 'effective' collision spectrum one can calculate the straggling distributions  $s(E; \bar{E})$  to different mean energy losses  $\bar{E}$ . This is described in section D.3. One may then first calculate the single event spectrum  $f_1'(E)$  without consideration of the straggling. In a second step the straggling can be taken into account according to the relation:

$$f_1(E) = \int_0^{\infty} s(E; \bar{E}) \cdot f_1'(\bar{E}) d\bar{E} \quad (34)$$

The properties of the straggling kernel  $s(E; \bar{E})$  and the influence of the straggling on the width of  $f_1(E)$  is discussed in D.3. Analytical techniques to eliminate straggling from a distribution  $f_1(E)$  are mentioned in section E.

The analysis of  $f_1(E)$  cannot be fully discussed in this survey. The following two sections are therefore restricted to the two random factors cord length fluctuations and energy deposition straggling. These are the two main aspects in which microdosimetry adds to the classical LET concept.

## 2. Cord length distributions

If a convex body is uniformly and isotropically traversed by straight particle tracks one obtains a distribution,  $c(\ell)$ , of cord length,  $\ell$ . For a sphere of diameter  $d$  one has:

$$c(\ell) = 2\ell/d^2 \quad \text{and} \quad C(\ell) = \ell^2/D^2 \quad \text{for} \quad 0 < \ell < d$$

which leads to: (35)

$$\bar{\ell} = \frac{2 \cdot d}{3} \quad \text{and} \quad \sigma^2 / \bar{\ell}^2 = 0.125$$

For cylinders cord length distributions have been calculated numerically by WILSON and EMERY<sup>10</sup>. BIRKHOFF et al.<sup>11</sup> have derived cord length distributions by Monte-Carlo methods; they also present a useful discussion of analytical expressions for some special cases. Numerical derivation of cord length distributions by direct integration over a body of arbitrary convex shape is straight forward. It is performed by a computer program which is available in ALGOL 60. The program divides the surface of any given body into small elements by collapsing a ruled-globe net over it. By summing the cord length contributions from all possible pairs of surface elements the probability distribution is derived. Distributions for spheroids together with the values of the mean, the relative variance, the skewness, and the kurtosis have been published<sup>9</sup>.

The mean value of the cord length in a convex body is equal to four times its volume divided by its surface:

$$\bar{l} = 4V/S \quad (36)$$

This relation which has already been given by CAUCHY has found applications in neutron physics. In the following the term  $4V/S$  will be called mean diameter,  $\bar{l}$ , of the body. The theorem can be generalized to tracks of finite length. If the mean length of the straight tracks is  $\bar{r}$ , one obtains the following formula for the mean segment length  $\bar{s}$ :

$$\frac{1}{\bar{s}} = \frac{1}{\bar{l}} + \frac{1}{\bar{r}} \quad (37)$$

The proof is omitted here. A broader generalization of the theorem to curved tracks will be given below.

If  $\bar{\Gamma}_T$  is the track average LET with appropriate cut-off, the mean energy deposition per event is  $\bar{\Gamma}_T \cdot \bar{s}$ . Accordingly one obtains the following formula for the mean number,  $\phi(0)$ , of events per unit dose:

$$\phi(0) = \frac{1}{16 \cdot \bar{\Gamma}_T} \left( \frac{S}{4} + \frac{V}{r} \right) \quad (38)$$

or if  $\bar{E}$  designates the mean initial energy of the charged particles:

$$\phi(0) = \frac{1}{16 \cdot \bar{E}} \left( \frac{S \cdot \bar{r}}{4} + V \right) \quad (39)$$

The units keV and  $\mu\text{m}$  are used here (as for the numerical constant see<sup>1</sup>).

One may suspect that the sphere has the smallest relative variance of cord length ( $V=0.125$ ) of all convex bodies. There is, however, no generally known proof of this assertion. The increase of  $V$  due to deviations from the spherical shape can be seen in the curve given for spheroids<sup>9</sup>.

The preceding discussion has been concerned with straight particle tracks. It is therefore mainly applicable to heavy charged particles. For the curled tracks of electrons the situation is more complicated, but statements on the mean segment length are still possible. Imagine that a track is cut in all points where it intersects the surface of the region of interest. The term 'segment' then designates a piece of the track which lies inside the region. If the total track lies inside the region it is also called a segment. The length of a track or a segment is understood to be its total integrated length. One can then show that the mean segment length,  $\bar{s}$ , in the case of a uniform, isotropic field is given by:

$$\frac{1}{\bar{s}} = \frac{1}{\bar{r}} + \frac{S}{4V} \quad (\bar{r}: \text{mean range of particles}) \quad (40)$$

The symbol  $\bar{r}$  has been avoided here because the relation in its general form also holds for concave volumes and the term mean diameter has little meaning in this case. For long tracks the relation reduces to:

$$\bar{s} = 4V/S \quad (41)$$

The general proof of this somewhat surprising extension of the theorem (36) is not too difficult but must be omitted here for brevity. The proof consists essentially of an enumeration of the number of intersection points, starting points, and stopping points of the tracks. The theorem even holds if one includes the length of all branches and subbranches of the track length or segment length.

One can show that under the conditions of FANO's theorem<sup>12</sup> one obtains exactly the same shapes and relative frequencies of segments in a region and in a cavity which simulates this region. The wall-effects merely consist in an increase in the frequency of associated segments, that is of segments which belong to the same track and thus occur simultaneously. This increase in the frequency of simultaneous passages leads to a corresponding increase in mean event size,  $\bar{z}_F$ .

A detailed study of the probabilities of multiple passages will be necessary in order to determine the extent of wall-effects in proportional counters. A first estimate should be possible on the basis of the following relation which holds for spherical cavities equivalent to volumes which are small enough that the change of energy and direction of a traversing particle can be neglected. One can prove that in this case the probabilities for multiple traversals through the sphere are equal to the probabilities for multiple passages through a plane. For anisotropic radiation fields one has to average the latter probabilities over planes of all orientations. The probabilities for multiple traversal through a plane (charged particle albedo) may be derived from cloud chamber photographs or from Monte Carlo simulations of tracks.<sup>14</sup>

### 3. Energy straggling

The term energy straggling designates fluctuations of energy loss along the track of a charged particle. The following section deals with energy straggling along track segments which are short enough that the mean energy loss of the charged particle is small as compared to the kinetic energy of the particle: The stopping power of the particle can then be assumed to be constant along the track segment. The case of larger mean energy loss is irrelevant to microdosimetry since the relative fluctuations of energy loss are then small enough to be neglected.

As can be seen from equ.(24) LET and cord length variations present no difficulties in the calculation of z-spectra. Straggling is therefore the central problem in theoretical microdosimetry. The straggling problem is complicated in microdosimetry by the fact that one is interested not in the distribution of energy loss of a particle, but in the distribution of energy deposition. The escape of delta-rays from the region of interest and the corresponding influx of delta-rays formed outside the critical volume presents considerable theoretical difficulties. The problem has to be studied by the deployment of wall-less proportional counters<sup>13</sup> and by Monte-Carlo simulations of delta-ray tracks<sup>14</sup>.

The collision spectrum,  $w(E)$ , is the probability distribution of energy transfers in the collisions encountered by the charged particles. For a general discussion see<sup>15,16</sup>. In the special case of a non-relativistic heavy charged particle:

$$w(E) \sim 1/E^2 \quad \text{for} \quad E_{\text{MIN}} < E < E_{\text{MAX}} \quad (42)$$

$$\text{with} \quad E_{\text{MAX}} = 4 \frac{m}{M} \cdot E_{\text{KIN}} \quad \text{and} \quad E_{\text{MIN}} = I^2/E_{\text{MAX}}$$

$E_{\text{KIN}}$  is the kinetic energy of the heavy particle,  $M$  is its mass,  $m$  is the electron mass, and  $I$  is the ionization potential of the medium. The relation is meaningful for  $E \gg I$ . The value of  $E_{\text{MIN}}$  has been assumed merely to arrive at the right stopping power. In reality  $w(E)$  has resonances in the vicinity of  $I$ .

At higher energies  $w(E)$  has to be corrected for delta-ray escape and influx if it is to describe energy deposition in the region of interest and not total energy loss of the charged particle. One may choose an appropriate cut-off energy or derive the effective spectrum by integrating escape and

influx probabilities over the particle track in the vicinity of the segment of interest.

The mean energy loss,  $\delta_1$ , in a collision derived from equ. (42) has no meaning since the unrealistic low energy part of this spectrum strongly affects  $\delta_1$ . Values of typically 60eV are indicated by experimental results<sup>17</sup>.

The 'energy mean' is, however, mainly dependent on the shape of  $w(E)$  at high values of  $E$  and can therefore in good approximation be taken from equ.(42):

$$\delta_2 = \frac{\int E^2 \cdot w(E) dE}{\int E w(E) dE} \approx \frac{E_{MAX}}{2 \ln(E_{MAX}/I)} \quad (43)$$

As an example one may give the value of  $\delta_2=480\text{eV}$  for a 2MeV proton in water ( $I=60.5\text{ eV}$ ). The actual value of  $\delta_2$  is somewhat larger due to the influence of the resonance collisions<sup>15</sup>

The straggling distribution reflects the succession of statistically independent collision events of varying size. It is therefore the solution of a compound Poisson process, and in full analogy to equ.(17) one obtains:

$$s(E; \bar{E}) = \sum_{v=0}^{\infty} e^{-n} \cdot \frac{n^v}{v!} \cdot w^{*v}(E) \quad \text{with } n = \bar{E}/\delta_1. \quad (44)$$

and also

$$s(\tau; \bar{E}) = e^{n(\omega(\tau)-1)} \quad (45)$$

where  $s(\tau; \bar{E})$  and  $\omega(\tau)$  are the characteristic functions of  $s(E; \bar{E})$  and  $w(E)$ . This relation applies not only to the characteristic functions (Fourier transforms) but also to the Laplace transforms. The latter is being used in the classical straggling theory of LANDAU<sup>18</sup> (assumption:  $E_{MAX}=\infty$ ) and in the more generalized theory of VAVILOV<sup>19</sup>. Both theories are restricted to the  $1/E^2$ -spectrum and its relativistic modifications and to the case of many collisions. Rough cor-

rections for the initial part of  $w(E)$  are introduced by BLUNCK and LEISEGANG<sup>20</sup> for the LANDAU theory and by SHULEK et al.<sup>21</sup> for the VAVILOV theory. In microdosimetry the classical theories are inadequate since one often deals with small energy losses where few collisions occur and where the initial part of  $w(E)$  is important. Furthermore one has to use appropriate corrections of  $w(E)$  at high energies to account for the delta-ray escape and influx problem. This has made a more general solution of the straggling problem necessary. The available computer programs for direct numerical derivation of the straggling distributions for arbitrary collision spectra  $w(E)$  are discussed in section E.

In analogy to the results derived in section C one finds that the semiinvariants  $\kappa_\nu(\bar{E})$  of the straggling distributions are equal to the mean collision number times the non-central moments of  $w(E)$ . Specifically with  $\bar{E} = n \cdot \delta_1$ :

$$V = \delta_2 / \bar{E} \quad (46)$$

Whenever the straggling distribution is near to a normal distribution the 'resolution' is a useful characteristic:

$$R = 2.77 \cdot \sqrt{\delta_2 / \bar{E}} \quad (47)$$

The value of  $\delta_2$  from equation (43) is usually sufficiently accurate for a rough estimate. For small volumes  $\delta_2$  can however be markedly decreased due to the delta-ray escape and the corresponding cut-off in  $w(E)$  (see<sup>22</sup>).

The combined influence of the various statistical factors on the width of the single event spectrum  $f_1(E)$  is described elsewhere<sup>9</sup>. Here it may suffice to give the formula for the relative variance of the distribution  $f_1(E)$  or  $f_1(z)$  which results from equ.(31) and 34):

$$V = \frac{\delta_2}{\bar{E}} + V_{\text{LET}} \cdot V_{\text{Cord length}} + V_{\text{LET}} + V_{\text{Cord length}} \quad (48)$$

For the 'dose mean',  $\bar{E}_D$ , of the single event spectrum  $f_1(E)$  one obtains:

$$\bar{E}_D = \delta_2 + \bar{\Gamma}_D \cdot \bar{\bar{x}} \quad (49)$$

Where  $\bar{\Gamma}_D$  is the dose mean LET, and  $\bar{\bar{x}} = \frac{\overline{x^2}}{\bar{x}}$  is the analogon of a dose mean for the cord length distribution (see equ.(30)).

For a sphere:

$$\bar{x} = \frac{2}{3} \cdot d \quad \text{and} \quad \bar{\bar{x}} = \frac{3}{4} \cdot d \quad (d: \text{diameter of the sphere}) \quad (50)$$

and consequently:

$$\bar{E}_D = \delta_2 + \frac{3}{4} \cdot d \cdot \bar{\Gamma}_D \quad (51)$$

For the dose mean,  $\bar{y}_D$ , of the event size one has:

$$\bar{y}_D = \delta_2 / \bar{x} + \bar{\Gamma}_D \cdot \bar{\bar{x}} / \bar{x} \quad \text{and for a sphere} \quad \bar{y}_D = \frac{3 \cdot \delta_2}{2 \cdot d} + \frac{9}{8} \cdot \bar{\Gamma}_D \quad (52)$$

These formulae are important for radiation quality considerations, where the dose mean LET,  $\bar{\Gamma}_D$ , may be the quantity of interest, while  $\bar{y}_D$  is experimentally observed. For brevity the influence of the FANO fluctuations<sup>23</sup> and of the multiplication statistics on experimental pulse height spectra is not discussed here (see<sup>9</sup>). It may, however, be remarked that due to the fluctuations in the number of ions (FANO fluctuations) the value of  $V$  in equ.(48) is increased by  $w/2\bar{E}$  (with  $w \approx 34\text{eV}$ ), and due to the multiplication statistics  $V$  is increased by  $w/\bar{E}$ .

The latter value corresponds to an exponential single-event spectrum. With optimal performance of the proportional counter the term is somewhat smaller. One may, however, state in general that the straggling term  $\delta_2/\bar{E}$  always exceeds the term  $w/\bar{E}$  by far. This is the reason for the applicability of proportional counters in microdosimetric measurements.

## E. COMPUTATIONAL TECHNIQUES

The following is a brief discussion of some computational procedures developed for microdosimetric calculations. Details for the actual use of these procedures must be taken from the available program listings.

### 1. Solution of the compound Poisson process by successive convolutions.

An early attempt to integrate equ.(44) has been made by WILLIAMS<sup>24</sup>. A computer program to solve the mathematically identical equ.(17) has been developed by B.BIAVATI<sup>25</sup>. Direct integration has the disadvantage that a great number of distributions  $f_n(z)$  must be calculated; moreover execution of the convolution operation on a linear scale is ineffective since the spectra  $w(E)$  or  $f_1(z)$  can be extremely wide. Shorter computation times have been achieved by Monte-Carlo solutions of the compound Poisson process<sup>7</sup>; the accuracy of Monte Carlo methods is however limited.

A new program has therefore been developed which derives straggling distributions by a series of successive convolutions. The program is exact, and since the convolutions are performed on a logarithmic scale the computation times are acceptable. This program is available in FORTRAN IV and can without alterations be used to derive straggling distributions for any given collision spectrum  $w(E)$  or to derive dose dependent distributions  $f(z;D)$  for any given single event spectrum  $f_1(z)$ . For details see<sup>26</sup> and<sup>9</sup>.

### 2. Solution of the compound Poisson process by use of the fast Fourier transform algorithm.

The program mentioned under 1. derives solutions of the compound Poisson process for a given characteristic spectrum. It can not be used in the opposite direction. That is, it can not derive the characteristic spectrum from a solution.

It is, however, possible to derive  $w(E)$  if in the equation:

$$s(E; \bar{E}) = \sum_{\nu=0}^{\infty} e^{-n} n^{\nu} / \nu! \cdot w^{*\nu}(E) \quad (53)$$

$s(E; \bar{E})$  is known for some value of  $\bar{E}$ . This can be seen from equ.(45) which holds for the characteristic functions (or Fourier transforms):

$$s(\tau; \bar{E}) = e^{n(\omega(\tau)-1)} \quad \text{or} \quad (54)$$

$$\omega(\tau) = \frac{\ln s(\tau; \bar{E})}{n} + 1 \quad (55)$$

Thus the characteristic function of the unknown collision spectrum  $w(E)$  can be expressed in terms of the characteristic function of the solution  $s(E; \bar{E})$ . Equ.(55) is evaluated by a computer program which uses the fast Fourier transform algorithm of COOLEY and TUCKEY<sup>27</sup>. The logarithm,  $\ln s(\tau; \bar{E})$ , is not uniquely defined for complex  $\tau$ . In the computer program it is made unique by the choice of a suitable continuous representation of  $s(\tau; \bar{E})$  in the complex plane. Thus if one reads in a particular solution  $s(E; \bar{E})$  one obtains a unique result  $w(E)$ .

It is not without interest to note the similarity of equ.(54) with the formalism used in the Vávilov theory. The equation holds not only for the Fourier transform but also for the Laplace transform. The latter could therefore in principle equally well be used for numerical evaluation. The Fourier transform has been chosen because of the great advantages of the Cooley and Tuckey algorithm. Conventional techniques require computation times proportional to the square of the length,  $N$ , of the transformed array. In the present program the computation time is proportional to  $N \cdot \ln(N)$ .

The solutions of the compound Poisson process converge against Gaussian distributions with increasing mean value  $\bar{E}$ . For large mean values the method is therefore limited by the fact that small inaccuracies in  $s(E; \bar{E})$  lead to very large deviations in

$w(E)$ . If due to inaccuracies  $s(E; \bar{E})$  is not a solution of a compound Poisson process (i.e. is not infinitely divisible, see<sup>28</sup>) one obtains solutions  $w(E)$  which are not positive definite. This is not a limitation of the numerical technique; on the contrary the blurring of the resulting  $w(E)$  indicates lack of information in the input data  $s(E; \bar{E})$ . This is a check for the dependability of the results.

The method is most suitable for the derivation of collision spectra from straggling distributions with low mean collision numbers. It can of course as well be used in the forward direction, but it is less suitable than the method described under 1. if one deals with extremely wide spectra. The distributions are on a linear scale and may therefore in certain cases take too much storage space. The program is written in FORTRAN IV.

### 3. Elimination of cord length fluctuations from pulse height spectra.

An LET-distribution may be derived from an observed spectrum according to equ.(24) or (28). This possibility is limited by the influence of straggling. In certain cases straggling may be relatively insignificant, in other cases the influence of straggling may be eliminated by the method mentioned in the next paragraph.

The problem has a simple analytical solution for a sphere or a slab (see general discussion in<sup>29</sup>). It has been solved in general by Monte-Carlo methods (see<sup>29</sup> and<sup>30</sup>). In addition there is the possibility of a direct numerical solution based on the characteristic functions.

If  $\phi(t)$ ,  $\gamma(t)$ , and  $\tau(t)$  are the characteristic functions of the distributions  $f(\ln E)$ ,  $c(\ln l)$ , and  $z(\ln L)$  introduced in equ.(27) then from equ.(28) one obtains:

$$\phi(t) = \gamma(t) \cdot \tau(t) \quad \text{and} \quad \tau(t) = \phi(t) / \gamma(t) \quad (56)$$

Thus the characteristic function of the LET-distribution (on a logarithmic scale) is equal to the quotient of the characteristic functions of the pulse height distribution and of the cord length distribution (again on a logarithmic scale). The relation shows that the solution of this unfolding problem is unique. Naturally the solution is a probability distribution only for suitable input distributions  $f(\ln E)$  and  $c(\ln l)$ . In general the resulting LET-distribution  $t(\ln L)$  has some negative values. As mentioned under 2. this shows that for the given set of input data the problem can not be strictly solved. This is again an important control for the results. In certain cases it clearly indicates the limitations of the simplified model expressed by equ.(24). The fast Fourier transform algorithm mentioned in the preceding paragraph is also used to evaluate equ.(56). The program is extremely fast and needs little storage since one deals with logarithmic distributions which are very narrow.

#### 4. Elimination of the influence of straggling from an experimental distribution.

Equ.(34) can be rewritten into a matrix equation. One represents the straggling kernel  $s(E; \bar{E})$  by a two dimensional array  $S_{E, \bar{E}}$  and the distributions  $f(E)$  and  $f'(E)$  by one-dimensional arrays  $F_E$  and  $F'_E$ :

$$F_E = S_{E, \bar{E}} \cdot F'_E \quad (57)$$

The matrix  $S_{E, \bar{E}}$  is too large for numerical evaluation, if a linear grid of  $E$  and  $\bar{E}$  is used. Matrix and vectors are therefore transformed to a logarithmic grid. Then the dimension of the matrix and vectors can be less than hundred, and the accuracy of the representation is still sufficient. The computer program first derives the distributions  $s(E; \bar{E})$  on a linear scale. This is done by the program mentioned in paragraph 2. Then these distributions are transformed to the suitable logarithmic representation. Finally  $S_{E, \bar{E}}$  is inverted; since  $S_{E, \bar{E}}$

is fairly near to a diagonal matrix inversion presents no great problems. Thus one obtains the distribution  $F_{\bar{E}}^1$  from the experimental distribution  $F_E$ .

$$F_{\bar{E}}^1 = S_{\bar{E}, E}^{-1} \cdot F_E \quad (58)$$

The method is, of course, limited by the assumptions discussed in section C.1 case c). But it is applicable in many instances where naive application of the unfolding procedure discussed in the preceding paragraph is not justified. The resulting distribution  $F_{\bar{E}}^1$  or  $f^1(E)$  can then be analyzed according to the unfolding procedure.

Without going into details one may remark that equ.(57) and its solution can also be applied in order to correct for the multiplication statistics of the proportional counter. In this case the kernel  $s(E; \bar{E})$  is derived not from the collision spectrum but from the single electron spectrum of the proportional counter.

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