1. Introduction.-

It is not always easy to solve the problem of approximating a function $y(x)$ of which a discrete set of approximate values is known if the degree of reliability with which they are known is uncertain.

In particular it is often impossible to apply its result to numerical derivation. It is moreover particularly inefficient to determine an approximation of a function by an exact fitting of the available data when the function $y(x)$ one wishes to approximate is known at many points of the interval.

It is then clearly preferable to consider the majority of the given values rather than to choose an arbitrary set, composed of the smallest number of discrete values necessary to determine a set of conditions.

In this note we present a method of computation that improves the precision of the data y_i which approximate a differentiable function at same points x_i, $(i = 0,1,...n)$ and which computes the values taken at the points x_i $(i = 0,1,...,n)$ by the derivative $y'(x)$.

The method we propose uses both the quadrature formulas that connect the values of the derivative of a function to the values of the function itself and Cook's method [1].

The present method has been developped in order to determine the energy level of a trapping centre in a semiconductor by studying the trapped charge.

It has been tested on some analytical functions, tabulated at points that differed from the true values by less than 1%.

2. Theory of the method of numerical derivation.

Let the values taken by the differentiable function $y = y(x)$ be assigned in correspondence of the values $x_0, x_1, \ldots, x_n$ of x, where

$$x_i = ih \qquad (i = 0,1,\ldots,n), \qquad h \in R^+ \ . \tag{2.1}$$

In the following we shall denote, for each i, by y_i and Δy_i, respectively the given numerical values and the deviation of every given y_i from the corresponding theoretical value $y(x_i)$.

We shall denote by

$$Y_S = \begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{pmatrix} \qquad Y_T = \begin{pmatrix} y(x_0) \\ y(x_1) \\ \vdots \\ y(x_n) \end{pmatrix} \qquad \begin{pmatrix} y'(x_0) \\ y'(x_1) \\ \vdots \\ y'(x_n) \end{pmatrix} \qquad \Delta Y = \begin{pmatrix} y_0 - y(x_0) \\ y_1 - y(x_1) \\ \vdots \\ y_n - y(x_n) \end{pmatrix}$$

the $(n+1)$-dimensional column vector and by E the identity matrix of order $n+1$.

Let A be an invertible linear operator such that

$$A\sigma = Y \ . \tag{2.2}$$

In the sequel we shall assume, for short, A to be an invertible matrix of order $n+1$.

It is our aim to give a numerical evaluation of vector σ, or of the

values that the derivative $y' = y'(x)$ takes at the points (2.1) with the highest possible precision.

It follows from (2.2) and from the relation $Y_T = Y_S + \Delta Y$ that

$$A\sigma = Y_S + \Delta Y \tag{2.3}$$

or

$$\sigma = A^{-1}Y_S + A^{-1}\Delta Y \quad . \tag{2.4}$$

Even though ΔY can be regarded as negligible with respect to Y_S and therefore a relationship of the type

$$A\sigma \tilde{=} Y_S \tag{2.5}$$

may be thought to hold, $A^{-1}\Delta Y$ is in general not negligible with respect to $A^{-1}Y_S$; the solution $A^{-1}Y_S$ is thus not "acceptable".

We denote by W the diagonal matrix $(E \cdot \Delta Y)^{-1}$ and by $\| \cdot \|$ the euclidean norm in R^{n+1}.

We shall say that $\sigma_S = (y'_0, y'_1, \ldots, y'_n)^T$ is an "acceptable" solution of the problem if

$$\chi^2 = \|W(Y_S - A\sigma_S)\|^2 \tilde{=} n + 1. \tag{2.6}$$

In order to obtain, among all the possible solutions σ that satisfy (2.6), the one that offers the " best possible solution", we define a structure function $S(\sigma)$, which is, to a certain extent, arbitrary,and we require that the solution vector σ_S be such as to minimize the function $S(\sigma)$ and satisfy (2.6). Using the method of Lagrange's multipliers one obtains the equation

$$\delta\chi^2 + \mu\delta S = 0 \qquad (2.7)$$

We shall denote by S the matrix (which we shall call, for short, smoothing matrix) such that

$$\delta S = S\sigma\delta\sigma$$

and by A^T the transposed matrix A. One obtains

$$\delta\chi^2 = \left[2A^T W^2(A\sigma - Y_S)\right]\ \delta\sigma$$

and hence

$$\delta\chi^2 + \mu\delta S = \left[2A^T W^2(A\sigma - Y_S) + \mu S\sigma\right]\ \delta S.$$

In order for (2.7) to be verified it is necessary and sufficient that

$$A\sigma - Y_S + \lambda\ (A^T W^2)^{-1}\ S\sigma = 0\ ;$$

then

$$Y_S = \left[A + \lambda\ (A^T W^2)^{-1} S\right]\sigma\ . \qquad (2.8)$$

The solution σ_S that we are looking for is then obtained as a solution of the system (2.8), (which is a system of $n+1$ equations in the $n+2$ unknown $y'_0, y'_1, \ldots, y'_n, \lambda$) if one chooses λ in such a way that $\chi^2 \simeq n+1$.

The matrix A we have considered is the matrix of order $n+1$

$$A = \frac{n}{2}\begin{pmatrix} \gamma & 0 & 0 & \ldots\ldots & 0 \\ 1+\gamma & 1 & 0 & \ldots\ldots & 0 \\ 1+\gamma & 2 & 1 & \ldots\ldots & 0 \\ - & - & - & - & - \\ 1+\gamma & 2 & 2 & \ldots\ldots & 1 \end{pmatrix}$$

where $\gamma = \dfrac{2y(x_o)}{hy'(x_o)}$ if $y(x_o) \cdot y'(x_o) \neq 0$. If, on the contrary, $y(x_o)\cdot y'(x_o) = 0$ one considers the matrix of order n obtained from A by deleting the first row and the first column (provided $y(x_1)\cdot y'(x_1)\neq 0$)

The structure functions considered by us are

$$S_1(\sigma) = \sum_{0}^{n-1} k \, (y_{k+1} - y_k)^2$$

$$S_2(\sigma) = \sum_{1}^{n-1} k \, (y_{k+1} - 2y_k + y_{k-1})^2$$

The corresponding smoothing matrices we obtained by considering $\dfrac{\partial S_1}{\partial y_i}$ and $\dfrac{\partial S_2}{\partial y_i}$; they are respectively

$$S_1 = 2 \begin{pmatrix} 1 & -1 & 0 & \cdots & & \\ -1 & 2 & -1 & 0 & \cdots & \\ 0 & -1 & 2 & -1 & 0 & \cdots \\ \multicolumn{6}{c}{- - - - - - - - - - - - - - -} \\ 0 & 0 & & -1 & 2 & -1 \\ \multicolumn{3}{c}{\cdots\cdots\cdots\cdots} & 0 & -1 & 1 \end{pmatrix}$$

$$S_2 = 2 \begin{pmatrix} 1 & -2 & 1 & 0 & 0 & \cdots & \\ -2 & 5 & -4 & 1 & 0 & \cdots & \\ 1 & -4 & 6 & -4 & 1 & 0 & \cdots \\ \multicolumn{7}{c}{- - - - - - - - - - - - - - -} \\ 0 & \cdots\cdots & 0 & 1 & -4 & 6 & -4 & 1 \\ 0 & \cdots\cdots & 0 & 0 & 1 & -4 & 5 & -2 \\ 0 & \cdots\cdots & 0 & 0 & 0 & 1 & -2 & 1 \end{pmatrix}$$

After determining $\sigma = (y'_0, y'_1, \ldots, y'_n)$ by the method outlined above we can determine with a higher precision the numerical values y_i setting

$$y_i^* = \frac{h}{2} \sum_{0}^{n} {}_j \; a_{ij} y'_j \qquad i = 0,1,\ldots,n$$

3. Numerical results

We have tested the method for the evaluation of the derivatives y'_i $(i = 1,40)$ of some analytical functions $y(x)$ at the points $x_i = ih$ $(i = 1,40)$ for $h = 0,05$ starting from a set of approximate values y_i as reported in table I,II,III.

The values y_i^* obtained by the present method are clearly better than the given y'_i s.

The method has been used in order to determine the maximum value of the modulus of the derivative of a function measured experimentally. In every case, we have adopted the smoothing matrix S_2.

Figure 1 shows the experimental values y_i, $i = 1,25$ the accumulated charge in terms of the energy of the quasi Fermi level in a semiconducting crystal in space-charge conditions due to trapping levels, the function (solide line) and the modulus of the derivative (dashed line), calculated by the present method.

The maximum value of the modulus of the derivative y' is connected to the energy position of the trapping level that governs the phenomenon.

The result we obtain agrees with that determined by other methods, [2].

TABLE I

$\lambda = 2.10^{7}$ $\quad y(x) = x^{3}/3$ $\quad \chi^{2} = 38,52$

x_i	$y(x_i)$	y_i	y_i^*	$y'(x_i)$	y'_i
0.05	0.000041	0.000041	0.000041	0.002500	0.002475
0.25	0.005208	0.005156	0.005209	0.062500	0.061252
0.45	0.030375	0.030071	0.030370	0.202500	0.201944
0.65	0.091541	0.090626	0.091522	0.422500	0.422007
0.85	0.204708	0.202661	0.204682	0.722500	0.722012
1.05	0.385875	0.382016	0.385747	1.102500	1.100949
1.25	0.651041	0.644531	0.650644	1.562500	1.561237
1.45	1.016208	1.006046	1.016215	2.102500	2.107910
1.65	1.497375	1.482401	1.499130	2.722500	2.731212
1.85	2.110541	2.089436	2.111794	3.422500	3.399466

(a) We have reported in each table only a few results as the space would be insufficient to report all of them.

Table I reports for the function $y(x) = x^3/3$ the values of the abscissae x_i, of the theoretical ordinates $y(x_i)$, of the experimental ordinates y_i, that differ from the true value by less than 1%, those calculated by the present method y_i^*, the theoretical values of the derivative $y'(x_i)$ and the values of the derivative y'_i obtained by the present method. The value of the Lagrange multiplier and the relative value of χ^2 are also reported.

TABLE II

$\lambda = 10^6$		$y(x) = e^x - x - 1$		$\chi^2 = 39,42$	
x_i	$y(x_i)$	y_i	y_i^*	$y'(x_i)$	y_i'
0.05	0.001271	0.001258	0.001259	0.051271	0.050820
0.25	0.034025	0.033685	0.034045	0.284025	0.281952
0.45	0.118312	0.117129	0.118290	0.568312	0.567674
0.65	0.265540	0.262885	0.265488	0.915540	0.914879
0.85	0.489646	0.484750	0.489543	1.339646	1.338830
1.05	0.807651	0.799574	0.807525	1.857651	1.857131
1.25	1.240342	1.227939	1.240083	2.490342	2.487356
1.45	1.813114	1.794983	1.812066	3.263114	3.258322
1.65	2.556979	2.531410	2.556752	4.206979	4.221641
1.85	3.509819	3.474721	3.513975	5.359819	5.373412

Table II reports the analogous results for the function $y(x) = e^x - x - 1$. For the meaning of symbols see table II.

TABLE III

$\lambda = 4.10^7$ $\quad y(x)=1-\cos(x)$ $\quad x^2 = 40$

x_i	$y(x_i)$	y_i	y_i^*	$y'(x_i)$	y_i'
0.05	0.001249	0.001237	0.001241	0.049979	0.049642
0.25	0.031087	0.030776	0.031078	0.247403	0.247244
0.45	0.099552	0.098557	0.099533	0.434965	0.435012
0.65	0.203916	0.201877	0.203869	0.605186	0.605094
0.85	0.340016	0.336616	0.339946	0.751280	0.751536
1.05	0.502428	0.497404	0.502448	0.867423	0.868300
1.25	0.684677	0.677830	0.684731	0.948984	0.948271
1.45	0.879497	0.870702	0.878949	0.992712	0.987785
1.65	1.079120	1.068329	1.077571	0.996865	0.994580
1.85	1.275590	1.262834	1.275774	0.961275	0.986571

Table III reports the analogous results for the function $y(x) = 1-\cos(x)$. For the meaning of symbols see table I.

REFERENCES

1. B.C.Cook, Nuclear Instrum. and Methods 24 (1963),256

2. C.Manfredotti,C.De Blasi,S.Galassini,G.Micocci,L.Ruggiero and A. Lepore, Phys. Stat. Sol. (a) 36 (1976),569.

Figure caption

The figure 1 reports the experimental values (dots), measured with an error estimated about 5%, of the accumulated charge versus the quasi Fermi level. In the same figure we show also the values of the function $\rho(E)$ calculated by the present method (solid line) and those of the modulus of the derivative (dashed line) for $\lambda = 4.10^{18}$ to which there corresponds the value $\chi^2 = 24{,}39$, to be compared with the number of experimental points N = 25.

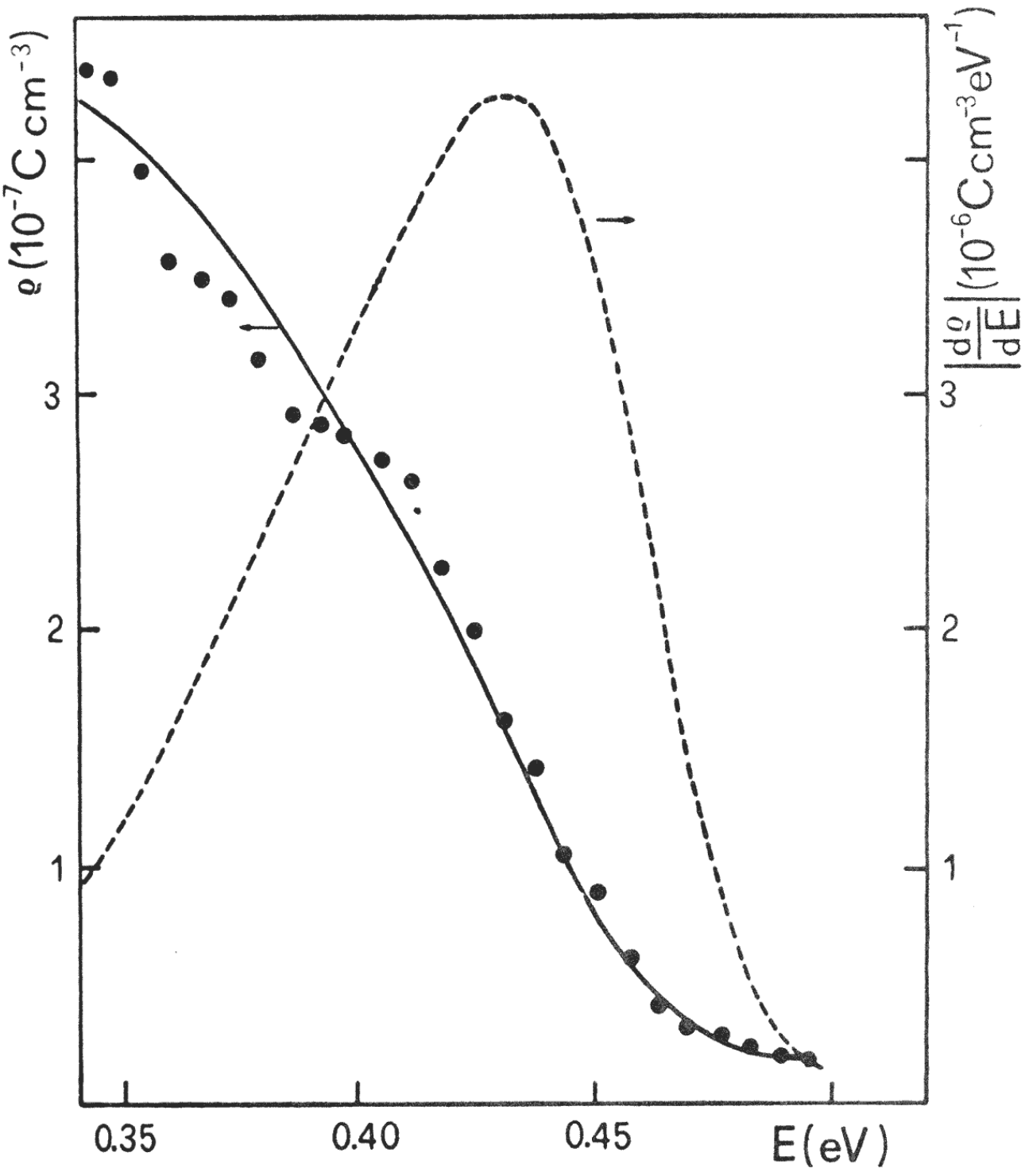

Fig.1