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 $x_0, x_1, \dots, x_n$ of x, where

$$x_i = ih \qquad (i = 0,1,\dots,n), \qquad h \in R^+ \quad . \qquad (2.1)$$

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

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

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

$$A\sigma = Y \quad . \qquad (2.2)$$

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

$$A\sigma \cong Y_S \tag{2.5}$$

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

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

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

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

and hence

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

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

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

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 $\chi^2 \cong n+1$.

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

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

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

$$S_1 = 2 \begin{pmatrix} 1 & -1 & 0 \ldots. & & & \\ -1 & 2 & -1 & 0 \ldots. & & \\ 0 & -1 & 2 & -1 & 0\ldots.. & \\ - - - & - - - & - - - & - - - & - - - & \\ 0 & 0 & & -1 & 2 & -1 \\ \ldots\ldots & \ldots\ldots & \ldots\ldots & 0 & -1 & 1 \end{pmatrix}$$

$$S_2 = 2 \begin{pmatrix} 1 & -2 & 1 & 0 & 0 \ldots & & & \\ -2 & 5 & -4 & 1 & 0 \ldots & & & \\ 1 & -4 & 6 & -4 & 1 & 0\ldots & & \\ - - - & - - - & - - - & - - - & - - - & - - - & - - - & \\ 0 \ldots\ldots & 0 & 1 & -4 & 6 & -4 & 1 & \\ 0 \ldots\ldots & 0 & 0 & 1 & -4 & 5 & -2 & \\ 0 \ldots\ldots & 0 & 0 & 0 & 1 & -2 & 1 & \end{pmatrix}$$

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

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

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].