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DEFINITION OF A CHARACTERISTIC REFERENCE CENTRE AND CHARACTERISTIC EXTERIOR POTENTIAL COEFFICIENTS A_{nm}, B_{nm}, MULTIPOLE MOMENTS)

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RÉSUMÉ

A partir d'un ensemble donné de coefficients A_{nm} et B_{nm} du potentiel extérieur d'une distribution de charge, il est possible de définir un centre de référence caractéristique et les valeurs caractéristiques correspondantes des coefficients. La définition proposée repose sur la condition de minimum de l'énergie électrostatique relative à un espace extérieur associé approprié. Les moments multipolaires caractéristiques s'obtiennent à partir des coefficients A_{nm} et B_{nm} caractéristiques par des relations connues. Les caractéristiques sont déterminées pour deux systèmes constitués : (a) de deux charges, (b) de deux dipôles dirigés suivant l'axe. Les formules de transformation relatives à une translation du centre de référence sont données pour les coefficients A_{nm}, B_{nm}, les polynomes harmoniques et les dérivées correspondantes.

SUMMARY

From a given set of coefficients A_{nm} and B_{nm} of the exterior potential of a charge distribution, it is possible to define a characteristic reference centre and corresponding characteristic values of the coefficients. The definition proposed rests on the minimum condition of the electrostatic energy relative to an appropriate associated exterior space. The characteristic multipole moments are obtained from the characteristic coefficients A_{nm} and B_{nm} by known relations. The characteristics are determined for two systems consisting in (a) two charges, (b) two dipoles parallel to the axis. Transformation formulae relative to a translation of the reference centre are given for the coefficients A_{nm}, B_{nm}, the harmonic polynomials and their derivatives.

§ 1. — The following abbreviations will be used below.

EPC : exterior potential coefficients
CEPC : characteristic exterior potential coefficients
CRC : characteristic reference centre
RCQ : reference centre corresponding to Q
AES : associated exterior space
SES : smallest excluded sphere

Let 0, r, ϑ, φ, r', ϑ', φ' denote the origin and spherical coordinates,

$$\tau = \cos\vartheta\,;\; z = r\tau\,;\; \tau' = \cos\vartheta'\,;\; z' = r'\tau' \tag{1.1}$$

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$\rho(r', \tau', \varphi)$, the space charge density of a system,

a, the radius of a sphere containing the whole of the charge,

$V(r, \tau, \varphi)$, the potential in the space outside the sphere, produced by $\rho(r', \tau', \varphi)$.

We first recall some classical results [1],[4] needed below. Using spherical harmonics

$$Y^e_{mn}(\tau, \varphi) = \cos(m\varphi)P^m_n(\tau); \quad Y^o_{mn}(\tau, \varphi) = \sin(m\varphi)P^m_n(\tau) \tag{1.2}$$

the exterior potential is given by the expansion

$$V(r, \tau, \varphi) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} [A_{nm}Y^e_{mn}(\tau, \varphi) + B_{nm}Y^o_{mn}(\tau, \varphi)] \frac{1}{r^{n+1}} \tag{1.3}$$

where

$$\begin{Bmatrix} A_{nm} \\ B_{nm} \end{Bmatrix} = \varepsilon_m \frac{(n-m)!}{(n+m)!} \int_{r'=0}^{\infty} \int_{\tau'=-1}^{1} \int_{\varphi'=0}^{2\pi} \rho(r', \tau', \varphi') \begin{Bmatrix} \cos(m\varphi') \\ \sin(m\varphi') \end{Bmatrix} P^m_n(\tau')(r')^{n+2} d\varphi' d\tau' dr' \tag{1.4}$$

$$\varepsilon_0 = 1; \ \varepsilon_m = 2 \ (m = 1, 2, 3, \ldots) \tag{1.5}$$

It is to be noted that the charge density appears in V only through the integrals A_{nm} and B_{nm}. These are fundamental parameters of the charge distribution. Alternately, V can be expressed as a Taylor expansion in cartesian coordinates with multipoles as parameters. However, the set of functions is redundant. Therefore, we choose expansion (1.3) for the discussion.

Set

$$A^+_{nm} = A_{nm}; \quad A^-_{nm} = B_{nm} \tag{1.6}$$

The symbols $A^{\pm}_{nm}$, more compact and convenient (especially in Appendices A and B) will be used below. In particular cases, when only the coefficients A^+_{n0} differ from zero, we will omit the useless superscript + and thus return to the conventional symbol. The above coefficients will be called the exterior potential coefficients (EPC's).

Among the coefficients $A^{\pm}_{nm}$ a few are independent of the reference centre chosen. These are fundamental characteristics of the charge distribution. The others vary. So the question arises : is it not possible to recognize or define a remarkable reference system such that the corresponding non invariant coefficients $A^{\pm}_{nm}$ can be considered as valuable characteristics of the charge distribution? Such a reference system, its centre and the corresponding coefficients $A^{\pm}_{nm}$ will be called « characteristic ». The problem to be studied in this note is the choice of the reference centre. The orientation of the axes also deserves attention but in this respect, we simply observe that the choice must be based on the symmetry of the system. There may well be several orientations with different corresponding characteristic sets.

§ 2. — For a clear understanding of the problem consider the case of a system possessing rotational symmetry around the z axis. We choose an origin more or less arbitrarily. Symmetry allows the coefficients A^+_{n0} to have arbitrary values but requires the other coefficients $A^{\pm}_{nm}$ to vanish. Accordingly, (1.3) and (1.4) become

$$V(r, \tau) = \sum_{n=0}^{\infty} A_{n0} \frac{P_n(\tau)}{r^{n+1}} \tag{2.1}$$

$$A_{n0} = 2\pi \int_{r'} \int_{\tau'=-1}^{1} \rho(r', \tau') P_n(\tau') (r')^{n+2} d\tau' dr' \tag{2.2}$$

The axial moments are given by

$$\mu_n = \frac{A_{n0}}{n!} \tag{2.3}$$

Beside the initial coordinate system, consider another one with its centre at $z = c$. The various symbols will be completed when necessary. As concerns A_{n0}, we use $A_{n0}(0)$ and $A_{n0}(c)$. $A_{n0}(c)$ may be obtained from $A_{n0}(0)$ by

$$A_{n0}(c) = \sum_{l=0}^{n} \frac{n!}{(n-l)!\,l!} (-c)^{n-l} A_{l_0}(0) \tag{2.4}$$

This relation is well known. It results from (A.21) in Appendix A.

From (2.4) we may draw some well known conclusions concerning the coefficients A_{n0} and μ_n as well :

(1a) if the first k coefficients vanish for one value of c, the same is true for all values of c;

(1b) the first coefficient different from zero is independent of c;

(1c) the coefficients of higher order have values depending upon c. Clearly, the invariant coefficients, charge of an ion, dipole moment of an AB molecule or quadrupole moment of an AA molecule are fundamental characteristics. As regards the coefficients of higher order, there is a general tendency in the literature to consider, implicitely or explicitely, that they have no interest in themselves because they are not invariant. In the present article, we develop an opposite point of view. Our approach is based on the following remarks.

(2a) There are various levels in significance. The invariant coefficients have an absolute significance at the level of facts. Coefficients of higher order are certainly at a lower level. However, if they can be adequately defined, they will have some interest for purposes of characterization, description, comparison, etc.

(2b) There are charge distributions which obviously possess a CRC. Consider for instance a system composed of two equal charges. The centre of symetry is the only remarkable point to choose as the CRC. With this reference centre, the coefficients $A_{2n+l,0}$ vanish, which is necessary and remarkable. Similarly, if the two charges have equal absolute values but opposite signs, the centre is necessarily the CRC.

Consider a charge distribution such that, for a given reference centre

$$A_{n0} \begin{cases} \neq 0 \text{ for } n = j \\ = 0 \text{ for } n > j \end{cases} \tag{2.5}$$

Suppose m is small, say $m = 2$. If we choose another reference centre, all the coefficients A_{n0} for $n > j$ (with a few possible exceptions) are different from zero. Clearly, (2.5) is a remarkable, unique characterization of the system and the corresponding reference centre is the CRC.

Some simple means of defining a reference centre may be examined here.

The centre of gravity of an axial charge distribution is given by

$$z = \frac{\sum z_i q_i}{\sum q_i} \tag{2.6.a}$$

consider a system defined by

$$q_1 < 0;\ q_2 > 0;\ |q_1 + q_2| \ll |q_1| + |q_2|$$
$$z_1 = -s;\ z_2 = s \tag{2.7}$$

Applying (2.6.a) we find

$$z = s\frac{|q_1| + |q_2|}{q_1 + q_2};\ |z| \gg s \tag{2.8}$$

The centre of gravity is far from the charges. It cannot be taken as the CRC.

To remove the difficulty, we modify the denominator in (2.6.a) by taking the absolute values q_i. Then, we must do the same in the numerator; otherwise, for $q_1 = -1$, $q_2 = 1$, $z_1 = -s$, $z_2 = s$, we would find $z = s$. Thus, we arrive at

$$z = \frac{\sum z_i |q_i|}{\sum |q_i|} \tag{2.6.b}$$

consider the system

$$q_1 = -q;\ q_2 = q;\ q_3$$
$$z_1 = -\frac{\delta}{2};\ z_2 = \frac{\delta}{2};\ z_3 \tag{2.9}$$

Keeping $$\delta q = \mu \text{ constant, let } \delta \to 0 \tag{2.10}$$

Applying (2.9), we find

$$z = \frac{z_3 |q_3|}{2|q| + |q_3|} = \frac{\delta z_3 |q_3|}{2\mu + \delta |q_3|} \tag{2.11}$$

According to (2.11), a system composed of an ideal dipole and a point charge would have its CRC at the dipole whatever the position, sign and finite value at the charge. This is unacceptable.

At this stage, it is appropriate to specify the properties to be expected for the CRC and devise a definition accordingly. Unfortunately, our ideas are very vague. Consider a system composed of two charges q_A and q_B at A and B, respectively (Fig. 1). Let 0 denote the origin, C the CRC; $(-s)$, s, 0 and c the coordinates.

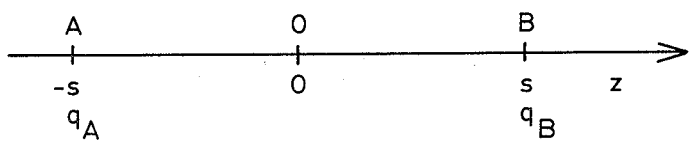

Fig. 1. — The two-charge system.

The value of c/s is determined by the ratio of the charges, say

$$q = q_A/q_B \tag{2.12}$$

According to point (2b) above, we write

$$c = s \quad \text{for} \quad q = 0 \tag{2.13.a}$$
$$c = 0 \quad \text{for} \quad q = \pm 1 \tag{2.13.b}$$
$$c = -s \quad \text{for} \quad q = \pm \infty \tag{2.13.c}$$

We may reasonably assume that c varies monotonically with q either positive or negative. This leads to the following conclusions :

$$-s \leqslant c \leqslant s \tag{2.14}$$

for each allowed value of c, there are two values of q having opposite signs. (2.15)

Parenthetically, consider the systems

$$\left.\begin{array}{l} S_I\ ;\ q_A = q_1 \quad ;\ q_B = q_1;\ c = 0\ \ ) \\ S_{II};\ q_A = -q_1;\ q_B = q_1;\ c = 0\ \ ) \end{array}\right. \tag{2.16}$$

and their sum

$$S_I + S_{II};\ q_A = 0;\ q_B = 2q_1;\ c = s \tag{2.17}$$

we find that the sum of two systems with the same CRC has a different CRC.

§ 3. — We try a variational approach. Consider a system such that the charge density and exterior potential can be treated as vanishingly small outside a limited region. The orientation of the reference axes and a preliminary reference centre $0(x_0, y_0, z_0)$ are chosen. The charge density and the EPC's are known.

Let $C(c_x, c_y, c_z)$ be a reference centre. We introduce a sphere of centre C and radius R. The radius is such that in the space outside the sphere, the potential may be treated as the exterior potential. This space is called the « associated exterior space » (AES). The sphere is the « excluded space ». The « smallest excluded sphere », (SES), is the excluded sphere with the smallest possible radius.

From c_x, c_y, c_z, R and the coefficients $A^{\pm}_{nm}$ we can calculate the electrostatic energy stored in the AES :

$$Q_E = \frac{1}{8\pi} \int_v |\ \text{grad}\ V\ |^2\, dv \tag{3.1}$$

This is a quadratic expression of the form

$$Q(c_x, c_y, c_z) = f \sum_{n=i}^{\infty} \sum_{m=0}^{n} W_{nm} \frac{[A^{+}_{nm}(c_x, c_y, c_z)]^2 + [A^{-}_{nm}(c_x, c_y, c_z)]^2}{R^{2n}} \tag{3.2}$$

with

$$W_{nm} = \frac{n+1}{n+1/2} \cdot \frac{1}{\varepsilon_m} \cdot \frac{(n+m)!}{(n-m)!} \tag{3.3}$$

$$i = 0;\ f = 1/4\ R$$

as shown in Appendix C.

Similarly, the integral

$$Q_V = \int_v V^2 dv \tag{3.4}$$

is given by (3.2) with

$$W_{nm} = \frac{1}{n^2 - 1/4} \frac{1}{\varepsilon_m} \frac{(n+m)!}{(n-m)!} \tag{3.5}$$

$$i = 1;\ f = \pi R.$$

In this case, we omit the term in $i = 0$ which is infinite but independent of C and disappears when we go to (3.6).

Consider a quadratic expression Q. Imagine that C is displaced infinitesimally in an arbitary direction, keeping R constant. In general Q varies. Suppose now that there exists a position of C such that Q is stationary.

The conditions of stationarity

$$\sum_{n=i}^{\infty} \sum_{m=0}^{n} \frac{W_{nm}}{R^{2n-1}} \left[A^{+}_{nm} \left(\frac{\partial A^{+}_{nm}}{\partial c_u} \right)_R + A^{-}_{nm} \left(\frac{\partial A^{-}_{nm}}{\partial c_u} \right)_R \right] = 0;\ u = x, y, z \tag{3.6}$$

allow c_x, c_y, c_z to be determined from the coefficients $A^{\pm}_{nm}$ given for a more or less arbitrary reference centre. The necessary transformation relations of these coefficients and of their derivatives are given in Appendices A and B. At this stage, the weights W_{nm} and the radius R are unknown. Our main problem will be to determine them. Point C thus defined may be called the « reference centre corresponding to Q » (RCQ).

Many questions arise here. With a view to finding answers as well as testing the approach, we begin a detailed study of the two-charge system.

§ 4. — Consider again the two-charge system represented in Fig. 1. The ratio of the charges, q, is defined by (2.12). According to (2.4)

$$A_{n0}(c) = (-1)^n (s + c)^n q_A + (s - c)^n q_B \tag{4.1}$$

Applying (3.6) we get

$$\frac{\partial}{\partial c} \left\{ \sum_{n=1}^{\infty} W_{n0} \frac{[(-1)^n (s + c)^n q_A + (s - c)^n q_B]^2}{R^{2n}} \right\} = 0 \tag{4.2}$$

which can be written

$$(s + c) S_{AA} q_A^2 + 2c S_{AB} q_A q_B - (s - c) S_{BB} q_B^2 = 0 \tag{4.3}$$

with

$$S_{AA} = \sum_{n=1}^{\infty} n W_{n0} \left(\frac{s + c}{R} \right)^{2n-2};\ S_{AB} = \sum_{n=1}^{\infty} (-1)^{n-1} n W_{n0} \left(\frac{s^2 - c^2}{R^2} \right)^{n-1};$$

$$S_{BB} = \sum_{n=1}^{\infty} n W_{n0} \left(\frac{s - c}{R} \right)^{2n-2} \tag{4.4}$$

For $c = 0$, (4.3) reduces to

$$q_A^2 = q_B^2 \tag{4.5}$$

Thus, condition (2.13.b) is satisfied independently of the values of R and W_{n0}.

In view of the symmetry of (4.3), the discussion will be limited to $c \geqslant 0$ in the rest of the article. We take c as a parameter and q as the unknown. It is convenient to set $q_B = 1$. Then $q = q_A$. The solutions $q^+(c)$ and $q^-(c)$ are given by

$$q^{\pm}(c) = \frac{-cS_{AB} \pm \sqrt{D}}{(s + c)S_{AA}} \tag{4.6}$$

where

$$D = c^2S_{AB}^2 + (s^2 - c^2)S_{AA}S_{BB} \tag{4.7}$$

For $c = s$, condition (2.13.a) must be satisfied. Therefore

$$q^+(s) = 0 \tag{4.8.a}$$

$$q^-(s) = 0 \tag{4.8.b}$$

Introducing (4.8.b) into (4.6) shows that S_{AA} must diverge for $c = s$.

Since S_{AA} increases with c, we get

$$S_{AA} \text{ diverges for } c \geqslant s \tag{4.9.a}$$

Accordingly, for $c > s$, $D < 0$; the solutions are not real. S_{AA} must not diverge for $c < s$ because one would have $q^{\pm}(c) = 0$ which means that adding a charge of value zero would displace the CRC from s to $c < s$.

Therefore

$$S_{AA} \text{ converges for } c < s \tag{4.9.b}$$

Accordingly, for $c < s$, $D > 0$; there are two real solutions of opposite signs :

$$q^+(c) > 0 \text{ and } q^-(c) < 0 \tag{4.10}$$

According to (4.4) and (4.9), S_{AA} is a series of the form

$$S_{AA} = \sum_i^{\infty} a_i x^i \tag{4.11.a}$$

with a limit of convergence x_L given by

$$x_L = \left(\frac{2s}{R}\right)^2 \tag{4.11.b}$$

We observe here that for

$$R = 2s \tag{4.12}$$

and $c = \pm s$, one of the charges is on the surface of the excluded sphere. For $R > 2s$, the charges are in the excluded sphere. For $R < 2s$, one of the charges is in the AES which is forbidden. Therefore, (4.12) defines a critical value of R. Here we assume that the critical value corresponds to the limit of convergence. Introducing (4.12) into (4.11.b), we find that $x_L = 1$, a plausible and pleasing conclusion.

We now examine the situation for $|c| < s$. The smallest sphere of centre C such that there is no charge outside has a radius $R_m(c)$ given by

$$R_m(c) = s + |c| \tag{4.13}$$

(4.12) is a particular case of (4.13). This suggests that the general expression of R might be

$$R = s + |c| \tag{4.14}$$

Introducing (4.14) into S_{AA} given by (4.4) and taking (4.9 a) into account, we find that S_{AA} diverges for all values of c. This is not acceptable. We therefore reject (4.14) as a possible alternative to (4.12).

Some remarks are appropriate here. The data consist of a constant length, $2s$, and a variable ratio, q, of the charges. It is normal for R to be determined by the length independently of q and therefore of c. A condition at one appropriate point is sufficient for finding R. It is clear that a limit of convergence is an essential property which must lead to an important conclusion or assumption helping to formulate the problem. Although the above considerations do not bring the proof of (4.12), they bring a fairly suggestive basis. On the other hand, this relation appears to be necessary and satisfactory for the development of a treatment. For these reasons and because no objection will arise later, we adopt (4.12). As a corollary of (4.12), the weights must be such as to have no influence on the limit of convergence.

In conclusion, the variational approach satisfies conditions (2.13), (2.14), (2.15) and determines R.

§ 5. — We examine the form of D. Let

$$P = (s^2 - c^2)S_{AA}S_{BB} \tag{5.1}$$

$$x = \frac{s + c}{R} \tag{5.2}$$

For $c \to s$, P contains a factor tending towards 0 and another one towards infinity. We derive an alternative expression free from this drawback.

$$s^2 - c^2 = \frac{s + c}{3s + c}[(2s^2) - (s + c)^2] = \frac{4s^2(s + c)}{3s + c}\left(1 - \frac{R^2}{4s^2}x^2\right) \tag{5.3}$$

$$P = \frac{4s^2(s + c)}{3s + c} SS_{BB} \tag{5.4}$$

where

$$S = \left(1 - \frac{R^2}{4s^2}x^2\right) S_{AA} \tag{5.5}$$

Using (4.4) we get

$$S = W_{10} + \sum_{n=1}^{\infty} \omega_n x^{2n} \tag{5.6}$$

with

$$\omega_{n0} = (n + 1)W_{n+1,0} - \frac{R^2}{4s^2} nW_{n0} \tag{5.7}$$

When the weights W_{n0} are given, (5.7) enables us to determine whether P converges or not.

For $\sqrt{D}$ in (4.9), we may use a two-term approximation if one of the two quantities involved is much smaller than the other one. This gives rise to two approximations for $q^{\pm}(c)$.

If
$$P \ll c^2 S_{AB}^2 \tag{5.8}$$
$$q^{\pm}(c) \cong -(1 \mp 1)\frac{cS_{AB}}{(s+c)S_{AA}} \pm \frac{(s-c)S_{BB}}{2cS_{AB}} \tag{5.9}$$

If
$$P \gg c^2 S_{AB}^2 \tag{5.10}$$
$$q^{\pm}(c) \cong \pm\left[\frac{(s-c)S_{BB}}{(s+c)S_{AA}}\right]^{1/2} - \frac{cS_{AB}}{(s+c)S_{AA}} \pm \frac{c^2 S_{AB}^2}{2(s+c)S_{AA}P^{1/2}} \tag{5.11}$$

The terms in (5.9) and (5.11) are ordered by decreasing magnitude. The important point here is that $|q^+(c)|$ and $|q^-(c)|$ are nearly equal in approximation (5.11), while they are very different in approximation (5.9). Thus if the weights are such that P diverges for $c = s$, $|q^+(c)|$ and $|q^-(c)|$ are nearly equal for c not too different from s.

Suppose that we take R slightly too large which means that the associated exterior space used is somewhat too small. What is the error? The question can be answered for $c = s$, since we know R by (4.12).

Set
$$R = 2s(1+\varepsilon),\ 0 < \varepsilon \ll 1 \tag{5.12}$$

The solutions $q^{\pm}(c)$ are defined up to
$$x = \frac{s+c}{2s(1+\varepsilon)} = 1 \tag{5.13}$$

For $c = s$, $x < 1$, S_{AA} converges, $P = 0$ and therefore
$$q^+(s) = 0;\ q^-(s) = -\frac{S_{AB}}{S_{AA}} \tag{5.14}$$

Set
$$\zeta = -\frac{q^-(s)}{\varepsilon} = -\frac{W_{10}}{\varepsilon S_{AA}} \tag{5.15}$$

where S_{AA} is taken for $x = 1/(1+\varepsilon)$.

ζ defines the sensitivity of $q^-(s)$ towards a slight increase in R by a factor $(1+\varepsilon)$.

§ 6. — The system composed of two charges q_A and q_B, which may be denoted by $A_{00}^{+(A)}$ and $A_{00}^{+(B)}$ respectively, is the first of a family of systems defined by one coefficient at A, $A_{km}^{\pm(A)}$, and one of same species, $A_{km}^{\pm(B)}$, at B. We propose here to generalize the results obtained above for the two-charge system.

From the two chosen coefficients, using (A.21), we find the coefficients of the system corresponding to reference centre C
$$A_{jm}^{\pm}(c) = \frac{(j-m)!}{(j-k)!(k-m)!}\left[(-1)^{j-k}(s+c)^{j-k}A_{km}^{\pm(A)} + (s-c)^{j-k}A_{km}^{\pm(B)}\right] \tag{6.1}$$

where
$$A_{jm}^{\pm}(c) = 0 \text{ for } j < k,\ m > k. \tag{6.2}$$

The condition of stationarity is

$$\frac{\partial}{\partial c}\left\{\sum_{j=k+1}^{\infty} W_{jm}\left[\frac{(j-m)!}{(j-k)!(k-m)!}\right]^2 \frac{[(-1^{j-k}(s+c)^{j-k}A_{km}^{\pm(A)}+(s-c)^{j-k}A_{km}^{\pm(B)})]^2}{R^{2j}}\right\}=0 \tag{6.3}$$

Using the summation index $n = j - k$ and the effective weight system

$$W_{nm}^{(k)} = W_{n+k,m}\left[\frac{(n+k-m)!}{n!(k-m)!}\right]^2 \tag{6.4}$$

(6.3) becomes

$$\frac{\partial}{\partial c}\left\{\sum_{n=1}^{\infty} W_{nm}^{(k)} \frac{[(-1)^n(s+c)^nA_{km}^{\pm(A)}+(s-c)^nA_{km}^{\pm(B)}]^2}{R^{2n}}\right\}=0 \tag{6.5}$$

Clearly, (6.5) has the same form as (4.4). The primitive treatment is directly applicable if we replace W_{n0} by $W_{nm}^{(k)}$, q_A by $A_{km}^{\pm(A)}$, q_B by $A_{km}^{\pm(B)}$. The problem is solved. We observe here that systems with different values of k and different weight sets have identical graphs $c(q)$ if their effective weight sets are equal. This particular form of equivalence has interesting consequences concerning the problem of selecting appropriate weight sets. Applying (6.4) to Q_E and Q_V, we get

$$\text{For } Q_E, \quad W_{nm}^{(k)} = \frac{2n+2k+2}{2n+2k+1}\cdot\frac{(n+k+m)!(n+k-m)!}{(n!)^2}\cdot\frac{1}{\varepsilon_m[(k-m)!]^2} \tag{6.6}$$

$$\text{For } Q_V, \quad W_{nm}^{(j)} = \frac{(n+j)^2-m^2}{(n+j)^2-1/4}\cdot\frac{(n+j-1+m)!(n+j-1-m)!}{(n!)^2}\cdot\frac{1}{\varepsilon_m[(j-m)!]^2} \tag{6.7}$$

The last factors in (6.6) and (6.7) are independent of n. They may be omitted. The first factors are close to 1 for n great. The second factors are identical if

$$j = k + 1 \tag{6.8}$$

Thus, to each system with indices k and m treated by Q_E, we can associate a system with indices $j = k + 1$ and m treated by Q_V. The effective weight systems are practically equal. Therefore, if we neglect minor differences, the two systems have the same solution, the ratios q being defined by

$$q = \begin{cases} A_{k+1,m}^{\pm(A)}/A_{k+1,m}^{\pm(B)} & \text{for system } (k+1, m) \text{ treated with } Q_V \\ A_{km}^{\pm(A)}/A_{km}^{\pm(B)} & \text{for system } (k, m) \text{ treated with } Q_E \end{cases} \tag{6.9}$$

The second factor in (6.6) may be written

$$(n+k+m)\ldots(n+1)(n+k-m)\ldots(n+1)=n^{2k}+(k^2+k+m^2)n^{2k-1}+\ldots \tag{6.10}$$

Accordingly

$$W_{nm}^{(k)} = n^{2k} + (k^2 + k + m^2 + 1/2)n^{2k-1} + \ldots \tag{6.11}$$

Therefore the influence of m is of secondary importance. A similar observation is made with (6.7).

The correspondence relations will find application in § 7 when we try to use the shapes of the curves $c(q)$ for rejecting inappropriate weight sets. Consider the

interesting correlations between Q_E and Q_V, assuming that the shape of the common solutions is acceptable or not for both weight sets. Taking (6.8) into account, we arrive at the following conclusions. (a) All the solutions obtained with Q_E are also obtained with Q_V. If the latter quadratic expression is adequate, so is Q_E. (b) There is one solution, for $j = 0$, obtained with Q_V and not with Q_E. If this solution alone has an unacceptable shape, Q_V is ruled out while Q_E is acceptable.

§ 7. — The problem, now, is the choice of the appropriate quadratic function. The algebraic treatment has not been fruitful in this respect. So, before going further, it is desirable clearly to formulate the objective. We are looking for the definition of a characteristic, unique reference centre. The corresponding Q ought to be a significant expression, such as Q_E or Q_V. Conditions (2.13), (2.14) and (2.15) being satisfied independently of Q, we really have no information which would enable us to prove that the right Q is either Q_E, Q_V or some other Q. However, in a sufficiently broad and detailed treatment, we could perhaps find selective objections.

Numerical solutions have been obtained for the three systems $(A_{k0}^{(A)} + A_{k0}^{(B)})$ with $k = 0, 1, 2$ using four weight systems and seven relations $R(c)$.

Beside those relative to Q_E and Q_V, the following weight sets

$$W_{nm} = \frac{2}{2n+1}\frac{(n+m)!}{(n-m)!} \tag{7.1}$$

and

$$W_{nm} = (n+1)\frac{(n+m)!}{(n-m)!} \tag{7.2}$$

have been used for comparison. The four weight sets are such that

$$W_{nm} \to n^p \text{ for } n \to \infty \tag{7.3}$$

with values of $p = -2, -1, 0, 1$. According to § 6, the effective weight sets have the asymptotic expressions.

$$W_{nm}^{(k)} \to n^{p+2k} \text{ for } n \to \infty. \tag{7.4}$$

For the purpose of testing the conclusion of § 4 and obtaining a better understanding of the R problem, the solutions $q^{\pm}(c)$ have been calculated for seven linear combinations of (4.12) and (4.16).

$$R = \alpha(2s) + (1-\alpha)(s + |c|) = 2s + (\alpha - 1)(s - |c|) \tag{7.5}$$

with

$$\alpha = \frac{1}{8}, \frac{1}{4}, \frac{1}{2}, 1, 2, 4, 8. \tag{7.6}$$

The value

$$s = 0.5 \tag{7.7}$$

has been chosen.

The calculations can be carried out easily. The sums S_{AA}, S_{AB} and S_{BB} have been obtained algebraically as well as numerically. The results may be condensed in 12 diagrams each containing 7 curves corresponding to the several values of α. As anticipated the diagrams corresponding to equal values of $(p + 2k)$ are very

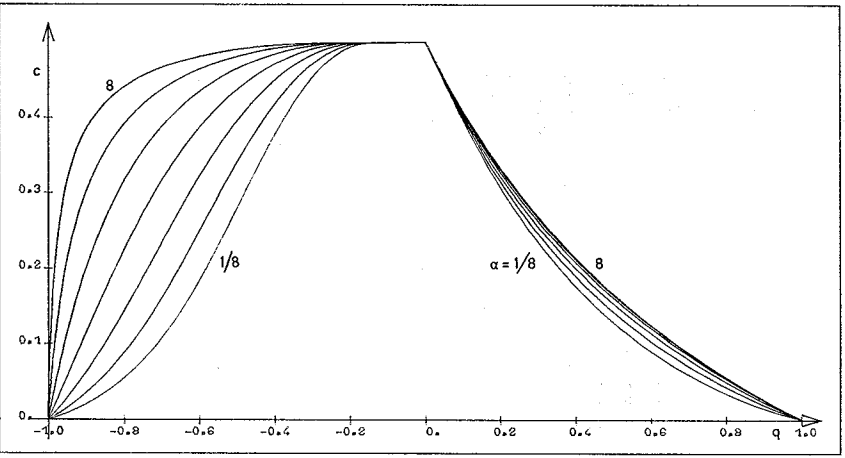

Fig. 2. — c vs. q for $W_{n0} = 4/(4n^2 - 1)$ corresponding to Q_V.

$$\zeta = \frac{4}{3\varepsilon\left[\ln\left(\frac{2}{\varepsilon}\right) - 1\right]}$$

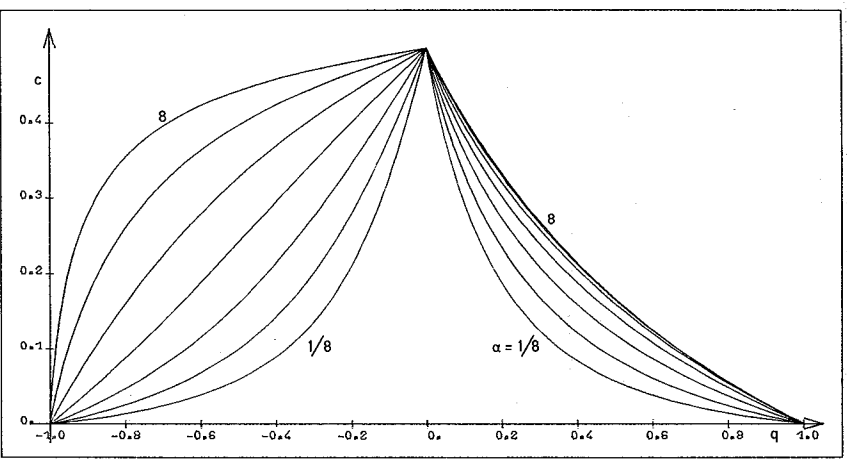

Fig. 3. — c vs. q for $W_{n0} = 2/(2n + 1)$.
$\zeta = 4/3$

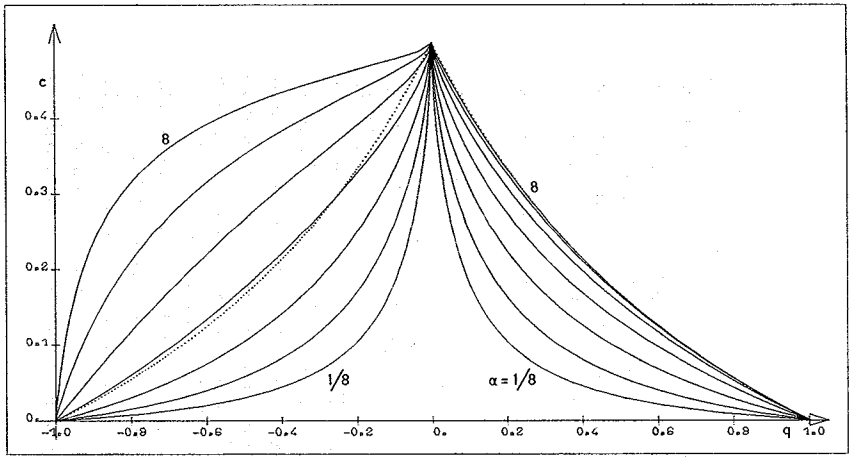

Fig. 4. — c vs. q for $W_{n0} = (2n + 2)/(2n + 1)$ corresponding to Q_E.
$\zeta = 16\varepsilon/3$

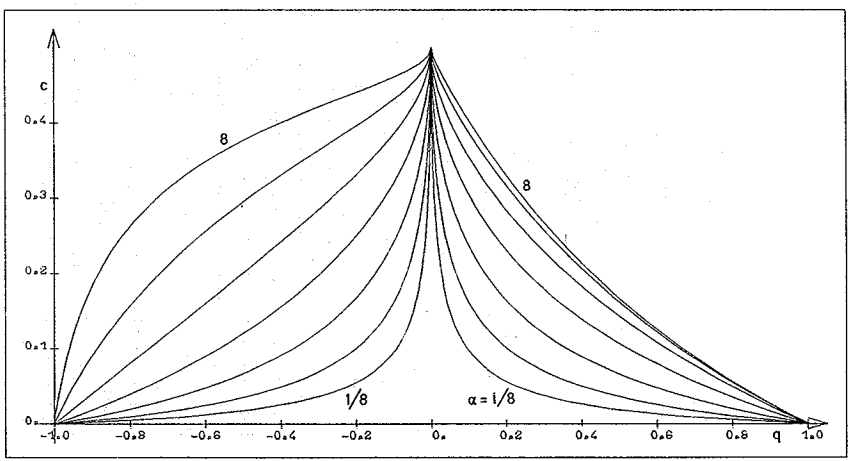

Fig. 5. — c vs. q for $W_{n0} = (n + 1)$.
$\zeta = 8\varepsilon^2$

similar. For the present analysis, it will suffice to consider the case of the two-charge system treated with the four weight sets (Fig. 2 to 5). As regards the diagrams with $(p + 2k) > 1$, we simply note that the trends observed in Fig. 3 to 5 continue to amplify as $(p + 2k)$ increases. In the presentation of the results, we return to q as the independent variable. A curve $c(q)$ is thus composed of two branches corresponding to $q^-(c)$ and $q^+(c)$. In the figures below, there are seven curves for R given by (7.5) and (7.6). The curves are in the order of the values of α, the curve for $\alpha = \frac{1}{8}$ being closest to the q axis. Expressions of the sensitivity defined by (5.15) are given in the captions.

We first examine the case of $(q_A + q_B)$ treated with Q_V (Fig. 2). The seven curves exhibit a horizontal part from $q = 0$ to $q \cong -0.15$. Such an insensitivity of c cannot be accepted for the solution of our problem. Therefore we reject Q_V as inappropriate. The origin of the situation encountered here is very simple. With $p = -2$, the weight set is at the limit permitting divergence of S_{AA} for $c = s$. As a result, P tends towards zero. Approximation (5.9) is valid, with its inherent dissymmetry between q^+ and q^-. A very small decrease in c, near $c = s$, is sufficient for causing an important variation in S_{AA} and consequently in q^-. Another consequence is the very great value of the sensitivity ζ. The curves relative to system $(q_A + q_B)$ treated with Q_E are given in Fig. 4. We first examine the curve for R given by (4.12), i.e. for $\alpha = 1$. The question is : can we find an objection to the shape of the curve? When we discussed simple means of defining the CRC, we were ready to accept (2.6.b) as a satisfactory relation for the two-charge system. The corresponding curve is represented as a dotted line in Fig. 4. The two curves are fairly similar. They are even close to each other for $q < 0$. This observation is gratifying.

Next we compare the two branches. The absolute values of the slopes lead to the following inequalities

$$\left|\frac{dc}{dq}\right| q = -0 < \left|\frac{dc}{dq}\right| q = +0 \tag{7.8}$$

$$\left|\frac{dc}{dq}\right| q = -1 > \left|\frac{dc}{dq}\right| q = 1. \tag{7.9}$$

These account for the observed greater curvature of the positive branch. It is to be noted that (7.8) and (7.9) are not independent because the two branches have the same mean slope in absolute value, i.e. s, and approximately the same shape. What is the origin of (7.8)? Consider a system $(q_A = \gamma,\ q_B = 1)$; γ very small, positive or negative. The boundary of the AES is close to A. We add a very small charge, δq, at A, of the same sign as γ. The electric field increases near A in the AES. The increase is smaller if δq is negative because of some mutual cancellation with the fields due to charge 1 at B. The increase in energy is smaller. The displacement of the sphere is smaller. We thus arrive at (7.8). It is to be pointed out that (7.8) is a property of the approach developped here since it is verified for all values of α and for the other two weight sets ($p = -1$ and $+1$). Can we find an objection to (7.8)? No. (7.8) is quite plausible and there appears to be no basis for comparison.

Fig. 4 allows us to analyse the effect of a variation of R with $|c|$. Starting with very small values of α, we note that the slopes are very small at $q \simeq \pm 1$ and, by compensation, very great in absolute values for $q \simeq 0$. This is normal. Consider, for instance, the situation at $q \simeq \pm 1$, $R \simeq s$. The boundary of the AES is very

close to both charges. A very small displacement of the AES suffices to balance a small variation in q. The sign of q is of secondary importance. With increasing values of α, the curves change gradually. For great values of α and therefore of R, the two branches have quite different shapes. Noteworthy is the steep slope at $q \simeq -1$. The explanation is simple. The system is equivalent to the sum of a non-ideal dipole $(q, -q)$ at 0 and a charge $(1 - q)$ at B. Now, the field of a dipole decreases much more rapidly with increasing distance than does the field of a charge. Therefore, Q_E is very sensitive towards the net charge $(1 - q)$ situated at B. There is no such effect for $q \simeq 1$.

From a careful numerical study, it is seen that the left branch has an inflection point for $\alpha > 1.4758$. This can hardly be considered as a normal property. No lower bound has been found. Clearly, large variations in R are excluded and small variations cause only meaningless effects.

There remains to examine Fig. 3 and 5 in order to complete the picture as regards the influence of the exponent p.

Consider particularly the curves for $\alpha = 1$. The curve in Fig. 3 has an inflection point. The curve in Fig. 5 is similar to the curve in Fig. 4 except that the curvatures of the branches are greater. In this respect, it may be mentioned that the curvatures go on increasing with p. It would thus seem that $p = 0$ is the best value as regards the shape of the curve.

The curve for $\alpha = 1$ and $Q = Q_E$ (Fig. 4) is now used with (4.1) to obtain the corresponding EPC's. The relevant curves are given in Fig. 6. The system composed of two dipoles parallel to the z axis can be treated similarly. The corresponding characteristic curves are given in Fig. 7. There is no apparent objection to the curves in either figure.

The results of the above numerical study may be summed up as follows.

(i) Q_V has been eliminated.

(ii) No objection has appeared against the use of either Q_E or (4.12). On the contrary, there is some positive evidence.

(iii) Frequently in the above discussion, we could do no more than conclude : no objection. This is normal. The definition leads to results going beyond our expectation.

At this stage, we may consider that the variational method based on Q_E and (4.12) satisfies the general conditions of suitability, consistency, uniqueness and significance. We therefore adopt it for the simple systems studied so far. We thus consider that Fig. 6 and 7 give the characteristic reference centre and exterior potential coefficients.

§ 8. — We propose here to extend the method to the case of fairly general systems. Prerequisite is the knowledge of the general transformation relations of the $A^{\pm}_{nm}$ and of their derivatives. The appropriate relations are established in Appendices A and B.

The main problem is the determination of R from the data. As an interesting example, consider a family of systems composed of two charges q_A and q_B distributed spherically around points A and B with densities

$$\rho_X = q_X \frac{p_X(r_X)e^{-\omega_X r_X}}{4\pi \int_0^\infty p_X(r_X)e^{-\omega_X r_X} r_X^2 dr_X}; \quad X = A, B \tag{8.1}$$

where $p_A(r_A)$ and $p_B(r_B)$ are two polynomials.

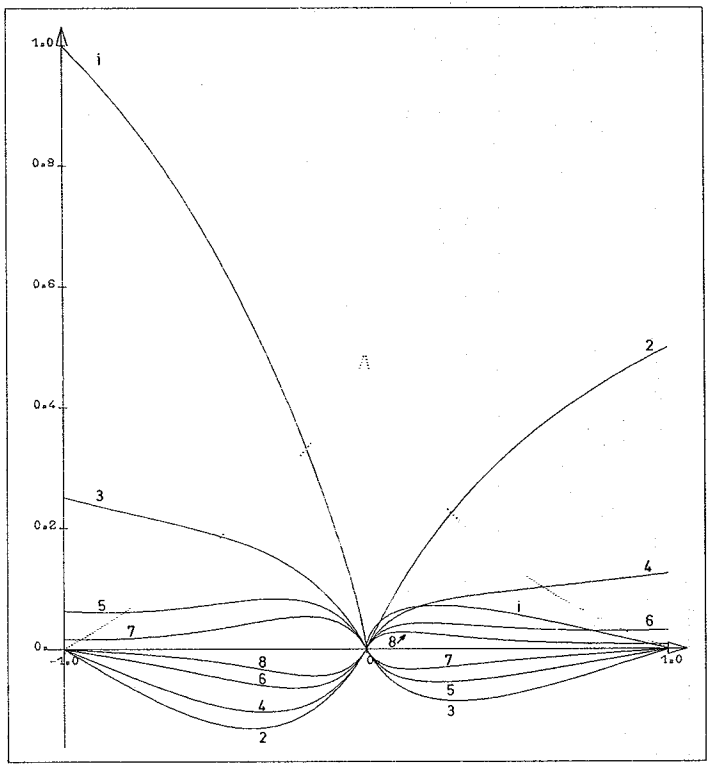

Fig. 6. — Characteristic curves for the two charge system $A_{n0}(q)$ for $n = 1, \ldots, 8$; $c(q)$ dotted line; $q = q_A/q_B$.

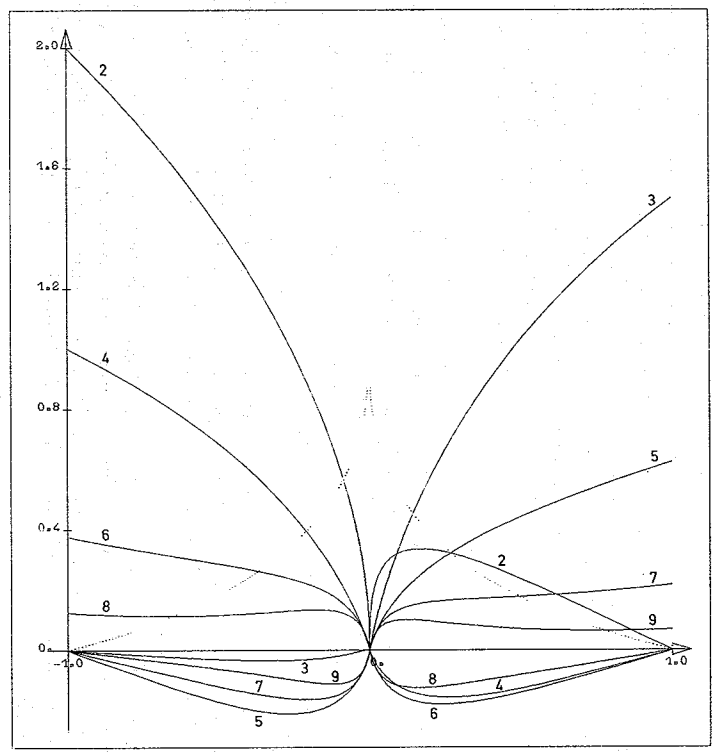

Fig. 7. — Characteristic curves for two dipoles parallel to the axis $A_{n0}(q)$ for $n = 2, \ldots 9$; $c(q)$ dotted line; $q = A_{10}^{-(A)}/A_{10}^{-(B)}$.

The set of constants A_{n0} is the same for all these systems for all reference centres whereas the extent of the charged space varies considerably. With small values of ω_A and ω_B, the charge outside a sphere of radius $R = 2s$ may still be considerable.

In this complicated situation, there seems to be no satisfactory way out unless we assign the following property to the CRC.

(1) All systems with the same set of constants $A^{\pm}_{nm}$ have the same CRC. In other words, the CRC is a property of the $A^{\pm}_{nm}$ set, the other characteristics of the charge distribution having no effect.

This leads us to giving up the classical exterior space — which may be called the exterior charge space — based on the vanishing of the charge density and adopting the following basic specification.

(2) The exterior space relevant to the problem under consideration is the exterior potential space defined as the space outside a sphere of centre 0 and radius R_0, such that the series (1.3) expressing the exterior potential, converges. 0 is the reference centre. R_0 is the distance between 0 and the farthest point for which the series diverges. This space is defined completely by the set of potential coefficients $A^{\pm}_{nm}$ corresponding to centre 0.

The value of R_0 depends upon the position of the centre. We assume here that R_0 has a smallest value, R_S, for the centre at point 0_S. The sphere of centre 0_S and radius R_S is the smallest excluded sphere (SES). R_S is a characteristic length of the system.

Examining our results on simple axial systems from the present point of view, we note that the two exterior spaces coincide. Thus (4.12) may be written

$$R = 2R_S \tag{8.2}$$

The question arises : may (8.2) be general? From the axial systems studied, we can generate fairly general axial or non-axial systems by adding charges anywhere in the SES (including the surface). The additional off-axis points change nothing as regards R_S and R; (8.2) still holds. In view of the great number and variety of the new systems, the validity of (8.2) cannot be limited to particular $A^{\pm}_{nm}$ sets.

(3) Accordingly, (8.2) may be taken as general.

The problem, now, is to find R_S. If the set of coefficients $A^{\pm}_{nm}$ corresponds to a finite number of coefficients relative to a finite number of points, we simply determine the smallest sphere such that none of these points is outside. In the general case, the resolution may be more laborious. Various methods may be devised. For instance, we may use the limit of convergence of Q_E at decreasing radius R_v and proceed by iteration. We start cycle i with a new reference centre $0^{(i)}$. We calculate the new coefficients $A^{\pm}_{nm}$. From these we compute Q_E for successively smaller values of R_v. We thus determine the smallest value $R_v^{(i)}$ for which Q_E converges. Normally, $R_v^{(i)} > R_S$ because $0^{(i)}$ does not coincide with the centre 0_S of the SES. We therefore choose another reference centre $0^{(i+1)}$ either according to a systematic exploration program or by application of a procedure leading to a better reference centre. For instance we may determine $0^{(i+1)}$ by the condition of minimum of Q_E using $0^{(i)}$ and $R_v^{(i)}$; the calculation, using (3.6), is formally identical with the determination of the CRC. We proceed to cycle $(i + 1)$ which gives $R_v^{(i+1)}$, and so on. The smallest

$R_v^{(k)}$ is the best approximation to R_S. From the definition (5.15) of the sensitivity ξ and its value $(16\varepsilon/3)$, it seems that R_S need not be determined with a very great accuracy.

It is possible that, for R_S, we find a vanishingly small value. Then the reference centre is the CRC. This case is met when the coefficients $A_{nm}^{\pm}$ vanish for n greater than a certain integer j. This has been discussed above. Thus we realize the importance of using the complete $A_{nm}^{\pm}$ set. If we truncate the set, Q_E necessarily converges everywhere, except at the reference centre chosen. Some judgement must therefore be exercised.

§ 9. — Consider a double system composed of a constant part consisting in a small number of coefficients $A_{nm}^{\pm}$ located at B and a variable part located at A. For the latter, we simply take a charge q. Fig. 1 is used again as regards A, 0, C, B and their coordinates.

Initially, $q = 0$. Part B is alone; $R_S = 0$; $c = s$. We then vary q continuously, R_S varies discontinuously : $R_S = s$ for $q \neq 0$. The question arises : is the resulting variation in c continuous or discontinuous? Part A in itself is unable to produce a discontinuity in c. Therefore the question is : does the CRC of part B alone vary when R_S varies from 0 to s? To clarify the question consider a system defined by

$$A_{00} \text{ and } A_{10} \text{ at B, nothing at A.} \tag{9.1}$$

The problem is to find c as a function of R. It is solved easily using the method of § 4 adapted to a monocentric system. Now, point B is taken as the origin. c is the coordinate of the CRC defined from the new origin. The appropriate variables are (c/R) and $(RA_{00}/A_{10}) = q_{01}$, playing the role of the former variables c and q. The result is given in Fig. 8, curve 01. We observe that (c/R) reaches notable values for $q_{01} \sim 2$. The explanation is simple. The exterior potential is made up of a contribution from A_{10} having the same sign over the whole of the exterior space, and a contribution from A_{00} which changes signs with z. The field is dissymmetric with respect to B. Therefore the CRC is not at B. It is displaced towards the region of greatest absolute values of the potential. For $q_{01} = 0$ and ∞, the system reduces to one component, $(c/R) = 0$. The extremum is accounted for directly.

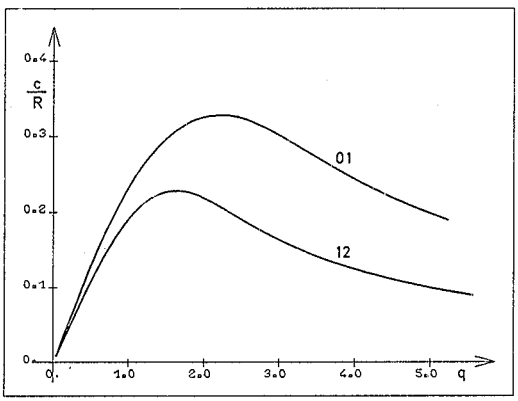

Fig. 8. — Curve 01 : (c/R) vs. $q_{01} = RA_{00}/A_{10}$
curve 12 : (c/R) vs. $q_{12} = RA_{10}/A_{20}$.

Curve 12 obtained for the system

$$A_{10} \text{ and } A_{20} \text{ at B, nothing at A} \tag{9.2}$$

is similar to curve 01. The observations and explanations are confirmed.

We may generalize our conclusions as follows. The CRC of a system may be stable or unstable with respect to a sudden change in the radius R caused by the addition of a potential coefficient at a point outside the excluded sphere. For a system with $R = 0$, instability occurs if the exterior potential is dissymmetric; the jump in c may be notable.

§ 10. — The evidence collected in the above exploration clearly shows that there is a remarkable possibility of defining the CRC. Accordingly, the following definition of the characteristic reference centre (CRC) is proposed. Consider a system for which we know the exterior potential coefficients A_{nm} and B_{nm}, denoted here by $A^{\pm}_{nm}$. Assume that the $A^{\pm}_{nm}$ set allows to define a smallest excluded sphere (SES), of centre 0_S and radius R_S, such that the exterior potential converges everywhere outside the sphere. Consider now the space outside a sphere of variable centre C and radius $R = 2R_S$, called the associated exterior space (AES). Let Q_E be the expression corresponding to the electrostatic energy stored in the AES of centre C. The CRC is the centre for which Q_E is stationary. The characteristic exterior potential coefficients (CEPC) are the coefficients $A^{\pm}_{nm}$ corresponding to the CRC. From these, the characteristic multipole moments are obtained by known relations [1],[4].

R_S may be obtained as explained at the end of § 8. Q_E is defined by (3.1) which leads to (3.2) and (3.3). The stationarity conditions are given by (3.6) using the transformation relations obtained in Appendices A and B for the coefficients $A^{\pm}_{nm}$ and their derivatives.

With some simple systems, the condition of stationarity leads to a second degree equation. We took advantage as much as possible of this circumstance which enabled us to have a direct view into the problem. In practical applications, the data are the potential coefficients $A^{\pm}_{nm}$, the unknowns are the coordinates c_x, c_y, c_z. These have to be determined as the zeros of a system of three simultaneous equations (3.6). Symmetry may require the CRC to be on a known plane or axis. This reduces the number of unknowns to two or one. No comment is necessary here, except perhaps that iteration using the Newton approximation is possible since we can easily find the second order derivatives of the $A^{\pm}_{nm}$ as pointed out in Appendix B.

APPENDIX A

TRANSFORMATION OF THE SURFACE HARMONICS AND CORRESPONDING INTEGRALS

Consider two cartesian coordinate systems such that an arbitrary point P has coordinates x_1, y_1, z_1 in the first system and

$$x_2 = x_1 - c_x, \quad y_2 = y_1 - c_y, \quad z_2 = z_1 - c_z \tag{A.1}$$

in the second system. The corresponding spherical coordinates are $r_j, \vartheta_j, \varphi_j$, $j = 1,2$.

For convenience, we introduce the following symbols, for $j = 1, 2$:

$$S^{+(j)}_{mn} = r_j^n Y^e_{mn}(\vartheta_j, \varphi_j); \; S^{-(j)}_{mn} = r_j^n Y^0_{mn}(\vartheta_j, \varphi_j) \tag{A.2}$$

$$A^{+(j)}_{nm} = A^{(j)}_{nm}; \; A^{-(j)}_{nm} = B^{(j)}_{nm} \tag{A.3}$$

By definition

$$S_{0n}^{-(j)} = A_{n0}^{-(j)} = 0;\ S_{mn}^{\pm(j)} = A_{nm}^{\pm(j)} = 0 \text{ for } m > n \tag{A.4}$$

and their derivatives with respect to c_x, c_y and c_z are also equal to zero.

$$t^{+}(\mathrm{mu}) = \cos(\mathrm{mu});\ t^{-}(\mathrm{mu}) = \sin(\mathrm{mu}) \tag{A.5}$$

The integral representations given by Morse and Feshbach [2] are, in the present notations

$$S_{mn}^{\pm(j)} = \frac{1}{2\pi i^m} \cdot \frac{(n+m)!}{n!} \int_0^{2\pi} X_j^n t^{\pm}(\mathrm{mu}) du \tag{A.6}$$

where

$$X_j = z_j + ix_j t^{+}(u) + iy_j t^{-}(u), \quad j = 1, 2. \tag{A.7}$$

Firstly, we propose to find the relations between the $S_{mn}^{\pm(2)}$ and $S_{gh}^{\pm(1)}$, using integral representations as clearly explained by Morse and Feshbach. These authors [3] establish the relations for $c_z \neq 0$, $c_x = c_y = 0$, viz

$$S_{mn}^{\pm(2)} = \sum_{l=m}^{n} (-1)^{n-l} \cdot \frac{(n+m)!}{(n-l)!(l+m)!} \cdot c_z^{n-l} S_{ml}^{\pm(1)} \tag{A.8}$$

in our notations.

We apply the same method in the case $c_x \neq 0$, $c_y = c_z = 0$

$$X_2 = X_1 - ic_x t^{+}(u) \tag{A.9}$$

$$S_{mn}^{\pm(2)} = \frac{1}{2\pi i^m} \cdot \frac{(n+m)!}{n!} \int_0^{2\pi} [X_1 - ic_x t^{+}(u)]^n t^{\pm}(\mathrm{mu}) du$$

$$= \frac{1}{2\pi i^m} \sum_{l=0}^{n} \frac{(n+m)!}{l!(n-l)!} (-ic_x)^l \int_0^{2\pi} X_1^{n-l} \cdot [t^{+}(u)]^l t^{\pm}(\mathrm{mu}) du. \tag{A.10 a}$$

Now, using Simpson's formulae, we easily find by recurrence

$$[t^{+}(u)]^l t^{\pm}(\mathrm{mu}) = \frac{1}{2^l} \sum_{k=0}^{l} \frac{l!}{k!(l-k)!} t^{\pm}[(m+l-2k)u]. \tag{A.11 a}$$

Introducing (A.11 a) into (A.10 a) we get

$$S_{mn}^{\pm(2)} = \sum_{l=0}^{n} \sum_{k=0}^{l} \frac{(-1)^l}{2\pi i^{m-l}} \cdot \frac{(n+m)!}{k!(l-k)!(n-l)!} \cdot \frac{1}{2^l} \cdot c_x^l \int_0^{2\pi} X_1^{n-l} t^{\pm}[(m+l-2k)u] du \tag{A.12}$$

We write

$$t^{\pm}[(m+l-2k)u] = s_{m+l-2k}^{\pm} \cdot t^{+}(|m+l-2k \mid u) \tag{A.13}$$

with

$$s_{m+l-2k}^{\pm} = \begin{cases} 1 & \text{for } m+l-2k \geqslant 0 \\ \pm 1 & \text{for } m+l-2k < 0 \end{cases} \tag{A.14}$$

We introduce (A.13) into (A.11 a) and eliminate the integrals by (A.6).

We get

$$S^{\pm(2)}_{mn} = \sum_{l=0}^{n} \sum_{k=0}^{l} \sigma^{\pm}_{mlk} \cdot F_{nmlk} \cdot c_x^l \cdot S^{\pm(1)}_{|m+l-2k|,n-l} \tag{A.15a}$$

where
$$F_{nmlk} = \frac{(n+m)!}{k!(l-k)!(n-l+|m+l-2k|)!2^l} \tag{A.16}$$

$$\sigma^{\pm}_{mlk} = (-1)^k \cdot i^{|m+l-2k|-(m+l-2k)} \cdot s^{\pm}_{m+l-2k} \tag{A.17}$$

or
$$\sigma^{\pm}_{mlk} = \begin{cases} (-1)^k \text{ for } m+1-2k \geqslant 0 \\ \pm(-1)^{l+m+k} \text{ for } m+l-2k < 0 \end{cases} \tag{A.18}$$

The case of $c_y \neq 0$, $c_x = c_z = 0$ is treated similarly with appropriate modifications

$$S^{\pm(2)}_{mn} = \frac{1}{2\pi i^m} \sum_{l=0}^{n} \frac{(n+m)!}{l!(n-l)!} \cdot (-ic_y)^l \int_0^{2\pi} X_1^{n-l} [t^-(u)]^l t^{\pm}(mu) du \tag{A.10 b}$$

$$[t^-(u)]^l t^{\pm}(mu) = \frac{1}{2^l} \sum_{k=0}^{l} (-1)^k \cdot \frac{l!}{k!(l-k)!} \left\{ t^+\left(\frac{l\pi}{2}\right) t^{\pm}[(m+l-2k)u] \right.$$
$$\left. \pm t^-\left(\frac{l\pi}{2}\right) t^{\mp}[(m+l-2k)u] \right\} \tag{A.11 b}$$

$$S^{\pm(2)}_{mn} = \sum_{l=0}^{n} \sum_{k=0}^{l} (-1)^k \cdot F_{nmlk} \cdot c_y^l \left\{ t^+\left(\frac{l\pi}{2}\right) \cdot \sigma^{\pm}_{mlk} \cdot S^{\pm(1)}_{|m+l-2k|,n-l} \right.$$
$$\left. \pm t^-\left(\frac{l\pi}{2}\right) \cdot \sigma^{\mp}_{mlk} \cdot S^{\mp(1)}_{|m+l-2k|,n-l} \right\} \tag{A.15 b}$$

In conclusion, the transformation relations between $S^{\pm(2)}_{nm}$ and $S^{\pm(1)}_{gh}$ are given by (A.8) and (A.15).

We propose now to find the relations between $A^{\pm(2)}_{nm}$ and $A^{\pm(1)}_{hg}$. With the present notations, (1.4) may be written

$$\int S^{\pm(j)}_{gh} \rho dv = \frac{1}{\varepsilon_g} \frac{(h+g)!}{(h-g)!} A^{\pm(j)}_{hg} \tag{A.19}$$

Now, consider each relation (A.8) and (A.15), multiply by the space charge density at point P, integrate over the whole space and eliminate the integrals by (A.19). The relations obtained result directly from the substitution

$$S^{\pm(j)}_{gh} \to \frac{1}{\varepsilon_g} \cdot \frac{(h+g)!}{(h-g)!} \cdot A^{\pm(j)}_{hg} \tag{A.20}$$

for all relevant values in the primitive relations. There remains to multiply each equation by $\varepsilon_m(n-m)!/(n+m)!$ and we get

$$A^{\pm(2)}_{nm} = \sum_{l=m}^{n} (-1)^{n-l} \frac{(n-m)!}{(n-l)!(l-m)!} \cdot c_z^{n-l} \cdot A^{\pm(1)}_{lm} \tag{A.21}$$

$$A_{nm}^{(2)\pm} = \sum_{l=0}^{n} \sum_{k=0}^{l} G_{nmlk} \cdot c_x^l \cdot \sigma_{mlk}^{\pm} A_{n-l,|m+l-2k|}^{\pm(1)} \tag{A.22.a}$$

$$A_{nm}^{\pm(2)} = \sum_{l=0}^{n} \sum_{k=0}^{l} (-1)^k \cdot G_{nmlk} \cdot c_y^l \left\{ t^{+}\left(\frac{l\pi}{2}\right) \cdot \sigma_{mlk}^{\pm} \cdot A_{n-l,|m+l-2k|}^{\pm(1)} \right.$$

$$\left. \pm t^{-}\left(\frac{l\pi}{2}\right) \sigma_{mlk}^{\mp} A_{n-l,|m+l-2k|}^{\mp(1)} \right\} \tag{A.22.b}$$

where

$$G_{nmlk} = \frac{\varepsilon_m}{\varepsilon_{|m+l-2k|}} \cdot \frac{(n-m)!}{k!(l-k)!(n-l-|m+l-2k|)!2^l} \tag{A.23}$$

$S_{mn}^{\pm(2)}$ and $A_{mn}^{\pm(2)}$ corresponding to a displacement c_x, c_y, c_z can be obtained in three successive steps, using the above relations in any order.

APPENDIX B

THE DERIVATIVES $\frac{\partial}{\partial c_x}(S_{mn}^{\pm(2)})$, $\frac{\partial}{\partial c_x}(A_{nm}^{\pm(2)})$, ETC...

The definitions, methods and notations are those of Appendix A. We wish to find the derivatives as functions of the quantities relative to the same cartesian system.

1) $X_2 = X_1 - c_z$ (B.1)

According to (A.6)

$$\frac{\partial}{\partial c_z} S_{mn}^{\pm(2)} = -\frac{1}{2\pi i^m} \cdot \frac{(n+m)!}{(n-1)!} \int_0^{2\pi} X_2^{n-1} t^{\pm}(\mathrm{mu}) du \tag{B.2}$$

Thence

$$\frac{\partial}{\partial c_z}(S_{mn}^{\pm(2)}) = -(n+m)\, S_{m,n-1}^{\pm(2)} \tag{B.3}$$

2) $X_2 = X_1 - ic_x t^{+}(u)$ (B.4.a)

$$\frac{\partial}{\partial c_x}(S_{mn}^{\pm(2)}) = -\frac{1}{2\pi i^{m-1}} \cdot \frac{(n+m)!}{(n-1)!} \int_0^{2\pi} X_2^{n-1} t^{+}(u) t^{\pm}(\mathrm{mu}) du \tag{B.5.a}$$

For $m = 0$

$$\frac{\partial}{\partial c_x}(S_{0n}^{+(2)}) = S_{1,n-1}^{+(2)}; \quad \frac{\partial}{\partial c_x}(S_{0n}^{-(2)}) = 0 \tag{B.6.a}$$

For $m > 0$, using (A.11.a)

$$\frac{\partial}{\partial c_x}(S_{mn}^{\pm(2)}) = -\frac{1}{2\pi i^{m-1}} \frac{(n+m)!}{(n-1)!} \cdot \frac{1}{2} \int_0^{2\pi} X_2^{n-1} \left\{ t^{\pm}[(m+1)u] + t^{\pm}[(m-1)u] \right\} du \tag{B.7.a}$$

We eliminate the integrals using (A.6). We get

$$\frac{\partial}{\partial c_x}(S^{\pm(2)}_{mn}) = \frac{1}{2}[S^{\pm(2)}_{m+1,n-1} - (n+m)(n+m-1)S^{\pm(2)}_{m-1,n-1}] \tag{B.8.a}$$

3) $X_2 = X_1 - ic_y t^-(u)$ (B.4.b)

$$\frac{\partial}{\partial c_y}(S^{\pm(2)}_{mn}) = -\frac{1}{2\pi i^{m-1}} \cdot \frac{(n+m)!}{(n-1)!} \int_0^{2\pi} X_2^{n-1} t^-(u) t^{\pm}(mu) du \tag{B.5.b}$$

For $m = 0$

$$\frac{\partial}{\partial c_y}(S^{+(2)}_{0n}) = S^{-(2)}_{1,n-1}\ ;\ \frac{\partial}{\partial c_y}(S^{-(2)}_{0n}) = 0 \tag{B.6.b}$$

For $m > 0$, using (A.11.b)

$$\frac{\partial}{\partial c_y}(S^{\pm(2)}_{mn}) = -\frac{1}{2\pi i^{m-1}} \cdot \frac{(n+m)!}{(n-1)!} \cdot \frac{1}{2} \int_0^{2\pi} X_2^{n-1} \left\{ \pm t^{\mp}[(m+1)u] \mp t^{\mp}[(m-1)u] \right\} du \tag{B.7.b}$$

$$\frac{\partial}{\partial c_y}(S^{\pm(2)}_{mn}) = \pm \frac{1}{2}[S^{\mp(2)}_{m+1,n-1} + (n+m)(n+m-1)S^{\mp(2)}_{m-1,n-1}] \tag{B.8.b}$$

Relations (B.6) and (B.7) can be condensed into the following relations

$$\frac{\partial}{\partial c_x}(S^{\pm(2)}_{mn}) = \frac{(1 \pm \delta_{0m})}{2}[S^{\pm(2)}_{m+1,n-1} - (n+m)(n+m-1)S^{\pm(2)}_{m-1,n-1}] \tag{B.9.a}$$

$$\frac{\partial}{\partial c_y}(S^{\pm(2)}_{mn}) = \pm \frac{(1 \pm \delta_{0m})}{2}[S^{\mp(2)}_{m+1,n-1} + (n+m)(n+m-1)S^{\mp(2)}_{m-1,n-1}] \tag{B.9.b}$$

valid for $m = 0, 1, 2, \ldots$

We get the relations between the A's as explained in Appendix A :

$$\frac{\partial}{\partial c_z}(A^{\pm(2)}_{nm}) = -(n-m)A^{\pm(2)}_{n-1,m} \tag{B.10}$$

$$\frac{\partial}{\partial c_x}(A^{\pm(2)}_{nm}) = \frac{(1 \pm \delta_{0m})}{2}\left[\frac{\varepsilon_m}{\varepsilon_{m+1}}(n-m)(n-m-1)A^{\pm(2)}_{n-1,m+1} - \frac{\varepsilon_m}{\varepsilon_{m-1}}A^{\pm(2)}_{n-1,m-1}\right] \tag{B.11.a}$$

$$\frac{\partial}{\partial c_y}(A^{\pm(2)}_{nm}) = \pm \frac{(1 \pm \delta_{0m})}{2}\left[\frac{\varepsilon_m}{\varepsilon_{m+1}}(n-m)(n-m-1)A^{\mp(2)}_{n-1,m+1} + \frac{\varepsilon_m}{\varepsilon_{m-1}}A^{\mp(2)}_{n-1,m-1}\right] \tag{B.11.b}$$

Derivatives of higher order can be obtained easily from (B.3) and (B.9), (B.10) and (B.11) without recourse to the integral representations.

APPENDIX C.

THE EXPRESSION OF Q_E

Applying Green's theorem, (3.1) becomes

$$8\pi Q_E = \int_S V(\nabla V \cdot dS) - \int_v V\nabla^2 V dv. \tag{C.1}$$

The last term vanishes owing to Laplace's equation. In the remaining integral, the contribution from the surface at infinity vanishes. Therefore

$$8\pi Q_E = \int_{\tau=-1}^{+1} \int_{\varphi=0}^{2\pi} \left[V \left(\frac{\partial V}{\partial r} \right)_{\tau,\varphi} \right]_{r=R} R^2 d\tau d\varphi \qquad (C\,2)$$

The derivative is obtained directly from (1.3). Taking into account the orthogonality of the harmonic polynomials and the values of the normalizing integrals, we obtain (3.2) with (3.3).

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