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The electrostatic energy of a lattice of point charges

by

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ABSTRACT. — By a correct application of Poisson's formula, the Born-Landé expression (of the electrostatic lattice energy) is related to the Ewald energy. A general expression of the Ewald energy is given. The limit volumic energy is defined and related to the Born-Lande expression and to the Ewald energy. With the help of Plancherel's theorem and Poisson's formula, the results are given in two forms: in the usual space and in the dual space. Precise conditions about the existence of the energies and the validity of the results, are specified. Owing to the long-range $\frac{1}{r}$ dependence of the electrostatic energy, the volumic electrostatic energy depends on the atomic configuration of the surface of the crystal (its minimum—for a suitable choice of the surface—being the Ewald energy).

RÉSUMÉ. — Par une application correcte de la formule de Poisson, l'expression de Born et Landé (pour l'énergie électrostatique de réseau) est reliée à l'énergie d'Ewald. Une expression générale de l'énergie d'Ewald est donnée. L'énergie volumique limite est définie et reliée à l'expression de Born et Landé et à l'énergie d'Ewald. A l'aide du théorème de Plancherel et de la formule de Poisson, les résultats sont exprimés sous deux formes : dans l'espace habituel et dans l'espace dual. Les conditions concernant l'existence des énergies et la validité des résultats, sont précisées. A cause de la décroissance lente en $\frac{1}{r}$ de l'énergie électrostatique avec la distance, l'énergie électrostatique volumique dépend de la configuration atomique de la surface du cristal (son minimum — pour un choix convenable de la surface — étant l'énergie d'Ewald).

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1. GENERAL INTRODUCTION

We consider a crystal lattice of point charges (these may represent the ions of an ionic crystal). There exists a finite set of point charges S (origin cell) and a basis $\mathscr{B} = \{ \vec{a}_1, \vec{a}_2, \vec{a}_3 \}$ (cell basis) of the euclidean space E such that:

the positions of all the point charges are represented by the vectors $\vec{n} + \vec{s}$, where $\vec{n}$ belongs to the lattice $L = \mathbb{Z}\vec{a}_1 + \mathbb{Z}\vec{a}_2 + \mathbb{Z}\vec{a}_3$ and $\vec{s} \in S$; (1)

the representation $(\vec{n}, \vec{s})$ of each point charge is unique; (2)

the electric charge at $(\vec{n}, \vec{s})$ does not depend on the lattice vector $\vec{n}$, and is denoted by $q_{\vec{s}}$; (3)

S is electrically neutral:

$$\sum_{\vec{s} \in S} q_{\vec{s}} = 0 . \tag{4}$$

Note that. — *i)* for a given crystal, the cell S and the cell basis $\mathscr{B}$ (defined as above) are not unique (see fig. 1); *ii)* S is not necessarily included in a cell parallelepiped $C = [0, 1[\vec{a}_1 + [0, 1[\vec{a}_2 + [0, 1[\vec{a}_3$ (with arbitrary origin).

The electrostatic energy of the crystal may be written as

$$\mathscr{E} = \sum_{\substack{\{\vec{n}+\vec{s},\, \vec{p}+\vec{t}\} \\ \vec{n}+\vec{s} \neq \vec{p}+\vec{t}}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{n} + \vec{s} - \vec{p} - \vec{t} \|} = \frac{1}{2} \sum_{\vec{n}} \sum_{\vec{p}} \sum_{\vec{s}} \sum_{\substack{\vec{t} \\ \vec{n}+\vec{s} \neq \vec{p}+\vec{t}}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{n} + \vec{s} - \vec{p} - \vec{t} \|} \tag{5}$$

$$= \frac{1}{2} \sum_{\vec{p}} \sum_{\vec{m}} \sum_{\vec{s}} \sum_{\substack{\vec{t} \\ \vec{m}+\vec{s} \neq \vec{t}}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|},$$

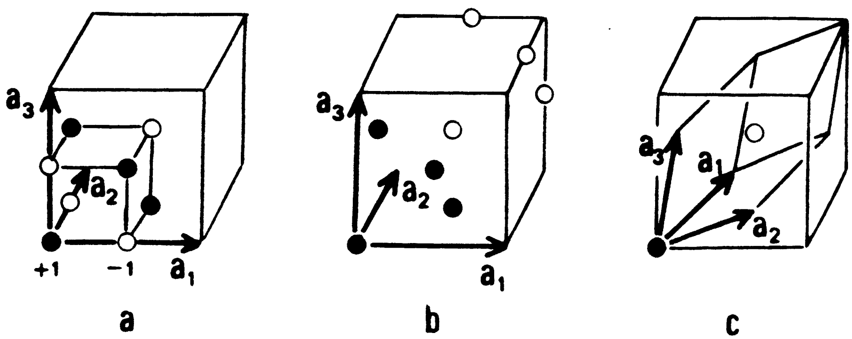

FIG. 1. — Three cells $(S, \mathscr{B})$—as defined by (1) to (4)—for NaCl. In each case (*a*, *b* or *c*), the ions of S are indicated by white and black circles, and $\mathscr{B} = \{ \vec{a}_1, \vec{a}_2, \vec{a}_3 \}$. Only the cell of case *a* has a dipole moment $\vec{M}$ equal to $\vec{O}$.

where: $\vec{n}$, $\vec{p}$, $\vec{m} \in \mathrm{L}$ (lattice vectors); $\vec{m} = \vec{n} - \vec{p}$; $\vec{s}$, $\vec{t} \in \mathrm{S}$. If $\vec{m}$ runs over the whole lattice L, we have

$$\mathscr{E} = \frac{1}{2}\mathrm{N} \sum_{\substack{\vec{m} \\ \vec{m}+\vec{s}\neq\vec{t}}} \sum_{\vec{s}} \sum_{\vec{t}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|}$$

where N is the number of cells. We are thus led to the following expression of the energy per cell:

$$\mathrm{E}_0 = \frac{1}{2} \sum_{\substack{\vec{m}\in\mathrm{L} \\ \vec{m}+\vec{s}\neq\vec{t}}} \sum_{\vec{s}\in\mathrm{S}} \sum_{\vec{t}\in\mathrm{S}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|}, \tag{6}$$

which was first proposed by Born and Landé [1]. After the particular calculation of Madelung [2], the first general result is that of Ewald [3], which may be written in the energy form

$$\mathrm{E}_0 = \mathrm{E}_\mathrm{E}, \tag{7}$$

the « Ewald energy » E_E being expressed in the form: $\mathrm{E}_\mathrm{E} = \mathrm{E}_1 - \mathrm{E}_2 + \mathrm{E}_3$, where E_1 is a sum in the dual lattice L^*, E_2 a finite sum, and E_3 a sum in L. Bertaut [4] obtained the same result (7), but with a more general expression for E_E.

Nevertheless, there are two errors in the preceding considerations:

1) In the Born-Landé expression E_0, the sum on $\vec{m}$ is generally not absolutely convergent: its value depends on the mode of summation on $\vec{m}$, which must be precised. Ewald's equality (7) is not correct and must be replaced by

$$\mathrm{E}_0 = \mathrm{E}_\mathrm{E} + \mathrm{E}'$$

where E' depends on the mode of summation on $\vec{m}$ ([5]: general lattice and ellipsoidal mode of summation, E' deduced from the potential; [6]: cubic lattice and spherical mode of summation; [7] [9] [10] and the present paper: general expressions).

2) The Born-Landé sum E_0 generally does not represent the energy per cell. We may note that the above considerations leading to (6) are contradictory: the crystal is supposed to be at the same time infinite ($\vec{m}$ runs over the whole lattice) and finite (N cells). A correct definition is that of the « limit energy per cell » E [9]; it is the limit of the energy of a finite crystal (formed by a finite number of cells) divided by its number of cells, when this number tends towards $+\infty$:

$$\mathrm{E} = \frac{1}{2} \lim_{k\to+\infty} \frac{1}{\mathrm{card}\, \mathrm{A}_k} \sum_{\substack{\vec{n}\in\mathrm{A}_k \\ \vec{n}+\vec{s}\neq\vec{p}+\vec{t}}} \sum_{\vec{p}\in\mathrm{A}_k} \sum_{\vec{s}\in\mathrm{S}} \sum_{\vec{t}\in\mathrm{S}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{n} + \vec{s} - \vec{p} - \vec{t} \|} \tag{8}$$

(according to (5); each $A_k + S$ represents a finite crystal, A_k being a finite subset of L; expressions of E are given in [*7* to *10*] and the present paper).

This paper presents the proof of our results [*9*] [*10*]. Section 2 introduces the method. We apply Poisson's formula to a sequence of functions f_N (sections 3 to 5) and take the limit of this formula when $N \to +\infty$ (sections 6 and 7). We obtain the relation between the Born-Landé expression E_0 and a generalized form of the Ewald energy E_E (section 7). This result is written in an integral form in section 8. With the help or Plancherel's theorem and Poisson's formula relative to the Dirac measure, a dual form of the result is obtained (section 9). The limit energy per cell E is then related to the Born-Landé expression E_0 (section 10; integral form in section 11). By application of Plancherel's theorem and Poisson's formula relative to the Dirac measure, a dual form of this result is given (sections 12 and 13). In section 14, these results are illustrated with the example of the spherical crystal. Section 15 summarizes the results.

2. INTRODUCTION TO THE METHOD USED

Our method consists of a correct application of Poisson's formula to a sequence of functions f_N, and then to take the limit when $N \to +\infty$. In order to define the functions f_N, we need to recall (very briefly) Bertaut's method [*4*]:

Bertaut considers the virtual charge density

$$\rho(\vec{x}) = \sum_{\vec{m}\in L} \sum_{\vec{s}\in S} q_{\vec{s}}\,\sigma(\vec{x} - \vec{m} - \vec{s})$$

and the corresponding « total energy »

$$E_t = \frac{1}{2}\int_{\vec{x}\in C} \frac{\rho(\vec{x})\rho(\vec{x} + \vec{u})}{\|\vec{u}\|}\, d\vec{x}d\vec{u}$$

$$= \frac{1}{2}\int \frac{P(\vec{u})}{\|\vec{u}\|}\, d\vec{u}$$

where

$$P(\vec{u}) = \int_C \rho(\vec{x})\rho(\vec{x} + \vec{u})d\vec{x}$$

and σ satisfies:

$\sigma(\vec{x})$ depends only on $\|\vec{x}\|$;

$\sigma \geqslant 0$;

$$\sigma \in \mathscr{L}^1(E) \quad \text{and} \quad \int \sigma(\vec{x})d\vec{x} = 1\,. \tag{9}$$

Then, he writes $P(\vec{u})$ in two different forms, in the dual lattice L^* (with the help of its Fourier series)

$$P(\vec{u}) = \frac{1}{V} \sum_{\vec{h} \in L^*} | F(\vec{h})\varphi(\vec{h}) |^2 e^{2\pi i \vec{h}.\vec{u}},$$

and in the lattice L

$$P(\vec{u}) = \sum_{\vec{s} \in S} q_{\vec{s}}^2 p(\vec{u}) + \sum_{\substack{\vec{m} \in L \\ \vec{m}+\vec{s} \neq \vec{t}}} \sum_{\vec{s} \in S} \sum_{\vec{t} \in S} q_{\vec{s}} q_{\vec{t}} p(\vec{u} - \vec{m} - \vec{s} + \vec{t}),$$

where: V is the volume of the cell parallelepiped

$$C = [0, 1[\vec{a}_1 + [0, 1[\vec{a}_2 + [0, 1[\vec{a}_3 ; L^* = \mathbb{Z}\vec{a}_1^* + \mathbb{Z}\vec{a}_2^* + \mathbb{Z}\vec{a}_3^*,$$

the dual basis $\mathscr{B}^* = \{ \vec{a}_1^*, \vec{a}_2^*, \vec{a}_3^* \}$ being defined by: $\vec{a}_i \vec{a}_j^* = \delta_{ij}$ (Kronecker delta);

$$F(\vec{h}) = \sum_{\vec{s} \in S} q_{\vec{s}} e^{-2\pi i \vec{h}.\vec{s}};$$

$$p = \sigma * \sigma \qquad \text{(convolution product)};$$

$$\varphi = \mathscr{F}\sigma \qquad \text{(Fourier transform)}. \tag{10}$$

Thus, he obtains two expressions for E_t, one in L^*:

$$E_t = E_1$$

where

$$E_1 = \frac{1}{2\pi V} \sum_{\vec{h} \in L^* \setminus \{\vec{0}\}} \frac{| F(\vec{h})\varphi(\vec{h}) |^2}{\vec{h}^2},$$

and the other in L:

$$E_t = E_2 + E_3'$$

where

$$E_2 = \frac{1}{2} \sum_{\vec{s} \in S} q_{\vec{s}}^2 \int \frac{p(\vec{u})}{\| \vec{u} \|} d\vec{u}$$

$$= \frac{1}{2\pi} \sum_{\vec{s} \in S} q_{\vec{s}}^2 \int \frac{(\varphi(\vec{h}))^2}{\vec{h}^2} d\vec{h},$$

$$E_3' = \frac{1}{2} \sum_{\substack{\vec{m} \in L \\ \vec{m}+\vec{s} \neq \vec{t}}} \sum_{\vec{s} \in S} \sum_{\vec{t} \in S} q_{\vec{s}} q_{\vec{t}} \int \frac{p(\vec{u})}{\| \vec{m} + \vec{s} - \vec{t} + \vec{u} \|} d\vec{u}$$

$$= \frac{1}{2\pi} \sum_{\substack{\vec{m} \in L \\ \vec{m}+\vec{s} \neq \vec{t}}} \sum_{\vec{s} \in S} \sum_{\vec{t} \in S} q_{\vec{s}} q_{\vec{t}} \int \frac{(\varphi(\vec{h}))^2}{\vec{h}^2} e^{-2\pi i \vec{h}.(\vec{m}+\vec{s}-\vec{t})} d\vec{h}.$$

Then

$$E_1 = E_2 + E'_3 \tag{11}$$

which leads to $E_0 = E_E$, with $E_E = E_1 - E_2 + E_3$ and $E_3 = E_0 - E'_3$. Note that the preceding method is erroneous because E_t does not exist, i. e. $\frac{P(\vec{u})}{\|\vec{u}\|}$ is not integrable, according to

$$\int \frac{|P(\vec{u})|}{\|\vec{u}\|} d\vec{u} \geqslant \int_C |P(\vec{u})| d\vec{u} \cdot \sum_{\vec{m} \in L} \frac{1}{\|\vec{m}\| + \gamma} = +\infty$$

(if $P \neq 0$; $\gamma = \sup_{\vec{x} \in C} \|\vec{x}\|$). Nevertheless, this method shows that Ewald's equality $E_0 = E_E$ is equivalent to the equality (11), in which we recognize Poisson's formula. Indeed

$$E_2 + E'_3 = \frac{1}{2\pi} \sum_{\vec{m} \in L} \int \frac{|F(\vec{h})\varphi(\vec{h})|^2}{\vec{h}^2} e^{-2\pi i \vec{h}.\vec{m}} d\vec{h},$$

so that (11) represents Poisson's formula

$$\sum_{\vec{h} \in L^*} f(\vec{h}) = V \sum_{\vec{m} \in L} \mathscr{F} f(\vec{m}) \tag{12}$$

applied to the function f:

$$f(\vec{h}) = \frac{|F(\vec{h})\varphi(\vec{h})|^2}{\vec{h}^2}, \qquad \vec{h} \neq \vec{0}$$

$$f(\vec{0}) = 0.$$

However, if the dipole moment of the cell

$$\vec{M} = \sum_{\vec{s} \in S} q_{\vec{s}} \vec{s}$$

is not equal to $\vec{0}$, the limit

$$\lim_{\zeta \to 0^+} \frac{F(\zeta \vec{h})}{\|\zeta \vec{h}\|} = 2\pi i \frac{\vec{M} \cdot \vec{h}}{\|\vec{h}\|}$$

(Taylor's formula applied to F) shows that f is not continuous at $\vec{h} = \vec{0}$, so that Poisson's formula cannot be applied to f (and the result of section 7 shows that (11)-(12) is not correct).

Before introducing the sequence of functions f_N, let us generalize the problem. We replace the conditions (9) and (10) by the more general conditions (without σ and without sign condition):

$$p \text{ is an application: } \mathrm{E} \to \mathbb{C};$$
$$p \in \mathscr{L}^1(\mathrm{E});$$
$$\int p(\vec{u})d\vec{u} = 1;$$
$$p(\vec{u}) \text{ depends only on } \|\vec{u}\|;$$
$$\psi = \mathscr{F}p; \tag{13}$$

f is now defined by:

$$f(\vec{h}) = \frac{|\mathrm{F}(\vec{h})|^2\psi(\vec{h})}{\vec{h}^2}, \qquad \vec{h} \neq \vec{0}$$
$$f(\vec{0}) = 0.$$

Then, we introduce the functions f_N

$$f_\mathrm{N}(\vec{h}) = (1 - e^{-\mathrm{N}\|\vec{h}\|})f(\vec{h})$$

which are continuous on E and satisfy, for any $\vec{h}$

$$\lim_{\mathrm{N}\to+\infty} f_\mathrm{N}(\vec{h}) = f(\vec{h}).$$

In order to apply correctly Poisson's formula to f_N, we have to prove that the following conditions are satisfied:

1) $f_\mathrm{N} \in \mathscr{L}^1(\mathrm{E})$;
2) the restriction to L of the Fourier transform $\mathscr{F}f_\mathrm{N}$, belongs to $\mathscr{L}^1(\mathrm{L})$;
3) for all $\vec{x} \in \mathrm{E}$, the function $\vec{h} \to f_\mathrm{N}(\vec{x} + \vec{h})$ on L* belongs to $\mathscr{L}^1(\mathrm{L}^*)$;
4) the function $\vec{x} \to \sum_{\vec{h}\in\mathrm{L}^*} f_\mathrm{N}(\vec{x} + \vec{h})$ is continuous on E (see [*11*], section 12).

3. THE CONDITIONS 1°, 3° AND 4° OF POISSON'S FORMULA

Since $\dfrac{\mathrm{F}(\vec{h})}{\|\vec{h}\|}$ is bounded (Taylor's formula applied to F), the functions f and f_N belong to $\mathscr{L}^1(\mathrm{E})$ if we suppose that

$$\psi \in \mathscr{L}^1(\mathrm{E}). \tag{14}$$

According to the integrability of p, condition (14) is equivalent to: p is almost everywhere equal to a function of $\mathscr{P}(\mathrm{E})$ (space of linear combinations of continuous functions « of positive type »; see [11], sections 8 and 10). In the following, we identify p with that function of $\mathscr{P}(E)$:

$$p \in \mathscr{P}(E). \tag{15}$$

Let us suppose that

for all $\vec{x}_0 \in E$, there are $r > 0$ and $g \in \mathscr{L}^1(L^*)$,
such that, for all $\vec{x} \in E$ and $\vec{h} \in L^*$,

$$\| \vec{x} - \vec{x}_0 \| \leqslant r \quad \text{implies} \quad | \psi(\vec{x} + \vec{h}) | \leqslant g(\vec{h}). \tag{16}$$

This implies that the function $\vec{h} \to \psi(\vec{x}_0 + \vec{h})$ on L^* belongs to $\mathscr{L}^1(L^*)$, so that f and f_N satisfy the condition 3) of Poisson's formula. With the help of this condition, together with the continuity of f_N and (16), the application of Lebesgue's dominated convergence theorem shows that the condition 4) of Poisson's formula is satisfied by f_N.

Finally, under the conditions (13), (14) and (16), the functions f_N satisfy the three conditions 1), 3) and 4) of Poisson's formula.

A sufficient condition for (14) and (16) is:

$$\text{there is } \beta > 3 \text{ such that } \| \vec{h} \|^\beta \psi(\vec{h}) \text{ is bounded}. \tag{17}$$

Note that all these conditions are satisfied by Ewald's example [3]

$$\begin{aligned} p(\vec{u}) &= \frac{H^3}{\pi^{3/2}} e^{-H^2\vec{u}^2} \\ \psi(\vec{h}) &= e^{-\frac{\pi^2 \vec{h}^2}{H^2}} \end{aligned} \tag{18}$$

and by Bertaut's example [4]

$$\begin{aligned} p(\vec{u}) &= \frac{3}{8\pi R^6}\left(2R^3 - \frac{3R^2 \| \vec{u} \|}{2} + \frac{\| \vec{u} \|^3}{8}\right) \quad \text{if} \quad \| \vec{u} \| \leqslant 2R \\ p(\vec{u}) &= 0 \quad \text{if} \quad \| \vec{u} \| > 2R, \\ \psi(\vec{h}) &= \frac{9(\sin\sigma - \sigma\cos\sigma)^2}{\sigma^6}, \qquad \sigma = 2\pi R \| \vec{h} \|, \qquad \vec{h} \neq \vec{0} \\ \psi(\vec{0}) &= 1 \end{aligned} \tag{19}$$

(used by Bertaut in the case $2R \leqslant \inf_{\vec{m}+\vec{s}\neq\vec{t}} \| \vec{m} + \vec{s} - \vec{t} \|$).

4. THE CONDITION 2° OF POISSON'S FORMULA

We define

$$g_N(\vec{h}) = e^{-N\|\vec{h}\|} f(\vec{h}),$$

so that

$$\begin{aligned} f_N &= f - g_N \\ \mathscr{F} f_N &= \mathscr{F} f - \mathscr{F} g_N. \end{aligned}$$

4.1. The term $\mathcal{F}f(\vec{m})$.

$$\mathcal{F}f(\vec{m}) = \sum_{\vec{s}}\sum_{\vec{t}} q_{\vec{s}}q_{\vec{t}}\int \frac{\psi(\vec{h})}{\vec{h}^2}\, e^{-2\pi i \vec{h}.(\vec{m}+\vec{s}-\vec{t})}d\vec{h}\,,$$

because $\frac{\psi(\vec{h})}{\vec{h}^2}$ is integrable. Moreover,

$$\int \frac{\psi(\vec{h})}{\vec{h}^2} e^{-2\pi i \vec{h}.\vec{x}}d\vec{h} = \pi\int \frac{p(\vec{u})}{\|\vec{x}+\vec{u}\|}d\vec{u}$$
$$= \begin{cases} \frac{\pi}{\|\vec{x}\|}\left(1-\int_{\|\vec{x}\|}^{+\infty} 4\pi u(u-\|\vec{x}\|)p(u)du\right) & \text{if } \vec{x}\neq\vec{0}, \\ \pi\int_0^{+\infty} 4\pi u p(u)du & \text{if } \vec{x}=\vec{0} \end{cases} \tag{20}$$

(appendix 1; $u = \|\vec{u}\|$ and $p(u)$ is written for $p(\vec{u})$). Then,

$$\mathcal{F}f(\vec{m}) = \begin{cases} \pi\sum_{\vec{s}}\sum_{\vec{t}}\frac{q_{\vec{s}}q_{\vec{t}}}{\|\vec{m}+\vec{s}-\vec{t}\|} \\ -\pi\sum_{\vec{s}}\sum_{\vec{t}}\frac{q_{\vec{s}}q_{\vec{t}}}{\|\vec{m}+\vec{s}-\vec{t}\|}\int_{\|\vec{m}+\vec{s}-\vec{t}\|}^{+\infty} 4\pi u(u-\|\vec{m}+\vec{s}-\vec{t}\|)p(u)du, \end{cases}$$

if $\vec{m}\neq\vec{0}$. Taylor's formula at the third order applied to the function $\frac{1}{\|\vec{x}\|}$, leads to:

$$\sum_{\vec{s}}\sum_{\vec{t}}\frac{q_{\vec{s}}q_{\vec{t}}}{\|\vec{m}+\vec{s}-\vec{t}\|} = \vec{M}^2\frac{1-3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} + A(\vec{m}) \tag{21}$$

for all $\vec{m}\neq\vec{0}$, with

$$A(\vec{m}) = \sum_{\vec{s}}\sum_{\vec{t}} q_{\vec{s}}q_{\vec{t}}\left\{-\frac{5[\vec{x}'\cdot(\vec{s}-\vec{t})]^3}{2\|\vec{x}'\|^7} + \frac{3[\vec{x}'\cdot(\vec{s}-\vec{t})](\vec{s}-\vec{t})^2}{2\|\vec{x}'\|^5}\right\}$$

if $\|\vec{m}\| > \delta = \sup_{\vec{s},\vec{t}}\|\vec{s}-\vec{t}\|$; θ_m is the angle $(\vec{M},\vec{m})$ and $\vec{x}' = \vec{m}+\zeta(\vec{s}-\vec{t})$, $0<\zeta<1$. Since

$$|A(\vec{m})| \leqslant \sum_{\vec{s}}\sum_{\vec{t}} |q_{\vec{s}}q_{\vec{t}}|\,\|\vec{s}-\vec{t}\|^3\frac{4}{(\|\vec{m}\|-\delta)^4}$$

for $\|\vec{m}\|>\delta$, the family $(A(\vec{m}))$ is absolutely summable. But, if $\vec{M}\neq\vec{0}$, the family $\left(\frac{1-3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3}\right)$ is not absolutely summable (its sum depends on the mode of summation; [9], section 4, « Calculation of E_0 »: the values of E_5 and E_5^0 are different). With respect to the second term in $\mathcal{F}f(\vec{m})$, a sufficient condition for its absolute summability (on $\vec{m}$) is:

$$\text{there is } \beta' > 3 \text{ such that } \| \vec{u} \|^{\beta'} p(\vec{u}) \text{ is bounded}. \tag{22}$$

(appendix 2). Note that this condition is satisfied by the examples (18)-(19) of Ewald and Bertaut.

In the particular case $\vec{M} = \vec{0}$, $(\mathcal{F}f(\vec{m}))$ is absolutely summable, and the proof is completed: indeed, f is continuous and satisfy the four conditions of Poisson's formula; then, this formula may directly be applied to f. In the following, we suppose $\vec{M} \neq \vec{0}$.

4.2. The term $\mathcal{F}g_N(\vec{m})$.

$$\begin{aligned}\mathcal{F}g_N(\vec{m}) &= \sum_{\vec{s}} \sum_{\vec{t}} q_{\vec{s}} q_{\vec{t}} \int e^{-N\|\vec{h}\|} \frac{\psi(\vec{h})}{\vec{h}^2} e^{-2\pi i \vec{h}.(\vec{m}+\vec{s}-\vec{t})} d\vec{h} \\ &= \sum_{\vec{s}} \sum_{\vec{t}} q_{\vec{s}} q_{\vec{t}} \int p(\vec{u}) d\vec{u} \int \frac{e^{-N\|\vec{h}\|}}{\vec{h}^2} e^{-2\pi i \vec{h}.(\vec{m}+\vec{s}-\vec{t}+\vec{u})} d\vec{h},\end{aligned}$$

by the Lebesgue-Fubini theorem. The integral on $\vec{h}$ may easily be calculated with $\vec{x} = \vec{m} + \vec{s} - \vec{t} + \vec{u}$ as polar axis:

$$\int \frac{e^{-N\|\vec{h}\|}}{\vec{h}^2} e^{-2\pi i \vec{h}.\vec{x}} d\vec{h} = \frac{4\pi}{2\pi \|\vec{x}\|} \int_0^{+\infty} \exp\left(-\frac{N\xi}{2\pi \|\vec{x}\|}\right) \frac{\sin \xi}{\xi} d\xi .$$

With the help of

$$\int_0^{+\infty} e^{-\frac{\xi}{r}} \frac{\sin \xi}{\xi} d\xi = \text{Arctan } r \qquad r > 0$$

(appendix 3), we obtain

$$\begin{aligned}\mathcal{F}g_N(\vec{m}) &= 4\pi \sum_{\vec{s}} \sum_{\vec{t}} q_{\vec{s}} q_{\vec{t}} \int p(\vec{u}) \frac{\text{Arctan}\left(\frac{2\pi}{N} \|\vec{m}+\vec{s}-\vec{t}+\vec{u}\|\right)}{2\pi \|\vec{m}+\vec{s}-\vec{t}+\vec{u}\|} d\vec{u} \qquad (23) \\ &= \frac{4\pi}{N} \int p(\vec{u}) G_N(\vec{m}, \vec{u}) d\vec{u}\end{aligned}$$

where

$$G_N(\vec{m}, \vec{u}) = \sum_{\vec{s}} \sum_{\vec{t}} q_{\vec{s}} q_{\vec{t}} \frac{\text{Arctan}\left(\frac{2\pi}{N} \|\vec{m}+\vec{s}-\vec{t}+\vec{u}\|\right)}{\frac{2\pi}{N} \|\vec{m}+\vec{s}-\vec{t}+\vec{u}\|}.$$

With the help of the new assumption

$$p(\vec{u}) = 0 \quad \text{if} \quad \| \vec{u} \| \geqslant d, \tag{24}$$

we shall suppose that $\| \vec{u} \| < d$. Taylor's formula at the fourth order applied to the function $\dfrac{\text{Arctan} \| \vec{x} \|}{\| \vec{x} \|}$, leads to:

$$G_N(\vec{m}, \vec{u}) = G_N^{(2)}(\vec{m}) + G_N^{(3)}(\vec{m}) \cdot \vec{u} + G_N^{(4)}(\vec{m}, \vec{u})$$

for all $\vec{m} \neq \vec{0}$, with

$$G_N^{(2)}(\vec{m}) = -\left(\frac{2\pi}{N}\right)^2 \left[\left(-\frac{3}{r^4(r^2+1)} - \frac{2}{r^2(r^2+1)^2} + \frac{3 \,\text{Arctan}\, r}{r^5} \right) \left(\frac{2\pi}{N}\right)^2 (\vec{M} \cdot \vec{m})^2 + \left(\frac{1}{r^2(r^2+1)} - \frac{\text{Arctan}\, r}{r^3} \right) \vec{M}^2 \right];$$

$$G_N^{(3)}(\vec{m}) \cdot \vec{u} = -\left(\frac{2\pi}{N}\right)^4$$

$$\left\{ \left(\frac{15}{r^6(r^2+1)} + \frac{10}{r^4(r^2+1)^2} + \frac{8}{r^2(r^2+1)^3} - \frac{15 \,\text{Arctan}\, r}{r^7} \right) \left(\frac{2\pi}{N}\right)^2 (\vec{m} \cdot \vec{u})(\vec{M} \cdot \vec{m})^2 + \left(-\frac{3}{r^4(r^2+1)} - \frac{2}{r^2(r^2+1)^2} + \frac{3 \,\text{Arctan}\, r}{r^5} \right) [2(\vec{M} \cdot \vec{u})(\vec{M} \cdot \vec{m}) + \vec{M}^2 (\vec{m} \cdot \vec{u})]; \right\}$$

and, if $\| \vec{m} \| > \delta + d$

$$G_N^{(4)}(\vec{m}, \vec{u}) = \frac{1}{4!} \sum_{\vec{s}} \sum_{\vec{t}} q_{\vec{s}} q_{\vec{t}}$$

$$\left\{ \left(-\frac{105}{r'^8(r'^2+1)} - \frac{70}{r'^6(r'^2+1)^2} - \frac{56}{r'^4(r'^2+1)^3} - \frac{48}{r'^2(r'^2+1)^4} + \frac{105 \,\text{Arctan}\, r'}{r'^9} \right) (\vec{x}' \cdot \vec{k})^4 + \left(\frac{15}{r'^6(r'^2+1)} + \frac{10}{r'^4(r'^2+1)^2} + \frac{8}{r'^2(r'^2+1)^3} - \frac{15 \,\text{Arctan}\, r'}{r'^7} \right) 6 (\vec{x}' \cdot \vec{k})^2 \vec{k}^2 + \left(-\frac{3}{r'^4(r'^2+1)} - \frac{2}{r'^2(r'^2+1)^2} + \frac{3 \,\text{Arctan}\, r'}{r'^5} \right) 3 \| \vec{k} \|^4 \right\}$$

notations:

$$\vec{x} = \frac{2\pi}{N} \vec{m}, \; r = \| \vec{x} \|, \; \vec{k} = \frac{2\pi}{N} (\vec{s} - \vec{t} + \vec{u}), \quad \vec{x}' = \vec{x} + \zeta \vec{k}, \quad 0 < \zeta < 1, \quad r' = \| \vec{x}' \|.$$

Since

$$\int p(\vec{u})G_N^{(2)}(\vec{m})d\vec{u} \quad = G_N^{(2)}(\vec{m})$$

$$\int p(\vec{u})G_N^{(3)}(\vec{m})\cdot \vec{u}d\vec{u} = 0\,,$$

the function $\vec{u} \rightarrow p(\vec{u})G_N^{(4)}(\vec{m}, \vec{u})$ is integrable and

$$\mathscr{F}g_N(\vec{m}) = \mathscr{F}g_N^{(2)}(\vec{m}) + \mathscr{F}g_N^{(4)}(\vec{m})$$

for all $\vec{m} \neq \vec{0}$, where

$$\mathscr{F}g_N^{(2)}(\vec{m}) = \frac{4\pi}{N} G_N^{(2)}(\vec{m})$$

$$\mathscr{F}g_N^{(4)}(\vec{m}) = \frac{4\pi}{N}\int p(\vec{u})G_N^{(4)}(\vec{m}, \vec{u})d\vec{u}\,.$$

The inequalities

$$\begin{aligned} |\,G_N^{(4)}(\vec{m}, \vec{u})\,| &\leqslant \frac{1}{4\,!}\sum_{\vec{s}}\sum_{\vec{t}}|\,q_{\vec{s}}q_{\vec{t}}\,|\left(\frac{204}{r'^4(r'^2+1)} + \frac{136}{r'^2(r'^2+1)^2} + \frac{104}{(r'^2+1)^3}\right. \\ &\quad \left. + \frac{48r'^2}{(r'^2+1)^4} + \frac{204 \operatorname{Arctan} r'}{r'^5}\right)\left(\frac{2\pi}{N}\right)^4 (\delta+d)^4 \qquad (25) \\ &\leqslant \frac{1}{4\,!}\sum_{\vec{s}}\sum_{\vec{t}}|\,q_{\vec{s}}q_{\vec{t}}\,|\left(\frac{492}{r'^6} + \frac{102\pi}{r'^5}\right)\left(\frac{2\pi}{N}\right)^4 (\delta + d)^4 \\ &\leqslant \frac{1}{4\,!}\sum_{\vec{s}}\sum_{\vec{t}}|\,q_{\vec{s}}q_{\vec{t}}\,|\,(\delta+d)^4\left(\frac{492}{\left(\frac{2\pi}{N}\right)^2(\,\|\,\vec{m}\,\|-\delta-d)^6} + \frac{102\pi}{\left(\frac{2\pi}{N}\right)(\,\|\,\vec{m}\,\| - \delta - d)^5}\right) \end{aligned}$$

for $\|\,\vec{m}\,\| > \delta + d$, show that $(\mathscr{F}g_N^{(4)}(\vec{m}))_{\vec{m}}$ is absolutely summable. The term $\mathscr{F}g_N^{(2)}(\vec{m})$ may be written

$$\begin{aligned} \mathscr{F}g_N^{(2)}(\vec{m}) &= 2\left(\frac{2\pi}{N}\right)^3\vec{M}^2\left(-\frac{1-3\cos^2\theta_{\vec{m}}}{r^2(r^2+1)} + \frac{2\cos^2\theta_{\vec{m}}}{(r^2+1)^2} + \frac{(1-3\cos^2\theta_{\vec{m}})\operatorname{Arctan} r}{r^3}\right) \\ &= \mathscr{F}g_N^{(2.1)}(\vec{m}) + \mathscr{F}g_N^{(2.2)}(\vec{m}) + \mathscr{F}g_N^{(2.3)}(\vec{m}) + \mathscr{F}g_N^{(2.4)}(\vec{m}) \end{aligned}$$

where

$$\mathscr{F}g_N^{(2.1)}(\vec{m}) = -\,2\left(\frac{2\pi}{N}\right)^3\vec{M}^2\,\frac{1 - 3\cos^2\theta_{\vec{m}}}{r^2(r^2 + 1)}$$

$$\mathscr{F}g_N^{(2.2)}(\vec{m}) = 4\left(\frac{2\pi}{N}\right)^3\vec{M}^2\,\frac{\cos^2\theta_{\vec{m}}}{(r^2+1)^2}$$

$$\mathscr{F}g_N^{(2.3)}(\vec{m}) = -\,2\left(\frac{2\pi}{N}\right)^3\vec{M}^2\,\frac{\left(\frac{\pi}{2} - \operatorname{Arctan} r\right)(1-3\cos^2\theta_{\vec{m}})}{r^3}$$

$$\mathscr{F}g_N^{(2.4)}(\vec{m}) = \pi\vec{M}^2\,\frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\,\vec{m}\,\|^3}\,.$$

$(\mathscr{F} g_N^{(2.1)}(\vec{m}))_{\vec{m}}$ and $(\mathscr{F} g_N^{(2.2)}(\vec{m}))_{\vec{m}}$ are absolutely summable. According to

$$\frac{\pi}{2} - \text{Arctan}\, r < \frac{1}{r} \tag{26}$$

$\left(\text{mean value theorem applied to Arctan } \frac{1}{x}\right)$, $(\mathscr{F} g_N^{(2.3)}(\vec{m}))_{\vec{m}}$ is also absolutely summable. The last term $\mathscr{F} g_N^{(2.4)}(\vec{m})$ is the same as that found in the expression of $\mathscr{F} f(\vec{m})$, and corresponds to a non absolutely summable family. Nevertheless, this term disappears in the difference $\mathscr{F} f_N = \mathscr{F} f - \mathscr{F} g_N$. We may then conclude: $(\mathscr{F} f_N(\vec{m}))_{\vec{m}}$ is absolutely summable, i. e. f_N satisfies the condition 2) of Poisson's formula.

5. POISSON'S FORMULA

Let us consider a mode of summation for $\left(\frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3}\right)$, i. e. an increasing sequence (B_k) of finite subsets of L, such that $\bigcup_k B_k \overset{\uparrow}{=} L$ and

$$\sum_{\vec{m} \in B_k \setminus \{\vec{0}\}} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} \text{ has a finite limit when } k \to +\infty. \tag{27}$$

According to the preceding sections, (B_k) is also a mode of summation for E_0, $(\mathscr{F} f(\vec{m}))$ and $(\mathscr{F} g_N(\vec{m}))$. Poisson's formula applied to f_N may then be written:

$$\begin{aligned}
\sum_{\vec{h} \in L^*} f_N(\vec{h}) &= V \sum_{\vec{m} \in L} \mathscr{F} f_N(\vec{m}) \\
&= V \lim_{k \to +\infty} \sum_{\vec{m} \in B_k} \mathscr{F} f(\vec{m}) - V \lim_{k \to +\infty} \sum_{\vec{m} \in B_k} \mathscr{F} g_N(\vec{m}) \\
&= \left\{ \begin{aligned}
& V \lim_{k \to +\infty} \sum_{\vec{m} \in B_k} \mathscr{F} f(\vec{m}) - V \mathscr{F} g_N(\vec{0}) - V \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.1)}(\vec{m}) \\
& - V \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.2)}(\vec{m}) - V \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.3)}(\vec{m}) \\
& - \pi V \vec{M}^2 \lim_{k \to +\infty} \sum_{\vec{m} \in B_k \setminus \{\vec{0}\}} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} - V \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(4)}(\vec{m}).
\end{aligned} \right.
\end{aligned}$$

6. LIMIT OF THE DIFFERENT TERMS OF POISSON'S FORMULA WHEN $N \to +\infty$

6.1. Limit of $\sum_{\vec{h}} f_N(\vec{h})$, $\mathscr{F}g_N$, $\mathscr{F}g_N^{(2)}$ and $\mathscr{F}g_N^{(4)}$.

Since $|f_N| \leqslant |f|$ and $(f(\vec{h}))$ is absolutely summable on L*, Lebesgue's dominated convergence theorem may be applied:

$$\lim_{N\to+\infty} \sum_{\vec{h}} f_N(\vec{h}) = \sum_{\vec{h}} f(\vec{h}).$$

Since $\vec{u} \to \dfrac{|p(\vec{u})|}{\|\vec{m}+\vec{s}-\vec{t}+\vec{u}\|}$ is integrable (appendix 1), the same theorem may be applied to the integral in (23), and shows that

$$\lim_{N\to+\infty} \mathscr{F}g_N(\vec{m}) = 0 \quad \text{for all } \vec{m}.$$

Since

$$\lim_{N\to+\infty} \mathscr{F}g_N^{(2)}(\vec{m}) = 0 \quad \text{for all } \vec{m} \neq \vec{0},$$

we may conclude

$$\lim_{N\to+\infty} \mathscr{F}g_N^{(4)}(\vec{m}) = 0 \quad \text{for all } \vec{m} \neq \vec{0}.$$

6.2. Limit of $\sum_{\vec{m}\neq\vec{0}} \mathscr{F}g_N^{(4)}(\vec{m})$.

According to (25),

$$\begin{aligned}
|G_N^{(4)}(\vec{m},\vec{u})| &\leqslant \frac{1}{4!}\sum_{\vec{s}}\sum_{\vec{t}} |q_{\vec{s}}q_{\vec{t}}| \left(\frac{2\pi}{N}\right)^4 (\delta+d)^4 \left(\frac{204}{r'^4} + \frac{136}{r'^2(r'^2+1)} + \frac{104}{(r'^2+1)^2} + \frac{48r'^2}{(r'^2+1)^3} + \frac{204}{r'^4}\right) \\
&\leqslant \frac{1}{4!}\sum_{\vec{s}}\sum_{\vec{t}} |q_{\vec{s}}q_{\vec{t}}| \left(\frac{2\pi}{N}\right)^4 (\delta+d)^4 \frac{696}{r'^4} \\
&\leqslant \frac{1}{4!}\sum_{\vec{s}}\sum_{\vec{t}} |q_{\vec{s}}q_{\vec{t}}| (\delta+d)^4 \frac{696}{(\|\vec{m}\|-\delta-d)^4}
\end{aligned}$$

for $\| \vec{m} \| > \delta + d$. Then

$$\left| \sum_{\|\vec{m}\| > \delta + d} \mathscr{F} g_N^{(4)}(\vec{m}) \right| \leqslant \frac{4\pi}{N} \frac{1}{4!} \sum_{\vec{s}} \sum_{\vec{t}} | q_{\vec{s}} q_{\vec{t}} | (\delta + d)^4 696 \sum_{\|\vec{m}\| > \delta + d} \frac{1}{(\|\vec{m}\| - \delta - d)^4},$$

which shows that

$$\lim_{N \to +\infty} \sum_{\|\vec{m}\| > \delta + d} \mathscr{F} g_N^{(4)}(\vec{m}) = 0 .$$

Then

$$\lim_{N \to +\infty} \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(4)}(\vec{m}) = 0 .$$

6.3. Limit of $\sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.1)}(\vec{m})$.

NOTATIONS: $\vec{\mu} = \frac{2\pi}{N} \vec{m}$; $C_{\vec{\mu}} = \vec{\mu} + \frac{2\pi}{N} C$ ($C = [0, 1[\vec{a}_1 + [0, 1[\vec{a}_2 + [0, 1[\vec{a}_3$); φ_A is the characteristic function of a subset A of E. We may write

$$V \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.1)}(\vec{m}) = -2\vec{M}^2 \sum_{\vec{\mu} \neq \vec{0}} \int \frac{1 - 3\cos^2\theta_{\vec{\mu}}}{\vec{\mu}^2(\vec{\mu}^2 + 1)} \varphi_{C_{\vec{\mu}}}(\vec{x}) d\vec{x}$$

$$= -2\vec{M}^2 \int d\vec{x} \sum_{\vec{\mu} \neq \vec{0}} \frac{1 - 3\cos^2\theta_{\vec{\mu}}}{\vec{\mu}^2(\vec{\mu}^2 + 1)} \varphi_{C_{\vec{\mu}}}(\vec{x})$$

(Lebesgue's convergence theorem). In the appendix 4, we show that

$$\lim_{N \to +\infty} \int d\vec{x} \sum_{\vec{\mu} \neq \vec{0}} \frac{1 - 3\cos^2\theta_{\vec{\mu}}}{\vec{\mu}^2(\vec{\mu}^2 + 1)} \varphi_{C_{\vec{\mu}}}(\vec{x}) = \int \frac{1 - 3\cos^2\theta_{\vec{x}}}{\vec{x}^2(\vec{x}^2 + 1)} d\vec{x} .$$

This last integral (calculated with $\vec{M}$ as polar axis) is equal to 0. Then

$$\lim_{N \to +\infty} \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.1)}(\vec{m}) = 0 .$$

6.4. Limit of $\sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.2)}(\vec{m})$.

As in the preceding section, we may apply Lebesgue's convergence theorem:

$$V \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.2)}(\vec{m}) = 4\vec{M}^2 \int h_N(\vec{x}) d\vec{x}$$

where

$$h_N(\vec{x}) = \sum_{\vec{\mu} \neq \vec{0}} \frac{\cos^2 \theta_{\vec{\mu}}}{(\vec{\mu}^2 + 1)^2} \varphi_{C_{\vec{\mu}}}(\vec{x}).$$

According to

$$\lim_{N \to +\infty} h_N(\vec{x}) = \frac{\cos^2 \theta_{\vec{x}}}{(\vec{x}^2 + 1)^2} \quad \text{for} \quad \vec{x} \neq \vec{0},$$

$$h_N(\vec{x}) \leqslant 1 \quad \text{for all} \quad \vec{x},$$

$$h_N(\vec{x}) \leqslant \frac{1}{[(\| \vec{x} \| - 2\pi\gamma)^2 - 1]^2} \quad \text{for} \quad \| \vec{x} \| \geqslant 2\pi\gamma,$$

where $\gamma = \sup_{\vec{x} \in C} \| \vec{x} \|$, we may apply Lebesgue's dominated convergence theorem

$$V \lim_{N \to +\infty} \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.2)}(\vec{m}) = 4\vec{M}^2 \int \frac{\cos^2 \theta_{\vec{x}}}{(\vec{x}^2 + 1)^2} d\vec{x}$$

$$= \frac{4\pi^2 \vec{M}^2}{3}$$

(the integral is calculated with $\vec{M}$ as polar axis, and with the change of variables: $\| \vec{x} \| = \tan \xi$).

6.5. Limit of $\sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.3)}(\vec{m})$.

We write

$$V \mathscr{F} g_N^{(2.3)}(\vec{m}) = S_1 + S_2$$

where

$$S_1 = V \sum_{0 < \| \vec{m} \| \leqslant N} \mathscr{F} g_N^{(2.3)}(\vec{m})$$

$$S_2 = V \sum_{\| \vec{m} \| > N} \mathscr{F} g_N^{(2.3)}(\vec{m}).$$

As in the preceding sections, and according to (26), Lebesgue's convergence theorem may be applied to S_2:

$$S_2 = -2\vec{M}^2 \int h_N(\vec{x})d\vec{x}$$

where

$$h_N(\vec{x}) = \sum_{\|\vec{\mu}\| > 2\pi} \frac{\left(\frac{\pi}{2} - \operatorname{Arctan} \|\vec{\mu}\|\right)(1 - 3\cos^2\theta_{\vec{\mu}})}{\|\vec{\mu}\|^3} \varphi_{C_{\vec{\mu}}}(\vec{x}).$$

According to

$$\lim_{N\to+\infty} h_N(\vec{x}) = \frac{\left(\frac{\pi}{2} - \operatorname{Arctan} \|\vec{x}\|\right)(1 - 3\cos^2\theta_{\vec{x}})}{\|\vec{x}\|^3} \quad \text{for} \quad \|\vec{x}\| > 2\pi,$$

$$\lim_{N\to+\infty} h_N(\vec{x}) = 0 \quad \text{for} \quad \|\vec{x}\| < 2\pi,$$

$$|h_N(\vec{x})| \leqslant \frac{1}{4\pi^2} \quad \text{for all } \vec{x},$$

$$|h_N(\vec{x})| \leqslant \frac{4}{(\|\vec{x}\| - 2\pi\gamma)^4} \quad \text{for } \|\vec{x}\| > 2\pi\gamma,$$

(with the help of (26)), Lebesgue's dominated convergence theorem may be applied:

$$\lim_{N\to+\infty} S_2 = -2\vec{M}^2 \int_{\|\vec{x}\| > 2\pi} \frac{\left(\frac{\pi}{2} - \operatorname{Arctan} \|\vec{x}\|\right)(1 - 3\cos^2\theta_{\vec{x}})}{\|\vec{x}\|^3} d\vec{x}$$
$$= 0$$

(the integral is calculated with $\vec{M}$ as polar axis).

The other sum S_1 may be written

$$S_1 = -\pi V\vec{M}^2 \sum_{0<\|\vec{m}\|\leq N} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} + S_1'$$

with

$$S_1' = 2\vec{M}^2 \sum_{0<\|\vec{\mu}\|\leqslant 2\pi} \int \frac{(\operatorname{Arctan} \|\vec{\mu}\|)(1 - 3\cos^2\theta_{\vec{\mu}})}{\|\vec{\mu}\|^3} \varphi_{C_{\vec{\mu}}}(\vec{x})d\vec{x}$$

$$= 2\vec{M}^2 \int d\vec{x} \sum_{0<\|\vec{\mu}\|\leqslant 2\pi} \frac{(\operatorname{Arctan} \|\vec{\mu}\|)(1-3\cos^2\theta_{\vec{\mu}})}{\|\vec{\mu}\|^3} \varphi_{C_{\vec{\mu}}}(\vec{x})$$

(the sum is finite). In the appendix 5, we show that

$$\lim_{N \to +\infty} \int d\vec{x} \sum_{0 < \|\vec{\mu}\| \leq 2\pi} \frac{(\operatorname{Arctan} \|\vec{\mu}\|)(1 - 3\cos^2 \theta_{\vec{\mu}})}{\|\vec{\mu}\|^3} \varphi_{C_{\vec{\mu}}}(\vec{x})$$

$$= \int_{\|\vec{x}\| \leq 2\pi} \frac{(\operatorname{Arctan} \|\vec{x}\|)(1 - 3\cos^2 \theta_{\vec{x}})}{\|\vec{x}\|^3} d\vec{x}.$$

And this last integral (calculated with $\vec{M}$ as polar axis) is equal to 0. In conclusion

$$V \lim_{N \to +\infty} \sum_{\vec{m} \neq \vec{0}} \mathscr{F} g_N^{(2.3)}(\vec{m}) = -\pi V \vec{M}^2 \lim_{N \to +\infty} \sum_{0 < \|\vec{m}\| \leq N} \frac{1 - 3\cos^2 \theta_{\vec{m}}}{\|\vec{m}\|^3}.$$

The existence of this last limit is proved in the appendix 6.

7. LIMIT OF POISSON'S FORMULA: THE EWALD ENERGY E_E AND THE BORN-LANDÉ EXPRESSION E_0

The results of the preceding sections show that the limit of Poisson's formula when $N \to +\infty$, is

$$\sum_{\vec{h}} f(\vec{h}) = \left\{ \begin{array}{l} V \lim\limits_{k \to +\infty} \sum\limits_{\vec{m} \in B_k} \mathscr{F} f(\vec{m}) \\ -\dfrac{4\pi^2 \vec{M}^2}{3} + \pi V \vec{M}^2 \lim\limits_{N \to +\infty} \sum\limits_{0 < \|\vec{m}\| \leq N} \dfrac{1 - 3\cos^2 \theta_{\vec{m}}}{\|\vec{m}\|^3} \\ -\pi V \vec{M}^2 \lim\limits_{k \to +\infty} \sum\limits_{\vec{m} \in B_k \setminus \{\vec{0}\}} \dfrac{1 - 3\cos^2 \theta_{\vec{m}}}{\|\vec{m}\|^3}, \end{array} \right.$$

or, after dividing by $2\pi V$:

$$E_1 = E_2 + E_3' - E_4 + E_5^0 - E_5$$

with

$$E_1 = \frac{1}{2\pi V} \sum_{\vec{h}} f(\vec{h}),$$

$$E_2 = \frac{1}{2\pi} \sum_{\vec{s}} q_{\vec{s}}^2 \int \frac{\psi(\vec{h})}{\vec{h}^2} d\vec{h} = \frac{1}{2} \sum_{\vec{s}} q_{\vec{s}}^2 \int \frac{p(\vec{u})}{\|\vec{u}\|} d\vec{u},$$

$$\mathrm{E}_3' = \frac{1}{2\pi} \lim_{k \to +\infty} \sum_{\vec{m} \in \mathrm{B}_k} \sum_{\vec{s}} \sum_{\substack{\vec{t} \\ \vec{m}+\vec{s} \neq \vec{t}}} q_{\vec{s}} q_{\vec{t}} \int \frac{\psi(\vec{h})}{\vec{h}^2} e^{-2\pi i \vec{h}.(\vec{m}+\vec{s}-\vec{t})} d\vec{h}$$

$$= \frac{1}{2} \lim_{k \to +\infty} \sum_{\vec{m} \in \mathrm{B}_k} \sum_{\vec{s}} \sum_{\substack{\vec{t} \\ \vec{m}+\vec{s} \neq \vec{t}}} q_{\vec{s}} q_{\vec{t}} \int \frac{p(\vec{u})}{\| \vec{m} + \vec{s} - \vec{t} + \vec{u} \|} d\vec{u},$$

$$\mathrm{E}_4 = \frac{2\pi \vec{\mathrm{M}}^2}{3\mathrm{V}},$$

$$\mathrm{E}_5^0 = \frac{\vec{\mathrm{M}}^2}{2} \lim_{\mathrm{N} \to +\infty} \sum_{0 < \|\vec{m}\| \leqslant \mathrm{N}} \frac{1 - 3\cos^2 \theta_{\vec{m}}}{\|\vec{m}\|^3},$$

$$\mathrm{E}_5 = \frac{\vec{\mathrm{M}}^2}{2} \lim_{k \to +\infty} \sum_{\vec{m} \in \mathrm{B}_k \setminus \{\vec{0}\}} \frac{1 - 3\cos^2 \theta_{\vec{m}}}{\|\vec{m}\|^3}. \tag{28}$$

According to (21) and (27), the Born-Landé expression

$$\mathrm{E}_0 = \frac{1}{2} \lim_{k \to +\infty} \sum_{\vec{m} \in \mathrm{B}_k} \sum_{\vec{s}} \sum_{\substack{\vec{t} \\ \vec{m}+\vec{s} \neq \vec{t}}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|}$$

exists, and, with the help of (20),

$$\mathrm{E}_3' = \mathrm{E}_0 - \mathrm{E}_3 \tag{29}$$

where

$$\mathrm{E}_3 = \frac{1}{2} \sum_{\vec{m}} \sum_{\vec{s}} \sum_{\substack{\vec{t} \\ \vec{m}+\vec{s} \neq \vec{t}}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|} \int_{\|\vec{m}+\vec{s}-\vec{t}\|}^{+\infty} 4\pi u (u - \| \vec{m} + \vec{s} - \vec{t} \|) p(u) du$$

(absolutely summable on $\vec{m}$, according to (22)). Then

$$\mathrm{E}_0 = \mathrm{E}_\mathrm{E} + \mathrm{E}_4 + \mathrm{E}_5 - \mathrm{E}_5^0$$

with

$$\mathrm{E}_\mathrm{E} = \mathrm{E}_1 - \mathrm{E}_2 + \mathrm{E}_3 .$$

8. INTEGRAL FORM OF $\mathrm{E}_5 - \mathrm{E}_5^0$

NOTATIONS. — $d(k) = \sup_{\vec{m} \in \mathrm{B}_k} \| \vec{m} \|$; $\mathrm{B}(r) = \{ \vec{x} \in \mathrm{E} / \| \vec{x} \| \leqslant r \}$. We assume that there are $(f(k)) > 0$ and $(r_k) \geqslant 0$ such that:

$$b = \sup_k \frac{d(k)}{f(k)} \quad \text{is finite};$$

for almost every $\vec{x} \in \mathrm{E}$, $\varphi_{\frac{\mathrm{B}_k + \mathrm{C}}{f(k)}}(\vec{x})$ has a limit when $k \to +\infty$, which is denoted by $\varphi_{\mathrm{B}}(\vec{x})$;

$$\mathrm{B}(r_k) \cap \mathrm{L} \subset \mathrm{B}_k \quad \text{for all } k;$$

$$\lim_{k \to +\infty} \frac{r_k}{f(k)} = \varepsilon > 0. \tag{30}$$

Immediate consequences are: $\lim\limits_{k \to +\infty} f(k) = \lim\limits_{k \to +\infty} r_k = +\infty$; $\inf\limits_k f(k) = \eta > 0$;

$$\frac{\mathrm{B}_k + \mathrm{C}}{f(k)} \subset \mathrm{B}\left(b + \frac{\gamma}{\eta}\right);$$

$$\mathrm{B} \subset \mathrm{B}\left(b + \frac{\gamma}{\eta}\right) \text{ almost everywhere}.$$

According to Lebesgue's dominated convergence theorem, note that B is integrable. We may write

$$\begin{aligned} \mathrm{I}_k &= \mathrm{V} \sum_{\vec{m} \in \mathrm{B}_k \setminus \{\vec{0}\}} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} - \mathrm{V} \sum_{\vec{m} \in \mathrm{B}(r_k) \setminus \{\vec{0}\}} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} \\ &= \mathrm{V} \sum_{\vec{m} \in \mathrm{B}_k \setminus \mathrm{B}(r_k)} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} = \int \Phi_k(\vec{x}) d\vec{x} \end{aligned}$$

where

$$\begin{aligned} \Phi_k(\vec{x}) &= \sum_{\vec{\mu} \in \frac{\mathrm{B}_k \setminus \mathrm{B}(r_k)}{f(k)}} \frac{1 - 3\cos^2\theta_{\vec{\mu}}}{\|\vec{\mu}\|^3} \varphi_{\mathrm{C}_{\vec{\mu}}}(\vec{x}) \\ &= \sum_{\vec{\mu} \neq \vec{0}} \frac{1 - 3\cos^2\theta_{\vec{\mu}}}{\|\vec{\mu}\|^3} \varphi_{\mathrm{C}_{\vec{\mu}}}(\vec{x}) \varphi_{\frac{(\mathrm{B}_k \setminus \mathrm{B}(r_k)) + \mathrm{C}}{f(k)}}(\vec{x}) \end{aligned}$$

with the notations: $\vec{\mu} = \dfrac{\vec{m}}{f(k)}$, $\mathrm{C}_{\vec{\mu}} = \vec{\mu} + \dfrac{\mathrm{C}}{f(k)}$. Since

$$\lim_{k \to +\infty} \varphi_{\frac{(\mathrm{B}_k \setminus \mathrm{B}(r_k)) + \mathrm{C}}{f(k)}}(\vec{x}) = \varphi_{\mathrm{B} \setminus \mathrm{B}(\varepsilon)}(\vec{x})$$

almost everywhere (appendix 7), we have

$$\lim_{k \to +\infty} \Phi_k(\vec{x}) = \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} \varphi_{\mathrm{B} \setminus \mathrm{B}(\varepsilon)}(\vec{x})$$

for all $\vec{x} \neq \vec{0}$. Let us consider $\vec{x} \in \frac{(B_k \backslash B(r_k)) + C}{f(k)}$; $\vec{x} \in C_{\vec{\mu}}$, $\vec{\mu} = \frac{\vec{m}}{f(k)}$. Then

$$\| \vec{x} \| \leqslant b + \frac{\gamma}{\eta}$$

$$\| \vec{\mu} \| = \frac{\| \vec{m} \|}{f(k)} > \frac{r_k}{f(k)}.$$

There is k_0 such that, for all $k \geqslant k_0$,

$$\frac{r_k}{f(k)} \geqslant \frac{\varepsilon}{2},$$

so that

$$| \Phi_k(\vec{x}) | \leqslant \frac{4}{\| \vec{\mu} \|^3} < \frac{32}{\varepsilon^3}.$$

Then, for all $k \geqslant k_0$,

$$| \Phi_k(\vec{x}) | < \frac{32}{\varepsilon^3} \quad \text{if} \quad \| \vec{x} \| \leqslant b + \frac{\gamma}{\eta}$$

$$\Phi_k(\vec{x}) = 0 \quad \text{if} \quad \| \vec{x} \| > b + \frac{\gamma}{\eta},$$

and Lebesgue's dominated convergence theorem may be applied:

$$\lim_{k \to +\infty} I_k = \int_{B \backslash B(\varepsilon)} \frac{1 - 3 \cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} d\vec{x}.$$

According to the existence of E_5^0 (appendix 6), we may conclude from the assumptions (30), that E_5 exists and

$$E_5 - E_5^0 = \frac{\vec{M}^2}{2V} \int_{B \backslash B(\varepsilon)} \frac{1 - 3 \cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} d\vec{x}.$$

Note that $\mathring{B}(\varepsilon) \subset B$ (appendix 7), and that the above integral on $B \backslash B(\varepsilon)$ does not depend on $\varepsilon > 0$, provided that $B(\varepsilon) \subset B$ almost everywhere (take $\vec{M}$ as polar axis).

9. DUAL FORM OF THE RESULT

In this section, we only need the two conditions: B is integrable and $B(\varepsilon) \subset B$ almost everywhere. Then, the integral

$$I = \int_{B \backslash B(\varepsilon)} \frac{1 - 3 \cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} d\vec{x}$$

exists and, according to Lebesgue's dominated convergence theorem,

$$I = \lim_{r \to +\infty} I(r)$$

where

$$I(r) = \int g(\vec{x})\varphi_B(\vec{x})d\vec{x}$$

$$g(\vec{x}) = \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3}\varphi_{B(r)\setminus B(\varepsilon)}(\vec{x}).$$

Since g and φ_B belong to $\mathscr{L}^2(E)$, we may apply Plancherel's theorem:

$$I(r) = \int \mathscr{F}g(\vec{h})\mathscr{F}\varphi_B(\vec{h})d\vec{h}.$$

According to the expression of $\mathscr{F}g$ (appendix 8), we may write

$$I(r) = I_1(r) - I_1(\varepsilon)$$

where

$$I_1(\zeta) = \int (1 - 3\cos^2\theta_{\vec{h}})4\pi\frac{\sin\sigma_\zeta - \sigma_\zeta\cos\sigma_\zeta}{\sigma_\zeta^3}\mathscr{F}\varphi_B(\vec{h})d\vec{h}$$

$$= \int (1 - 3\cos^2\theta_{\vec{h}})\frac{1}{\zeta^3}\mathscr{F}\varphi_{B(\zeta)}(\vec{h})\mathscr{F}\varphi_B(\vec{h})d\vec{h},$$

$$\sigma_\zeta = 2\pi\zeta\,\|\vec{h}\|$$

($\mathscr{F}\varphi_{B(\zeta)}\mathscr{F}\varphi_B$ is integrable because $\mathscr{F}\varphi_{B(\zeta)}$ and $\mathscr{F}\varphi_B$ belong to $\mathscr{L}^2(E)$).
We have

$$\lim_{r \to +\infty}\frac{\sin\sigma_r - \sigma_r\cos\sigma_r}{\sigma_r^3} = 0 \quad \text{for all } \vec{h} \neq \vec{0}.$$

The function $\dfrac{\sin\sigma - \sigma\cos\sigma}{\sigma^3}$ is bounded (it has finite limits when $\sigma \to 0$ and $\sigma \to +\infty$):

$$\left|\frac{\sin\sigma - \sigma\cos\sigma}{\sigma^3}\right| \leqslant A.$$

We have also

$$\left|\frac{\sin\sigma_r - \sigma_r\cos\sigma_r}{\sigma_r^3}\right| \leqslant \frac{2}{\sigma_r^2}$$

$$\leqslant \frac{2}{4\pi^2\vec{h}^2} \quad \text{if} \quad r \geqslant 1.$$

If G denotes the function

$$G(\vec{h}) = \inf\left(A, \frac{2}{4\pi^2\vec{h}^2}\right),$$

we have, for all $\vec{h} \neq \vec{0}$ and $r \geqslant 1$,

$$\left| \frac{\sin \sigma_r - \sigma_r \cos \sigma_r}{\sigma_r^3} \mathscr{F}\varphi_B(\vec{h}) \right| \leqslant | G(\vec{h})\mathscr{F}\varphi_B(\vec{h}) | ,$$

and $G\mathscr{F}\varphi_B$ is integrable (G and $\mathscr{F}\varphi_B$ belong to $\mathscr{L}^2(E)$). We may then apply Lebesgue's dominated convergence theorem:

$$\lim_{r \to +\infty} I_1(r) = 0 .$$

The term $I_1(\varepsilon)$ may be written

$$I_1(\varepsilon) = I_2 - I_3$$

where

$$I_2 = \int \frac{1}{\varepsilon^3} \mathscr{F}\varphi_{B(\varepsilon)}(\vec{h})\mathscr{F}\varphi_B(\vec{h})d\vec{h} = \int \frac{1}{\varepsilon^3} \mathscr{F}(\varphi_B * \varphi_{B(\varepsilon)})(\vec{h})d\vec{h} ,$$

$$I_3 = \int 3\cos^2 \theta_{\vec{h}} \frac{1}{\varepsilon^3} \mathscr{F}\varphi_{B(\varepsilon)}(\vec{h})\mathscr{F}\varphi_B(\vec{h})d\vec{h} .$$

Poisson's formula relative to the Dirac measure

$$\varphi(\vec{0}) = \int \mathscr{F}\varphi(\vec{h})d\vec{h}$$

may be applied to the function φ if

1° φ is integrable;
2° $\mathscr{F}\varphi$ is integrable;
3° φ is continuous.

(see [*11*], section 12). The function $\varphi = \varphi_B * \varphi_{B(\varepsilon)}$ satisfies the condition 1°, and $\mathscr{F}\varphi = \mathscr{F}\varphi_B \mathscr{F}\varphi_{B(\varepsilon)}$ is integrable (condition 2°) because $\mathscr{F}\varphi_B$ and $\mathscr{F}\varphi_{B(\varepsilon)}$ belong to $\mathscr{L}^2(E)$. The condition 3° is also satisfied because φ_B and $\varphi_{B(\varepsilon)}$ belong to $\mathscr{L}^2(E)$. Then, Poisson's formula may be written:

$$I_2 = \frac{1}{\varepsilon^3}(\varphi_B * \varphi_{B(\varepsilon)})(\vec{0}) = \frac{1}{\varepsilon^3} \lambda(B \cap B(\varepsilon))$$

$$= \frac{1}{\varepsilon^3} \lambda(B(\varepsilon)) = \frac{4\pi}{3} \quad (\lambda \text{ is the Lebesgue measure on E}).$$

We may conclude

$$\int_{B \setminus B(\varepsilon)} \frac{1 - 3\cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} d\vec{x} = -\frac{4\pi}{3} + \int 3\cos^2 \theta_{\vec{h}} \frac{1}{\varepsilon^3} \mathscr{F}\varphi_{B(\varepsilon)}(\vec{h})\mathscr{F}\varphi_B(\vec{h})d\vec{h}$$

$$= -\frac{4\pi}{3} + 4\pi \int \cos^2 \theta_{\vec{h}} \mathscr{F}\varphi_\varepsilon(\vec{h})\mathscr{F}\varphi_B(\vec{h})d\vec{h} ,$$

where $\varphi_\varepsilon = \dfrac{3}{4\pi\varepsilon^3}\varphi_{B(\varepsilon)}$. The result of sections 7-8 may thus be written in the dual form:

$$E_0 = E_E + \frac{2\pi\vec{M}^2}{V}\int \cos^2\theta_{\vec{h}}\mathcal{F}\varphi_\varepsilon(\vec{h})\mathcal{F}\varphi_B(\vec{h})d\vec{h}\,.$$

10. THE LIMIT ENERGY PER CELL E

Let (A_k) be any increasing sequence of finite subsets of L such that $\bigcup_k A_k = L$. Our purpose is now to determine the conditions of existence and the value of the limit energy per cell E defined by (8). Since

$$\text{card}\,\{(\vec{n}, \vec{p}) \in A_k \times A_k / \vec{n} - \vec{p} = \vec{m}\} = \text{card}\,(A_k \cap \vec{m} + A_k),$$

we have

$$E = \lim_{k\to+\infty} E(k)$$

where

$$E(k) = \frac{1}{2}\sum_{\vec{m}\in B_k} c(A_k, \vec{m}) \sum_{\substack{\vec{s} \quad \vec{t}\\ \vec{m}+\vec{s}\neq\vec{t}}}\sum \frac{q_{\vec{s}}q_{\vec{t}}}{\|\vec{m}+\vec{s}-\vec{t}\,\|},$$

$$B_k = \{\vec{n}-\vec{p}/\vec{n}\in A_k \text{ and } \vec{p}\in A_k\} = A_k - A_k,$$

$$c(A_k, \vec{m}) = \frac{\text{card}\,(A_k\cap\vec{m}+A_k)}{\text{card}\,A_k}.$$

We write

$$E(k) = E_0(k) - E_6(k)$$

with

$$E_0(k) = \frac{1}{2}\sum_{\vec{m}\in B_k}\sum_{\substack{\vec{s} \quad \vec{t}\\ \vec{m}+\vec{s}\neq\vec{t}}}\sum \frac{q_{\vec{s}}q_{\vec{t}}}{\|\vec{m}+\vec{s}-\vec{t}\,\|}$$

$$E_6(k) = \frac{1}{2}\sum_{\vec{m}\in B_k\setminus\{\vec{0}\}}(1 - c(A_k, \vec{m}))\sum_{\vec{s}}\sum_{\vec{t}}\frac{q_{\vec{s}}q_{\vec{t}}}{\|\vec{m}+\vec{s}-\vec{t}\,\|}.$$

The existence and the value of $E_0 = \lim_{k\to+\infty} E_0(k)$ has been studied in the preceding sections. We now study the term $E_6(k)$.

Limit of $E_6(k)$ *when* $k \to +\infty$.

NOTATIONS. — $d'(k) = \sup_{\vec{n}\in A_k} \|\vec{n}\|$; $d(k) = \sup_{\vec{m}\in B_k} \|\vec{m}\|$. We assume that there are $(f(k)) > 0$, $a \geqslant 0$ and $\alpha > 0$ such that:

$$b' = \sup_k \frac{d'(k)}{f(k)} \quad \text{is finite;} \tag{31}$$

$$1 - c(A_k, \vec{m}) \leqslant a\left(\frac{\|\vec{m}\|}{f(k)}\right)^\alpha \quad \text{for all } k \text{ and } \vec{m}\in B_k. \tag{32}$$

Note that the first assumption is equivalent to

$$b = \sup_k \frac{d(k)}{f(k)} \quad \text{is finite}.$$

According to (21), we may write

$$E_6(k) = E_{6.1}(k) + E_{6.2}(k),$$

where

$$E_{6.1}(k) = \frac{\vec{M}^2}{2} \sum_{\vec{m}\in B_k\setminus\{\vec{0}\}} (1 - c(A_k, \vec{m}))\frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3},$$

$$E_{6.2}(k) = \frac{1}{2} \sum_{\vec{m}\in B_k\setminus\{\vec{0}\}} (1 - c(A_k, \vec{m}))A(\vec{m})$$

and

$$|A(\vec{m})| \leqslant \frac{A}{(\|\vec{m}\| - \delta)^4} \quad \text{if} \quad \|\vec{m}\| > \delta.$$

We write

$$E_{6.2}(k) = E_{6.2.1}(k) + E_{6.2.2}(k)$$

with

$$E_{6.2.1}(k) = \frac{1}{2} \sum_{\substack{\vec{m}\in B_k\setminus\{\vec{0}\} \\ \|\vec{m}\|\leqslant\delta}} (1 - c(A_k, \vec{m}))A(\vec{m})$$

$$E_{6.2.2}(k) = \frac{1}{2} \sum_{\substack{\vec{m}\in B_k\setminus\{\vec{0}\} \\ \|\vec{m}\|>\delta}} (1 - c(A_k, \vec{m}))A(\vec{m}).$$

From the assumptions (31)-(32), we may deduce

$$\lim_{k\to+\infty} c(A_k, \vec{m}) = 1$$

so that

$$\lim_{k\to+\infty} E_{6.2.1}(k) = 0,$$

and

$$| E_{6.2.2}(k) | \leqslant \frac{a\mathrm{AS}(k)}{2(f(k))^\alpha} \leqslant \frac{a\mathrm{A}b^\alpha \mathrm{S}(k)}{2(d(k))^\alpha}$$

where

$$\mathrm{S}(k) = \sum_{\delta < \|\vec{m}\| \leqslant d(k)} \frac{\|\vec{m}\|^\alpha}{(\|\vec{m}\| - \delta)^4}.$$

Since

$$\lim_{k \to +\infty} \frac{\mathrm{S}(k)}{(d(k))^\alpha} = 0$$

(appendix 9), we may conclude

$$\lim_{k \to +\infty} E_{6.2}(k) = 0.$$

Note first that the proof is completed if $\vec{\mathrm{M}} = \vec{0}$, for $E_6(k) = E_{6.2}(k)$ in this case. We suppose now $\vec{\mathrm{M}} \neq \vec{0}$ and we introduce the new assumptions:

for almost every $\vec{x} \in \mathrm{E}$, $\varphi_{\frac{\mathrm{B}_k + \mathrm{C}}{f(k)}}(\vec{x})$ has a limit when $k \to +\infty$, which is denoted by $\varphi_\mathrm{B}(\vec{x})$; (33)

for almost every $\vec{x} \in \mathrm{E}$, $c(\mathrm{A}_k, \vec{m}_k(\vec{x}))$ has a finite limit when $k \to +\infty$, which is denoted by $c(\vec{x})$; notation: $\vec{m}_k(\vec{x}) \in \mathrm{L}$ is defined by $\vec{x} \in \frac{\vec{m}_k(\vec{x}) + \mathrm{C}}{f(k)}$. (34)

NOTATIONS. — $\vec{\mu} = \frac{\vec{m}}{f(k)}$; $\mathrm{C}_{\vec{\mu}} = \vec{\mu} + \frac{\mathrm{C}}{f(k)}$. As in section 6.3, we write

$$E_{6.1}(k) = \frac{\vec{\mathrm{M}}^2}{2\mathrm{V}} \int d\vec{x} \sum_{\vec{\mu} \neq \vec{0}} (1 - c(\mathrm{A}_k, \vec{m})) \frac{1 - 3\cos^2\theta_{\vec{\mu}}}{\|\vec{\mu}\|^3} \varphi_{\mathrm{C}_{\vec{\mu}}}(\vec{x}) \varphi_{\frac{\mathrm{B}_k + \mathrm{C}}{f(k)}}(\vec{x}),$$

and, in the appendix 10, we show that

$$\lim_{k \to +\infty} E_{6.1}(k) = \frac{\vec{\mathrm{M}}^2}{2\mathrm{V}} \int (1 - c(\vec{x})) \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} \varphi_\mathrm{B}(\vec{x}) d\vec{x}.$$

Finally,

$$\lim_{k \to +\infty} E_6(k) = E_6$$

with

$$E_6 = \frac{\vec{\mathrm{M}}^2}{2\mathrm{V}} \int_\mathrm{B} (1 - c(\vec{x})) \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x}.$$

In conclusion,

$$E = E_0 - E_6.$$

11. INTEGRAL FORM OF $E_5 - E_5^0 - E_6$

According to section 8, we may write, with $0 < \varepsilon' \leqslant \varepsilon$:

$$E_5 - E_5^0 - E_6 = \frac{\vec{M}^2}{2V} \int_{B \setminus B(\varepsilon')} \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x} - \frac{\vec{M}^2}{2V} \int_B (1 - c(\vec{x})) \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x}$$

$$= \frac{\vec{M}^2}{2V} \int_{B \setminus B(\varepsilon')} c(\vec{x}) \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x} - \frac{\vec{M}^2}{2V} \int_{B(\varepsilon')} (1 - c(\vec{x})) \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x}$$

$$= \frac{\vec{M}^2}{2V} \lim_{\varepsilon' \to 0^+} \int_{B \setminus B(\varepsilon')} c(\vec{x}) \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x}$$

(the function $(1 - c(\vec{x})) \dfrac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3}$ is integrable in $B(\varepsilon)$: end of the appendix 10).

12. DUAL FORM OF THE RESULT

New assumption:

$$c \in \mathscr{C}(E) \quad \text{and} \quad \mathscr{F}c \in \mathscr{L}^1(E) \tag{35}$$

($\mathscr{C}(E)$ is the space of continuous functions). According to (33), for almost every $\vec{x} \notin B$, there is k_0 such that, for all $k \geqslant k_0$, $\vec{x} \notin \dfrac{B_k + C}{f(k)}$ i. e. $\vec{m}_k(\vec{x}) \notin B_k$; then, $c(A_k, \vec{m}_k(\vec{x})) = 0$ and, at the limit $k \to +\infty$, $c(\vec{x}) = 0$. Since B is bounded, we deduce

$$c \in \mathscr{K}(E) \tag{36}$$

($\mathscr{K}(E)$ is the space of continuous functions with compact support), which implies $c \in \mathscr{L}^1(E) \cap \mathscr{L}^2(E)$. As for the function p in section 3, note that (35) is equivalent to

$$c \in \mathscr{P}(E).$$

According to (36), we may write

$$I = \lim_{\varepsilon \to 0^+} \int_{B \setminus B(\varepsilon)} c(\vec{x}) \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x}$$

$$= \lim_{\substack{\varepsilon \to 0^+ \\ r \to +\infty}} I(\varepsilon, r)$$

where

$$I(\varepsilon, r) = \int_{B(r) \setminus B(\varepsilon)} c(\vec{x}) \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x}.$$

With the same notations as in section 9, we apply Plancherel's theorem:

$$I(\varepsilon, r) = \int \mathscr{F}g(\vec{h})\mathscr{F}c(\vec{h})d\vec{h}.$$

According to the expression of $\mathscr{F}g$ (appendix 8), we have

$$\lim_{\substack{\varepsilon \to 0^+ \\ r \to +\infty}} \mathscr{F}g(\vec{h})\mathscr{F}c(\vec{h}) = -\frac{4\pi}{3}(1 - 3\cos^2\theta_{\vec{h}})\mathscr{F}c(\vec{h})$$

and

$$|\mathscr{F}g(\vec{h})\mathscr{F}c(\vec{h})| \leqslant 4\pi \times 4 \times 2A\,|\mathscr{F}c(\vec{h})|.$$

We may then apply Lebesgue's dominated convergence theorem:

$$\begin{aligned} I &= \int -\frac{4\pi}{3}(1 - 3\cos^2\theta_{\vec{h}})\mathscr{F}c(\vec{h})d\vec{h} \\ &= -\frac{4\pi}{3}\int \mathscr{F}c(\vec{h})d\vec{h} + 4\pi\int \cos^2\theta_{\vec{h}}\mathscr{F}c(\vec{h})d\vec{h}. \end{aligned}$$

According to (35) and (36), the conditions 1°, 2° and 3° of Poisson's formula relative to the Dirac measure (see section 9) are satisfied by c, so that:

$$\int \mathscr{F}c(\vec{h})d\vec{h} = c(\vec{0}).$$

For all k, $\vec{0} \in \frac{C}{f(k)}$ i. e. $\vec{m}_k(\vec{0}) = \vec{0}$, so that

$$c(\vec{0}) = \lim_{k \to +\infty} c(A_k, \vec{0}) = 1.$$

Then

$$I = -\frac{4\pi}{3} + 4\pi\int \cos^2\theta_{\vec{h}}\mathscr{F}c(\vec{h})d\vec{h},$$

which may also be written

$$E_4 + E_5 - E_5^0 - E_6 = \frac{2\pi\vec{M}^2}{V}\int \cos^2\theta_{\vec{h}}\mathscr{F}c(\vec{h})d\vec{h}.$$

Finally, the results of sections 7 and 10 lead to the expression:

$$E = E_E + \frac{2\pi\vec{M}^2}{V}\int \cos^2\theta_{\vec{h}}\mathscr{F}c(\vec{h})d\vec{h}.$$

13. EXPRESSION OF c

Notation: $B(\vec{x}, r) = \{\vec{y} \in E / \|\vec{y} - \vec{x}\| \leqslant r\}$. In this section, we only consider the assumption (31) and the following one: there is $A \subset E$ such that for all $\vec{x} \in \mathring{A}$, there are $r > 0$ and k_0 such that $B(\vec{x}, r) \subset \frac{A_k + C}{f(k)}$ for all $k \geqslant k_0$;

for all $\vec{x} \in E \backslash \overline{A}$, there are $r > 0$ and k_0 such that $B(\vec{x}, r) \subset E \backslash \frac{A_k + C}{f(k)}$ for all $k \geqslant k_0$;

$\overline{A} \backslash \mathring{A}$ is negligible;

$$\mathring{A} \neq \phi . \tag{37}$$

Let us denote $A'_k = \frac{A_k + C}{f(k)}$. As a consequence of the preceding assumption (37), we have, for any $\vec{x} \in E$ and $(\vec{x}_k)$ such that $\lim_{k \to +\infty} \vec{x}_k = \vec{x}$,

$$\lim_{k \to +\infty} \varphi_{\vec{x}_k + A'_k}(\vec{y}) = \varphi_{\vec{x}+A}(\vec{y}) \qquad \text{for all} \qquad \vec{y} \in \vec{x} + (\mathring{A} \cup (E \backslash \overline{A})), \tag{38}$$

i. e. for almost every $\vec{y} \in E$. Indeed, if $\vec{y} \in \vec{x} + \mathring{A}$, $\vec{y} = \vec{x} + \vec{u}$ and there are $r > 0$ and k_0 such that

$$B(\vec{u}, r) \subset A'_k \qquad \text{for all} \quad k \geqslant k_0 .$$

We may write $\vec{y} = \vec{x}_k + \vec{u}_k$ with $\vec{u}_k = \vec{u} + \vec{x} - \vec{x}_k$, and there is k_1 such that

$$\vec{u}_k \in B(\vec{u}, r) \qquad \text{for all} \quad k \geqslant k_1 .$$

Then

$$\vec{y} \in \vec{x}_k + A'_k \qquad \text{for all} \quad k \geqslant \sup (k_0, k_1) .$$

The proof is similar in the case $\vec{y} \in \vec{x} + (E \backslash \overline{A})$. Let us return to the function c:

$$c(A_k, \vec{m}_k(\vec{x})) = \frac{\int \varphi_{A_k + C}(\vec{y}) \varphi_{\vec{m}_k(\vec{x}) + A_k + C}(\vec{y}) d\vec{y}}{\int \varphi_{A_k + C}(\vec{y}) d\vec{y}}$$

$$= \frac{\int \varphi_{A'_k}(\vec{y}) \varphi_{\frac{\vec{m}_k(\vec{x})}{f(k)} + A'_k}(\vec{y}) d\vec{y}}{\int \varphi_{A'_k}(\vec{y}) d\vec{y}} .$$

According to (38), we have

$$\lim_{k \to +\infty} \varphi_{A'_k} = \varphi_A \text{ almost everywhere},$$

and, for all $\vec{x} \in E$,

$$\lim_{k \to +\infty} \varphi_{\frac{\vec{m}_k(\vec{x})}{f(k)} + A'_k} = \varphi_{\vec{x}+A} \text{ almost everywhere} .$$

Since

$$\varphi_{A'_k} \leqslant \varphi_{B\left(b' + \frac{\gamma}{\eta}\right)},$$

we may apply Lebesgue's dominated convergence theorem: for all $\vec{x} \in \mathrm{E}$, $c(\vec{x})$ exists and is equal to

$$c(\vec{x}) = \frac{\lambda(\mathrm{A} \cap \vec{x} + \mathrm{A})}{\lambda(\mathrm{A})} = \frac{1}{\lambda(\mathrm{A})}(\varphi_{\mathrm{A}} * \varphi_{-\mathrm{A}})(\vec{x}).$$

Since $\varphi_{\mathrm{A}} \in \mathscr{L}^1(\mathrm{E})$, we may write

$$\mathscr{F}c = \frac{1}{\lambda(\mathrm{A})} |\mathscr{F}\varphi_{\mathrm{A}}|^2.$$

Since $\varphi_{\mathrm{A}} \in \mathscr{L}^2(\mathrm{E})$, we have also

$$c \in \mathscr{C}(\mathrm{E}) \quad \text{and} \quad \mathscr{F}c \in \mathscr{L}^1(\mathrm{E}).$$

The assertions (34) and (35) are then consequences of (31) and (37), and the result of section 12 may also be written:

$$\mathrm{E} = \mathrm{E}_{\mathrm{E}} + \frac{2\pi\vec{\mathrm{M}}^2}{\mathrm{V}\lambda(\mathrm{A})} \int \cos^2 \theta_{\vec{h}} |\mathscr{F}\varphi_{\mathrm{A}}(\vec{h})|^2 d\vec{h}.$$

14. AN EXAMPLE: THE SPHERICAL CRYSTAL

Let us order the set $\{ \|\vec{n}\| / \vec{n} \in \mathrm{L} \}$ into an increasing sequence, denoted by R_k, and define

$$\mathrm{A}_k = \{ \vec{n} \in \mathrm{L} / \|\vec{n}\| \leqslant \mathrm{R}_k \}.$$

In order to apply the results of sections 7 and 10, we have to prove (27), (31), (32), (33) and (34). The proof of (27) and (33) requires a preliminary result, which will be proved in the following section.

14.1. Properties concerning A_k, B_k and their convex hulls.

RESULT 1. — There is $\mathrm{R} > 0$ such that, for all k,

$$\mathrm{B}(\mathrm{R}_k - \mathrm{R}) \subset \operatorname{conv} \mathrm{A}_k.$$

Proof. — Since A_k is finite, we know that conv A_k is the intersection of a finite number of closed half-spaces H_i:

$$\operatorname{conv} \mathrm{A}_k = \bigcap_{i=1}^{l} \mathrm{H}_i \tag{39}$$

(see [*12*]). Let P_i denote the plane which bounds H_i, $d_i = \inf_{\vec{x} \in \mathrm{P}_i} \|\vec{x}\|$ and $d_{i_0} = \inf_{i=1,\dots,l} d_i$. Since $\vec{0} \in \mathrm{A}_k$, and with the help of (39), we have

$$\mathrm{B}(d_{i_0}) \subset \operatorname{conv} \mathrm{A}_k. \tag{40}$$

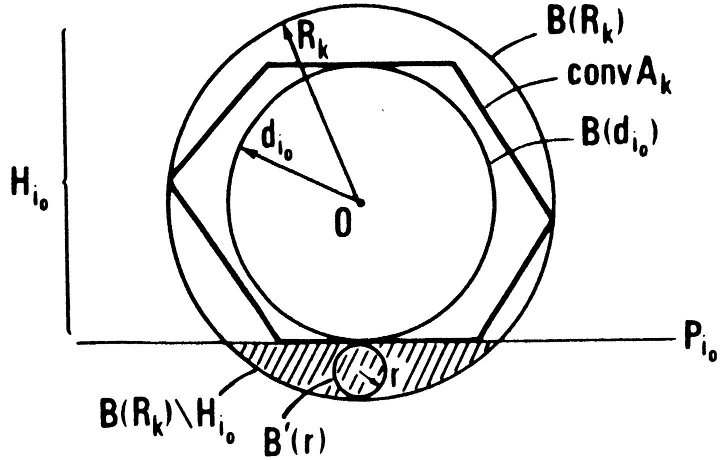

FIG. 2. — Spherical crystal: property concerning the convex hull of A_k (proof of the result 1 of section 14.1).

From the definition of A_k and conv $A_k \subset H_{i_0}$, we may deduce that

$$L \cap (B(R_k)\backslash H_{i_0}) = \phi\,,$$

and then

$$L \cap B'(r) = \phi\,, \tag{41}$$

where $B'(r)$ is the open ball of radius $r = \frac{1}{2}(R_k - d_{i_0})$, included in $B(R_k)\backslash H_{i_0}$, as shown in fig. 2. Denote by R the greatest diameter of an open ball which does not contain lattice points:

$$R = 2 \sup_{\vec{y} \in E} \inf_{\vec{n} \in L} \| \vec{y} - \vec{n} \|$$

(R is finite, for $\inf_{\vec{n} \in L} \| \vec{y} - \vec{n} \| \leqslant \| \vec{y} - \vec{n}(\vec{y}) \| \leqslant \gamma$, $\vec{n}(\vec{y})$ being defined by: $\vec{y} \in \vec{n}(\vec{y}) + C$). Then, according to (41),

$$R_k - d_{i_0} = 2r \leqslant R$$

or

$$R_k - R \leqslant d_{i_0}\,,$$

which leads to the result 1 (with the help of (40)).

RESULT 2.

$$\text{conv } B_k = 2 \text{ conv } A_k\,.$$

Proof. — We may write

$$2A_k \subset A_k + A_k = A_k - A_k = B_k\,,$$

and then

$$2 \text{ conv } A_k \subset \text{conv } B_k .$$

On the other hand

$$B_k = A_k + A_k \subset \text{conv } A_k + \text{conv } A_k = 2 \text{ conv } A_k$$

($A + A = 2A$ for any convex set A, since $x + y \in A + A$ may be written as $2\left(\frac{x + y}{2}\right)$, and then

$$\text{conv } B_k \subset 2 \text{ conv } A_k .$$

RESULT 3.

$$B_k = L \cap \text{conv } B_k .$$

Proof. — We have to prove

$$L \cap \text{conv } B_k \subset B_k . \tag{42}$$

Let $\vec{m} \in L \cap \text{conv } B_k$. According to the result 2, $\vec{m} = 2\vec{\mu}$ where

$$\vec{\mu} \in \text{conv } A_k . \tag{43}$$

By the definition of A_k, $\text{conv } A_k \subset B(R_k)$, so that

$$\| \vec{\mu} \| \leqslant R_k . \tag{44}$$

If $\vec{\mu} \in L$, then (by (44)) $\vec{\mu} \in A_k$ and

$$\vec{m} = 2\vec{\mu} = \vec{\mu} + \vec{\mu} \in A_k + A_k = B_k ,$$

which proves (42).

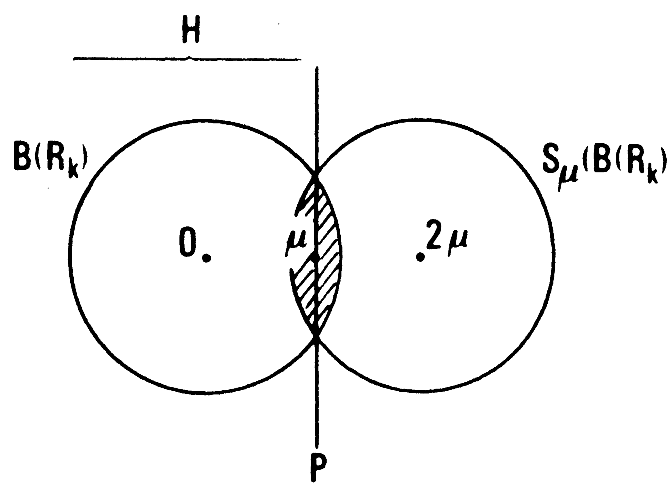

FIG. 3. — Spherical crystal: relation between B_k and its convex hull (proof of the result 3 of section 14.1).

Now, let us suppose that $\vec{\mu} = \frac{\vec{m}}{2} \in \frac{1}{2} L$ is such that

$$\vec{\mu} \notin L .$$

We have to prove that

$$\vec{m} = 2\vec{\mu} \in B_k = A_k + A_k ,$$

i. e. that $\vec{\mu}$ may be written as

$$\vec{\mu} = \frac{1}{2}(\vec{n} + \vec{p}), \qquad \vec{n} \quad \text{and} \quad \vec{p} \in A_k . \tag{45}$$

We argue by contradiction. Suppose that (45) is false, i. e. that

$$\text{for all} \quad \vec{n} \in A_k, \quad S_{\vec{\mu}}(\vec{n}) \notin A_k \tag{46}$$

where $S_{\vec{\mu}}$ is the symmetry with center $\vec{\mu}$. Since $\vec{\mu} \in \frac{1}{2} L$, $S_{\vec{\mu}}(L) = L$ and we may deduce, from (46) and the definition of A_k:

$$L \cap B(R_k) \cap S_{\vec{\mu}}(B(R_k)) = \phi . \tag{47}$$

Let P denote the plane containing $\vec{\mu}$ and perpendicular to the direction $\vec{\mu}$, and H the open half-space bounded by P, which contains $\vec{0}$ (see fig. 3). (47) implies

$$A_k \subset H ,$$

and hence

$$\text{conv } A_k \subset H . \tag{48}$$

The contradiction arises from (43) and (48), since $\vec{\mu}$ does not belong to the *open* half-space H.

RESULT 4.

$$L \cap B(2R_k - 2R) \subset B_k . \tag{49}$$

Proof. — This result (which will be used in the following sections) is a consequence of the preceding results 1, 2 and 3.

14.2. **Proof of** (27)

Let us consider the difference

$$\Delta_k = \left| \sum_{0 < \|\vec{m}\| \leqslant 2R_k} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} - \sum_{\vec{m} \in B_k \setminus \{\vec{0}\}} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} \right|$$

$$= \left| \sum_{\substack{\|\vec{m}\| \leqslant 2R_k \\ \vec{m} \notin B_k}} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} \right| .$$

According to the result (49), Δ_k may be majorized by

$$\Delta_k \leqslant \left| \sum_{2R_k - 2R < \|\vec{m}\| \leqslant 2R_k} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} \right|$$

$$\leqslant 4 \sum_{2R_k - 2R < \|\vec{m}\| \leqslant 2R_k} \frac{1}{\|\vec{m}\|^3}.$$

Let us denote

$$D_k = \bigcup_{2R_k - 2R < \|\vec{m}\| \leqslant 2R_k} \vec{m} + C$$

$$\Phi(\vec{x}) = \sum_{\vec{m} \neq \vec{0}} \frac{1}{\|\vec{m}\|^3} \varphi_{\vec{m}+C}(\vec{x})$$

$$F(\vec{x}) = \frac{1}{\|\vec{x}\|^3}.$$

With a method similar to that of appendix 9, we obtain

$$\Delta_k \leqslant \frac{4}{V} \int_{D_k} F(\vec{x}) d\vec{x} + \frac{4}{V} \int_{D_k} |\Phi(\vec{x}) - F(\vec{x})| \, d\vec{x}$$

$$\leqslant \frac{16\pi}{V} \operatorname{Log} \frac{2R_k + \gamma}{2R_k - 2R - \gamma} + \frac{48\pi\gamma}{V} \left[-\frac{1}{\rho} - \frac{\gamma}{\rho^2} - \frac{\gamma^2}{3\rho^3} \right]_{\rho = 2R_k - 2R - 2\gamma}^{2R_k}$$

which shows that

$$\lim_{k \to +\infty} \Delta_k = 0.$$

According to the result of appendix 6, the two following limits exist and are equal:

$$\lim_{k \to +\infty} \sum_{\vec{m} \in B_k \setminus \{\vec{0}\}} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3} = \lim_{r \to +\infty} \sum_{0 < \|\vec{m}\| \leqslant r} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3}.$$

By application of the result of section 7, we may conclude:

$$E_0 = \frac{1}{2} \lim_{k \to +\infty} \sum_{\vec{m} \in B_k} \sum_{\vec{s}} \sum_{\substack{\vec{t} \\ \vec{m} + \vec{s} \neq \vec{t}}} \frac{q_{\vec{s}} q_{\vec{t}}}{\|\vec{m} + \vec{s} - \vec{t}\|}$$

$$= \frac{1}{2} \lim_{r \to +\infty} \sum_{\|\vec{m}\| \leqslant r} \sum_{\vec{s}} \sum_{\substack{\vec{t} \\ \vec{m} + \vec{s} \neq \vec{t}}} \frac{q_{\vec{s}} q_{\vec{t}}}{\|\vec{m} + \vec{s} - \vec{t}\|}$$

$$= E_E + \frac{2\pi \vec{M}^2}{3V}.$$

14.3. **Proof of** (34).

We take $f(k) = R_k$. The assertion (31) is obviously satisfied. With the help of

$$c(A_k, \vec{m}) = \frac{\int_{(A_k+C)\cap(\vec{m}+A_k+C)} d\vec{x}}{\int_{A_k+C} d\vec{x}}$$

and the inclusions

$$B(R_k - \gamma) \subset A_k + C \subset B(R_k + \gamma),$$

we obtain, for $R_k > \gamma$:

$$c(A_k, \vec{m}) \geqslant \frac{(R_k-\gamma)^3}{(R_k+\gamma)^3} - \frac{3\|\vec{m}\|(R_k-\gamma)^2}{4(R_k+\gamma)^3} + \frac{\|\vec{m}\|^3}{16(R_k+\gamma)^3} \text{ if } \|\vec{m}\| < 2(R_k-\gamma); \tag{50}$$

$$c(A_k, \vec{m}) \leqslant \frac{(R_k+\gamma)^3}{(R_k-\gamma)^3} - \frac{3\|\vec{m}\|(R_k+\gamma)^2}{4(R_k-\gamma)^3} + \frac{\|\vec{m}\|^3}{16(R_k-\gamma)^3} \text{ if } \|\vec{m}\| < 2(R_k+\gamma); \tag{51}$$

$$c(A_k, \vec{m}) = 0 \quad \text{if} \quad \|\vec{m}\| \geqslant 2(R_k + \gamma). \tag{52}$$

The inequality

$$\|\vec{m}_k(\vec{x})\| \geqslant \|\vec{x}\| R_k - \gamma$$

shows that (52) is satisfied if $\|\vec{x}\| > 2$ and k is large enough, so that

$$c(\vec{x}) = 0 \quad \text{if} \quad \|\vec{x}\| > 2.$$

The inequality

$$\|\vec{m}_k(\vec{x})\| \leqslant \|\vec{x}\| R_k + \gamma$$

shows that (50) and (51) are satisfied if $\|\vec{x}\| < 2$ and k is large enough. Since

$$\|\vec{m}_k(\vec{x})\| \underset{k\to+\infty}{\sim} \|\vec{x}\| R_k,$$

we deduce that

$$c(\vec{x}) = 1 - \frac{3\|\vec{x}\|}{4} + \frac{\|\vec{x}\|^3}{16} \quad \text{if} \quad \|\vec{x}\| < 2.$$

14.4. **Proof of** (32).

With the help of (50), we may write

$$\begin{aligned} 1 - c(A_k, \vec{m}) &\leqslant 1 - \frac{(R_k - \gamma)^3}{(R_k + \gamma)^3} + \frac{3\|\vec{m}\|}{4R_k} \\ &= \frac{6R_k^2\gamma + 2\gamma^3}{(R_k + \gamma)^3} + \frac{3\|\vec{m}\|}{4R_k} \\ &\leqslant \frac{6\gamma}{R_k} + \frac{2\gamma}{R_k} + \frac{3\|\vec{m}\|}{4R_k}. \end{aligned}$$

If $\vec{m} \neq \vec{0}$, $\| \vec{m} \| \geqslant | m | \varepsilon_0 \geqslant \varepsilon_0$ (see the notations in appendix 4) and we deduce

$$1 - c(A_k, \vec{m}) \leqslant \frac{\| \vec{m} \|}{R_k} \left(\frac{8\gamma}{\varepsilon_0} + \frac{3}{4} \right)$$

if $R_k > \gamma$ and $\| \vec{m} \| < 2(R_k - \gamma)$ (the inequality also holds for $\vec{m} = \vec{0}$). In the case $\| \vec{m} \| \geqslant 2(R_k - \gamma)$, we have

$$1 - c(A_k, \vec{m}) \leqslant 1 \leqslant \frac{\| \vec{m} \|}{2(R_k - \gamma)} \leqslant \frac{\| \vec{m} \|}{R_k} \quad \text{if} \quad R_k \geqslant 2\gamma .$$

In the last case $R_k < 2\gamma$, we have

$$1 - c(A_k, \vec{m}) \leqslant 1 < \frac{2\gamma}{R_k} \leqslant \frac{\| \vec{m} \|}{R_k} \frac{2\gamma}{\varepsilon_0} .$$

These inequalities show that (32) is satisfied with $\alpha = 1$.

14.5. **Proof of** (33).

If $\| \vec{x} \| > 2$ and k is large enough, we have $\frac{\| \vec{m}_k(\vec{x}) \|}{R_k} > 2$, which implies $\vec{m}_k(\vec{x}) \notin B_k$ i. e.

$$\varphi_{\frac{B_k + C}{R_k}}(\vec{x}) = 0 .$$

The inequality

$$\| \vec{m}_k(\vec{x}) \| \leqslant \| \vec{x} \| R_k + \gamma$$

implies

$$\| \vec{m}_k(\vec{x}) \| \leqslant 2R_k - 2R$$

if $\| \vec{x} \| < 2$ and k is large enough. The result (49) shows that $\vec{m}_k(\vec{x}) \in B_k$ i. e.

$$\varphi_{\frac{B_k + C}{R_k}}(\vec{x}) = 1 .$$

Finally,

$$B = \{ \vec{x} \in E / \| \vec{x} \| \leqslant 2 \} \quad \text{(almost everywhere)} .$$

In conclusion, the result of section 10 may be applied:

$$E = E_0$$

($E_6 = 0$ for B is a sphere and $c(\vec{x})$ depends only on $\| \vec{x} \|$: take $\vec{M}$ as polar axis) with the value of E_0 given in section 14.2.

15. SUMMARY OF THE RESULTS

For clarity, we present first the notations and a classification of the assumptions.

NOTATIONS:

$B(r) = \{ \vec{x} \in E / \| \vec{x} \| \leqslant r \}$;

$B(\vec{x}, r) = \{ \vec{y} \in E / \| \vec{y} - \vec{x} \| \leqslant r \}$;

φ_D is the characteristic function of a subset D of E ;
λ or $d\vec{x}$ represents the Lebesgue measure on E ;

$\mathscr{F}f(\vec{h}) = \int f(\vec{x}) e^{-2\pi i \vec{h}.\vec{x}} d\vec{x}$ (Fourier transform of f);

$C = [0, 1[\vec{a}_1 + [0, 1[\vec{a}_2 + [0, 1[\vec{a}_3$ (cell parallelepiped);

$V = |(\vec{a}_1, \vec{a}_2, \vec{a}_3)| = \lambda(C)$;

$L^* = \mathbb{Z}\vec{a}_1^* + \mathbb{Z}\vec{a}_2^* + \mathbb{Z}\vec{a}_3^*$ (dual lattice) where $\vec{a}_i \cdot \vec{a}_j^* = \delta_{ij}$ (Kronecker delta);

$$F(\vec{h}) = \sum_{\vec{s} \in S} q_{\vec{s}} e^{-2\pi i \vec{h}.\vec{s}};$$

$$\vec{M} = \sum_{\vec{s} \in S} q_{\vec{s}} \vec{s} \text{ (dipole moment of the cell S)};$$

$\theta_{\vec{x}}$ is the angle $(\vec{M}, \vec{x})$.

Classification of the assumptions:

1) $\displaystyle\sum_{\vec{m} \in B_k \setminus \{\vec{0}\}} \frac{1 - 3\cos^2 \theta_{\vec{m}}}{\|\vec{m}\|^3}$ has a finite limit when $k \to +\infty$;

2) there is $(f(k)) > 0$ such that

2.1) $\left(\dfrac{d(k)}{f(k)}\right)$ is majorized; notation: $d(k) = \sup_{\vec{m} \in B_k} \|\vec{m}\|$ (or $\sup_{\vec{n} \in A_k} \|\vec{n}\|$);

2.2) for almost every $\vec{x} \in E$, $\varphi_{\frac{B_k + C}{f(k)}}(\vec{x})$ has a limit when $k \to +\infty$, which is denoted by $\varphi_B(\vec{x})$;

2.3) there is an increasing sequence $(r_k) \geqslant 0$ such that

2.3.1) $B(r_k) \cap L \subset B_k$ for all k;

2.3.2) $\dfrac{r_k}{f(k)}$ has a limit $\varepsilon > 0$, when $k \to +\infty$;

2.4) there are $a \geqslant 0$ and $\alpha > 0$ such that

$$1 - c(A_k, \vec{m}) \leqslant a \left(\frac{\|\vec{m}\|}{f(k)}\right)^{\alpha} \quad \text{for all } k \quad \text{and} \quad \vec{m} \in B_k ;$$

2.5) for almost every $\vec{x} \in E$, $c(A_k, \vec{m}_k(\vec{x}))$ has a finite limit when $k \to +\infty$, which is denoted by $c(\vec{x})$; $\vec{m}_k(\vec{x}) \in L$ being defined by: $\vec{x} \in \dfrac{\vec{m}_k(\vec{x}) + C}{f(k)}$;

2.6) $c \in \mathscr{C}(E)$ and $\mathscr{F}c \in \mathscr{L}^1(E)$ (the function c is continuous and its Fourier transform is integrable);

2.7) there is $A \subset E$ such that

2.7.1) for all $\vec{x} \in \mathring{A}$, there are $r > 0$ and k_0 such that

$$B(\vec{x}, r) \subset \frac{A_k + C}{f(k)} \quad \text{for all } k \geqslant k_0 ;$$

2.7.2) for all $\vec{x} \in E \backslash \overline{A}$, there are $r > 0$ and k_0 such that

$$B(\vec{x}, r) \subset E \backslash \frac{A_k + C}{f(k)} \quad \text{for all } k \geqslant k_0 ;$$

2.7.3) $\overline{A} \backslash \mathring{A}$ is negligible;

2.7.4) $\mathring{A} \neq \phi$.

15.1. General expression of the Ewald energy E_E.

Let S and $\mathscr{B}$ satisfy (1) to (4). We use the following expression of the Ewald energy

$$E_E = E_1 - E_2 + E_3$$

where

$$E_1 = \frac{1}{2\pi V} \sum_{\vec{h} \in L^* \backslash \{0\}} \frac{|F(\vec{h})|^2 \psi(\vec{h})}{\vec{h}^2},$$

$$E_2 = 2\pi \sum_{\vec{s} \in S} q_{\vec{s}}^2 \int_0^{+\infty} up(u) du$$

$$= 2 \sum_{\vec{s} \in S} q_{\vec{s}}^2 \int_0^{+\infty} \psi(h) dh,$$

$$E_3 = \frac{1}{2} \sum_{\substack{\vec{m} \in L \\ \vec{m} + \vec{s} \neq \vec{t}}} \sum_{\vec{s} \in S} \sum_{\vec{t} \in S} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|} \int_{\| \vec{m} + \vec{s} - \vec{t} \|}^{+\infty} 4\pi u (u - \| \vec{m} + \vec{s} - \vec{t} \|) p(u) du$$

$$= \frac{1}{2} \sum_{\substack{\vec{m} \in L \\ \vec{m} + \vec{s} \neq \vec{t}}} \sum_{\vec{s} \in S} \sum_{\vec{t} \in S} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|} \left(1 - \frac{2}{\pi} \int_0^{+\infty} \frac{\psi(h) \sin(2\pi \| \vec{m} + \vec{s} - \vec{t} \| h)}{h} dh \right)$$

(the expressions of E_2 and E_3 with the integrals on E, may directly be written from (28)-(29)), which has the same form as that of Bertaut [*4*], but in which the functions p and ψ satisfy the more general conditions:

a) $p \in \mathscr{L}^1_{\mathbb{C}}(E)$ (the values of p belong to $\mathbb{C}$ and p is integrable);

b) $\int p(\vec{u}) d\vec{u} = 1$;

c) $p(\vec{u})$ depends only on $\| \vec{u} \|$;
d) there is $\beta > 3$ such that $\| \vec{u} \|^{\beta} p(\vec{u})$ is bounded;
e) $\psi = \mathscr{F} p$;
f) $\psi \in \mathscr{L}^1_{\mathbb{C}}(\mathrm{E})$;
g) for all $\vec{x}_0 \in \mathrm{E}$, there is $r > 0$ such that the family

$$\vec{h} \in \mathrm{L}^* \to \sup_{\vec{x} \in \mathrm{B}(\vec{x}_0, r)} | \psi(\vec{x} + \vec{h}) |$$

is absolutely summable.

(In the above expressions of E_2 and E_3, $p(u)$ and $\psi(h)$ are written for $p(\vec{u})$ and $\psi(\vec{h})$, where $u = \| \vec{u} \|$ and $h = \| \vec{h} \|$). In our proof, we have also used the condition (more restrictive than *d*)):

d') there is $d \geqslant 0$ such that $\| \vec{u} \| \geqslant d$ implies $p(\vec{u}) = 0$.

Notes on the preceding expression.

A) According to *a*) and *e*), the condition *f*) is equivalent to: p is almost everywhere equal to a function of $\mathscr{P}(\mathrm{E})$ (space of linear combinations of continuous functions « of positive type »; see [*11*], sections 8 and 10). We identify p with that function of $\mathscr{P}(\mathrm{E})$, so that *f*) is equivalent to:

f') $$p \in \mathscr{P}(\mathrm{E})$$

(which implies that p is continuous). We have also: $\psi \in \mathscr{P}(\mathrm{E})$.

B) Note that a sufficient condition for *f*) and *g*) is:

g') there is $\beta' > 3$ such that $\| \vec{h} \|^{\beta'} \psi(\vec{h})$ is bounded.

C) Note that *a*), *b*) and *f*) are satisfied if

$$p = \sigma * \tau,$$
$$\sigma \text{ and } \tau \in \mathscr{L}^1_{\mathbb{C}}(\mathrm{E}) \cap \mathscr{L}^2_{\mathbb{C}}(\mathrm{E}),$$
$$\int \sigma(\vec{x}) d\vec{x} = \int \tau(\vec{x}) d\vec{x} = 1$$

($\psi = \mathscr{F}\sigma \mathscr{F}\tau$ is integrable because $\mathscr{F}\sigma$ and $\mathscr{F}\tau$ belong to $\mathscr{L}^2_{\mathbb{C}}(\mathrm{E})$).

D) The examples of Ewald (18) and Bertaut (19) satisfy the conditions *a*) to *g*) (and *g'*)).

15.2. The Born-Landé expression E_0.

Let S and $\mathscr{B}$ satisfy (1) to (4).

If $\vec{\mathrm{M}}$ (dipole moment of the cell S) $= \vec{0}$ the Born-Landé expression

$$\mathrm{E}_0 = \frac{1}{2} \sum_{\substack{\vec{m} \in \mathrm{L} \\ \vec{m} + \vec{s} \neq \vec{t}}} \sum_{\vec{s} \in \mathrm{S}} \sum_{\vec{t} \in \mathrm{S}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|} \tag{53}$$

exists and, for any functions p and ψ which satisfy *a*) to *g*), we have

$$E_0 = E_E. \tag{54}$$

If $\vec{M} \neq \vec{0}$: Let (B_k) be any increasing sequence of finite subsets of L such that $\bigcup_k B_k = L$. Then

i)
$$E_0 = \frac{1}{2} \lim_{k \to +\infty} \sum_{\vec{m} \in B_k} \sum_{\vec{s} \in S} \sum_{\substack{\vec{t} \in S \\ \vec{m} + \vec{s} \neq \vec{t}}} \frac{q_{\vec{s}} q_{\vec{t}}}{\| \vec{m} + \vec{s} - \vec{t} \|} \tag{55}$$

exists if and only if assertion 1) is satisfied;

ii) if 1) is satisfied: for any functions p and ψ which satisfy *a*) to *g*) and *d'*), we have

$$E_0 = E_E + E_4 + E_5 - E_5^0 \tag{56}$$

where

$$E_4 = \frac{2\pi \vec{M}^2}{3V}$$

$$E_5 = \frac{\vec{M}^2}{2} \lim_{k \to +\infty} \sum_{\vec{m} \in B_k \setminus \{\vec{0}\}} \frac{1 - 3\cos^2 \theta_{\vec{m}}}{\| \vec{m} \|^3}$$

$$E_5^0 = \frac{\vec{M}^2}{2} \lim_{r \to +\infty} \sum_{\substack{\vec{m} \in L \setminus \{\vec{0}\} \\ \|\vec{m}\| \leq r}} \frac{1 - 3\cos^2 \theta_{\vec{m}}}{\| \vec{m} \|^3} \tag{57}$$

(E_5^0 always exists);

iii) if 2.1), 2.2) and 2.3) are satisfied, then

iii.i) assertion 1) is satisfied and the preceding result *ii*) holds;

iii.ii) B is integrable and bounded (almost everywhere), and $\overset{\circ}{B}(\varepsilon) \subset B$;

iii.iii)
$$E_0 = E_E + \frac{2\pi \vec{M}^2}{3V} + \frac{\vec{M}^2}{2V} \int_{B \setminus B(\varepsilon)} \frac{1 - 3\cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} d\vec{x} \tag{58}$$

(the integral on $B \setminus B(\varepsilon)$ does not depend on $\varepsilon > 0$, provided that $B(\varepsilon) \subset B$ almost everywhere);

iii.iv)
$$\begin{aligned} E_0 &= E_E + \frac{2\pi \vec{M}^2}{V} \int \cos^2 \theta_{\vec{h}} \mathscr{F}(\varphi_B * \varphi_\varepsilon)(\vec{h}) d\vec{h} \\ &= E_E + \frac{2\pi \vec{M}^2}{V} \int \cos^2 \theta_{\vec{h}} \mathscr{F}\varphi_B(\vec{h}) \mathscr{F}\varphi_\varepsilon(\vec{h}) d\vec{h} \end{aligned} \tag{59}$$

where
$$\varphi_\varepsilon = \frac{3}{4\pi\varepsilon^3} \varphi_{B(\varepsilon)}$$

so that
$$\mathscr{F}\varphi_\varepsilon(\vec{h}) = \frac{3(\sin\sigma - \sigma\cos\sigma)}{\sigma^3} \quad \text{with} \quad \sigma = 2\pi\varepsilon \| \vec{h} \|$$

(the integral in (59) does not depend on $\varepsilon > 0$, provided that $B(\varepsilon) \subset B$ almost everywhere).

Consequences and notes:

A) Since E_0, E_4, E_5 and E_5^0 do not depend on p and ψ, the preceding result proves that E_E (defined in section 15.1) does not depend on the functions p and ψ which satisfy *a*) to *g*) if $\vec{M} = \vec{0}$, or *a*) to *g*) and *d'*) if $\vec{M} \neq \vec{0}$. If $\vec{M} \neq \vec{0}$, this result probably holds with functions p and ψ not restricted by the condition *d'*) (as we empirically know from numerical calculations with the gaussian functions (18) of Ewald).

B) Consider the group G (of order 48) of all symmetries of the cube. With orthonormal coordinates, the sum of

$$1 - 3\cos^2\theta_{\vec{x}} = 1 - \frac{3}{\vec{M}^2\vec{x}^2}(M_1x_1 + M_2x_2 + M_3x_3)^2$$

on the eight points $\vec{x}$ equivalent by the three reflexions in the planes $x_1 = 0$, $x_2 = 0$ and $x_3 = 0$, is equal to

$$8 - \frac{24}{\vec{M}^2\vec{x}^2}(M_1^2x_1^2 + M_2^2x_2^2 + M_3^2x_3^2);$$

and the sum of this last expression on the six points $\vec{x}$ equivalent by the three reflexions in the planes $x_1 = x_2, x_2 = x_3$ and $x_3 = x_1$, is equal to

$$48 - \frac{48}{\vec{M}^2\vec{x}^2}(M_1^2 + M_2^2 + M_3^2)(x_1^2 + x_2^2 + x_3^2) = 0.$$

Then, the sum of $1 - 3\cos^2\theta_{\vec{x}}$ on the 48 points equivalent by G, is equal to 0. We may conclude that, if B has all the symmetries of the cube, then the integral on $B \backslash B(\varepsilon)$ in (58) is equal to 0, and

$$E_0 = E_E + \frac{2\pi\vec{M}^2}{3V}. \tag{60}$$

Simple examples of such B are the sphere and the regular polyhedra with group G: the cube, the octahedron, the cuboctahedron, etc. ((60) was shown in the following cases: cubic lattice and B = sphere [*6*]; general lattice and B = sphere [*9*]; general lattice and B = cube [*7*]). The complete proof for the spherical case, is given in section 14.

C) Application of (58) to

$$B = B(1) \cup \left\{ \vec{x} \in E/1 < \|\vec{x}\| \leqslant 1 + r \quad \text{and} \quad |\cos\theta_{\vec{x}}| \geqslant \frac{1}{\sqrt{3}} \right\}$$

leads to

$$E_0 = E_E + \frac{2\pi\vec{M}^2}{3V}\left[1 - \frac{2}{\sqrt{3}}\operatorname{Log}(1 + r)\right],$$

which shows that $E_0 < E_E$ if r is large enough, and $E_0 - E_E \to -\infty$ when $r \to +\infty$.

D) The equation of Smith ([7], (3.12) and (3.15))

$$E_0 = E_E + \frac{2\pi \vec{M}^2}{V} \int \cos^2 \theta_{\vec{h}} \mathscr{F} \varphi_B(\vec{h}) d\vec{h}$$

is incorrect because $\mathscr{F}\varphi_B$ is not integrable. Indeed, the integrability of $\mathscr{F}\varphi_B$ would imply the continuity of a function almost everywhere equal to φ_B (as for the function p in note A) of section 15.1), which obviously is false (as a concrete example, if B is a sphere, $\mathscr{F}\varphi_B$—which has the same form as $\mathscr{F}\varphi_\varepsilon$ above— is not integrable). In the above equation (59),

$$\mathscr{F}(\varphi_B * \varphi_\varepsilon) = \mathscr{F}\varphi_B \mathscr{F}\varphi_\varepsilon \in \mathscr{L}^1(E)$$

because $\quad \mathscr{F}\varphi_B \in \mathscr{L}^2(E) \quad$ and $\quad \mathscr{F}\varphi_\varepsilon \in \mathscr{L}^2(E)$.

15.3. The limit energy per cell E.

Let S and $\mathscr{B}$ satisfy (1) to (4). Let (A_k) be any increasing sequence of finite subsets of L such that $\bigcup_k A_k = L$.

If $\vec{M} = \vec{0}$: If (2.4) is satisfied with $f(k) = \sup_{n \in A_k} \| \vec{n} \|$, then the limit energy per cell E—defined by (8)—exists and

$$E = E_0 = E_E \tag{61}$$

(E_0 given by (53)).

If $\vec{M} \neq \vec{0}$: Let define

$$B_k = \{ \vec{n} - \vec{p} / \vec{n} \in A_k \text{ and } \vec{p} \in A_k \} = A_k - A_k .$$

Then

i) if 2.1), 2.2), 2.4) and 2.5) are satisfied, then the following three assertions are equivalent:

i.i) E (defined by (8)) exists;

i.ii) E_0 (defined by (55)) exists;

i.iii) assertion 1) is satisfied;

ii) if 1), 2.1) 2.2), 2.4) and 2.5) are satisfied, then

ii.i) B is integrable and bounded (almost everywhere);

ii.ii) $1 - c(\vec{x}) \leqslant a \| \vec{x} \|^\alpha$ for almost every $\vec{x} \in B$;

ii.iii)
$$E = E_0 - E_6 = E_E + E_4 + E_5 - E_5^0 - E_6 \tag{62}$$

where E_4, E_5 and E_5^0 are given by (57), and

$$E_6 = \frac{\vec{M}^2}{2V} \int_B (1 - c(\vec{x})) \frac{1 - 3\cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} d\vec{x} ; \tag{63}$$

iii) if 2.1), 2.2), 2.3), 2.4) and 2.5) are satisfied, then

iii.i) assertion 1) is satisfied and the preceding result (*ii*) holds;

iii.ii) $\overset{\circ}{\mathrm{B}}(\varepsilon) \subset \mathrm{B}$;

iii.iii) $$\mathrm{E}=\mathrm{E_E} + \frac{2\pi\vec{\mathrm{M}}^2}{3\mathrm{V}} + \frac{\vec{\mathrm{M}}^2}{2\mathrm{V}} \lim_{\varepsilon'\to 0^+} \int_{\mathrm{B}\setminus\mathrm{B}(\varepsilon')} c(\vec{x}) \frac{1-3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3} d\vec{x}; \quad (64)$$

iv) if 2.1), 2.2), 2.3), 2.4), 2.5) and 2.6) are satisfied, then

iv.i) the preceding results (*ii*) and (*iii*) hold;

iv.ii) $$\mathrm{E} = \mathrm{E_E} + \frac{2\pi\vec{\mathrm{M}}^2}{\mathrm{V}} \int \cos^2\theta_{\vec{h}} \mathscr{F}c(\vec{h})d\vec{h}\,; \quad (65)$$

v) if 2.1), 2.2), 2.3), 2.4) and 2.7) are satisfied, then

v.i) A is integrable and bounded (almost everywhere);

v.ii) assertion 2.5) is satisfied for all $\vec{x} \in \mathrm{E}$, and

$$c(\vec{x}) = \frac{\lambda(\mathrm{A} \cap \vec{x} + \mathrm{A})}{\lambda(\mathrm{A})} = \frac{1}{\lambda(\mathrm{A})}(\varphi_{\mathrm{A}} * \varphi_{-\mathrm{A}})(\vec{x})\,; \quad (66)$$

assertion 2.6) is satisfied and the preceding results (*ii*), (*iii*) and (*iv*) hold;

v.iii) $$\mathrm{E} = \mathrm{E_E} + \frac{2\pi\vec{\mathrm{M}}^2}{\mathrm{V}\lambda(\mathrm{A})} \int \cos^2\theta_{\vec{h}} |\mathscr{F}\varphi_{\mathrm{A}}(\vec{h})|^2 d\vec{h}\,. \quad (67)$$

Consequences and notes.

A) As in note A) of section 15.2, if A and B have all the symmetries of the cube, then the integrals in (63) and (64)—with $c(\vec{x})$ given by (66)—are equal to 0, and

$$\mathrm{E} = \mathrm{E_0} = \mathrm{E_E} + \frac{2\pi\vec{\mathrm{M}}^2}{3\mathrm{V}} \quad (68)$$

(note that if $\mathrm{B} = \mathrm{A} - \mathrm{A}$, the symmetry conditions on A imply those on B). Simple examples of such A and B are given in note A) of section 15.2. The complete proof for the spherical case, is given in section 14.

B) According to (67), we have always $\mathrm{E} \geqslant \mathrm{E_E}$.

C) The general relation between E and $\mathrm{E_0}$ given by Smith ([*7*], (4.24)): $\mathrm{E} = \mathrm{E_0}$, is not correct. The exact relation is (62) (the equality $\mathrm{E} = \mathrm{E_0}$ only occurs in some particular cases, as indicated in the preceding note A)). The equality (67) is identical with that of Smith ([*8*], (1.7) and (2.4)).

15.4. **Conclusion.**

Born and Landé [*1*] thought that the expression $\mathrm{E_0}$ (given by (6)) represented the electrostatic energy per cell of an ionic crystal. Ewald [*3*] (and

Bertaut [4]) thought that the « Ewald energy » E_E was equal to E_0 (and then, to the energy per cell). These two affirmations are generally not correct (if the dipole moment of the cell is not equal to $\vec{0}$). The correct definition of the energy per cell is that of the « limit energy per cell » E (defined by (8)). We use general increasing sequences of finite crystals ((A_k) in the definition of E, and (B_k) for E_0) and a general definition of a cell (S, $\mathscr{B}$), which may be modified for a given crystal (see section 1: (1) to (4) and fig. 1). We obtain a general expression of the Ewald energy E_E, written with functions p and ψ with complex values (section 15.1), and we prove that the value of E_E is independent on the functions p and ψ (note A) of section 15.2). All the results of sections 15.2 and 15.3 are given in two forms: in the usual space and in the dual space. The general relations between the Born-Landé expression E_0 and the Ewald energy E_E are (56) and (58) in the usual space, and (59) in the dual space. The general relations between the limit energy per cell E, the Born-Landé expression E_0 and the Ewald energy E_E, are (62) and (64) in the usual space, and (65) and (67) in the dual space. Note that some consequences may be deduced from the usual space-form of the results, whereas other consequences are obtained from the dual space-form (see the following). In the case of a crystal shape which has all the symmetries of the cube, we deduce the relations (60)-(68) (complete proof for the spherical case, in section 14). In the general case, the limit energy per cell E, and the limit volumic energy $\frac{E}{V}$, depend on the increasing sequence of finite crystals $A_k + S$. Since changes of A_k and S are equivalent to a modification of the surface of the crystal, the volumic electrostatic energy $\frac{E}{V}$ depends on the surface of the crystal (the same occurs for E_0). This property is due to the long-range $\frac{1}{r}$ interaction of the electrostatic potential energy. The Born-Landé expression E_0 has generally no physical meaning (it may be lower than E_E: see note C) of section 15.2). According to (67), the Ewald volumic energy $\frac{E_E}{V}$ (which is charactistic of the crystal: it probably does not depend on (S, $\mathscr{B}$)) appears as the minimum value of the volumic energy $\frac{E}{V}$, for a suitable choice of the surface of the crystal (choice of (A_k) or A, and choice of a cell (S, $\mathscr{B}$)). In particular, this minimum is obtained if the dipole moment $\vec{M}$ of the cell S is equal to $\vec{0}$. If the crystal is such that there is a cell (S, $\mathscr{B}$) with a dipole moment equal to $\vec{0}$, a large crystal will preferably have a surface which corresponds to a crystal built with such a cell (S, $\mathscr{B}$) ([10], fig. 2). In the example of NaCl, the surface of a large finite crystal will preferably be that corresponding to a crystal built with the cell of fig. 1 *a* (i. e. a cubic octopole with { 100 } microscopic faces. A recent experimental work on the equilibrium shape of NaCl [*13*] shows that, at a ~ 100 Å scale of observation, the only observed plane faces are { 100 }; nevertheless, at such a scale of observation, the exact positions of the ions remain unknown).

APPENDIX 1

$$\begin{aligned} I &= \int \frac{\psi(\vec{h})}{\vec{h}^2} e^{-2\pi i \vec{h}.\vec{x}} d\vec{h} \\ &= \int \frac{e^{-2\pi i \vec{h}.\vec{x}}}{\vec{h}^2} d\vec{h} \int p(\vec{u}) e^{-2\pi i \vec{h}.\vec{u}} d\vec{u} \\ &= \lim_{H \to +\infty} \int_{\|\vec{h}\| \leqslant H} \frac{e^{-2\pi i \vec{h}.\vec{x}}}{\vec{h}^2} d\vec{h} \int p(\vec{u}) e^{-2\pi i \vec{h}.\vec{u}} d\vec{u} \\ &= \lim_{H \to +\infty} \int p(\vec{u}) d\vec{u} \int_{\|\vec{h}\| \leqslant H} \frac{e^{-2\pi i \vec{h}.(\vec{x}+\vec{u})}}{\vec{h}^2} d\vec{h} \end{aligned}$$

by the Lebesgue-Fubini theorem. After calculation of the integral on $\vec{h}$ with $\vec{x} + \vec{u}$ as polar axis, we obtain:

$$I = \lim_{H \to +\infty} \int g_H(\vec{u}) d\vec{u}$$

where

$$g_H(\vec{u}) = 2 \frac{p(\vec{u})}{\| \vec{x} + \vec{u} \|} \int_0^{2\pi \|\vec{x}+\vec{u}\| H} \frac{\sin \xi}{\xi} d\xi .$$

For all $\vec{u} \neq - \vec{x}$,

$$\lim_{H \to +\infty} g_H(\vec{u}) = g(\vec{u})$$

where

$$g(\vec{u}) = \pi \frac{p(\vec{u})}{\| \vec{x} + \vec{u} \|} .$$

The integrability of $| g |$ may be shown by taking $\vec{x}$ as polar axis, and the same method leads to the value of the integral of g given in the last member of the equalities (20) (see [4]). Since

$$| g_H(\vec{u}) | \leqslant \frac{2}{\pi} | g(\vec{u}) | \sup_x \left| \int_0^x \frac{\sin \xi}{\xi} d\xi \right| ,$$

Lebesgue's dominated convergence theorem may be applied:

$$I = \pi \int \frac{p(\vec{u})}{\| \vec{x} + \vec{u} \|} d\vec{u} .$$

APPENDIX 2

First, we observe that the function

$$H(\vec{x}) = \frac{1}{\|\vec{x}\|}\int_{\|\vec{x}\|}^{+\infty} u(u - \|\vec{x}\|)p(u)du$$

is of class C^2 on $E\backslash\{\vec{0}\}$, as a consequence of the continuity of p (15). Taylor's formula at the second order applied to H, leads to

$$\begin{aligned} I(\vec{m}) &= \sum_{\vec{s}}\sum_{\vec{t}} q_{\vec{s}}q_{\vec{t}}H(\vec{m} + \vec{s} - \vec{t}) \\ &= \frac{1}{2}\sum_{\vec{s}}\sum_{\vec{t}} q_{\vec{s}}q_{\vec{t}} \left\{ \begin{array}{l} \left(\dfrac{3}{\|\vec{x}'\|^3}\displaystyle\int_{\|\vec{x}'\|}^{+\infty} u^2p(u)du + p(\vec{x}')\right)\dfrac{(\vec{x}'\cdot\vec{k})^2}{\vec{x}'^2} \\ -\dfrac{1}{\|\vec{x}'\|^3}\displaystyle\int_{\|\vec{x}'\|}^{+\infty} u^2p(u)du\,\vec{k}^2 \end{array} \right\} \end{aligned}$$

for $\|\vec{m}\| > \delta$; notations: $\vec{k} = \vec{s} - \vec{t}$, $\vec{x}' = \vec{m} + \zeta\vec{k}$, $0 < \zeta < 1$. Then, the two inequalities

$$\begin{aligned} \left|\frac{1}{\|\vec{x}'\|^3}\int_{\|\vec{x}'\|}^{+\infty} u^2p(u)du\right| &\leqslant \frac{p_0}{(\beta' - 3)\|\vec{x}'\|^{\beta'}} \\ &\leqslant \frac{p_0}{(\beta' - 3)(\|\vec{m}\| - \delta)^{\beta'}} \end{aligned}$$

and

$$|p(\vec{x}')| \leqslant \frac{p_0}{(\|\vec{m}\| - \delta)^{\beta'}}$$

($p_0 = \sup_{\vec{u}} \|\vec{u}\|^{\beta'}|p(\vec{u})|$), show that $(I(\vec{m}))$ is absolutely summable.

APPENDIX 3

Consider the functions

$$g(\xi, a) = e^{-a\xi}\,\frac{\sin \xi}{\xi}, \qquad \xi > 0, \qquad a > 0,$$

$$f(a) = \int_0^{+\infty} g(\xi, a)\,d\xi .$$

The inequality

$$\left| \frac{\partial g}{\partial a}(\xi, a) \right| \leqslant e^{-\varepsilon\xi} \qquad \text{if} \qquad a > \varepsilon > 0,$$

shows (Lebesgue's dominated convergence theorem) that f is differentiable on $\mathbb{R}_+^*$ ($\varepsilon > 0$ is arbitrary) and

$$\begin{aligned} f'(a) &= \int_0^{+\infty} - e^{-a\xi} \sin \xi\, d\xi \\ &= \left[\frac{a e^{-a\xi} \sin \xi + e^{-a\xi} \cos \xi}{a^2 + 1} \right]_{\xi=0}^{+\infty} \\ &= - \frac{1}{a^2 + 1}. \end{aligned}$$

The function $F(r) = f\left(\frac{1}{r}\right)$ is then differentiable on $\mathbb{R}_+^*$ and

$$F'(r) = \frac{1}{r^2 + 1}.$$

Then

$$F(r) = \operatorname{Arctan} r + \text{constant}.$$

Since

$$\lim_{a \to +\infty} g(\xi, a) = 0$$

$$| g(\xi, a) | \leqslant \sup_t \left| \frac{\sin t}{t} \right| e^{-\xi} \quad \text{for} \quad a \geqslant 1,$$

we may apply Lebesgue's dominated convergence theorem:

$$\lim_{r \to 0} F(r) = \lim_{a \to +\infty} f(a) = 0.$$

We may conclude: $F(r) = \operatorname{Arctan} r$.

APPENDIX 4

We may write, with $\vec{M}$ as polar axis,

$$I_N = \int d\vec{x} \sum_{\vec{\mu} \neq \vec{0}} \frac{1 - 3\cos^2\theta_{\vec{\mu}}}{\vec{\mu}^2(\vec{\mu}^2 + 1)} \varphi_{C_{\vec{\mu}}}(\vec{x})$$

$$= \int_0^{+\infty} k_N(\rho) d\rho$$

with

$$k_N(\rho) = \int_{\substack{0 \leqslant \theta \leqslant \pi \\ 0 \leqslant \varphi \leqslant 2\pi}} h_N(\rho, \theta, \varphi) d\theta d\varphi$$

$$h_N(\rho, \theta, \varphi) = \sum_{\vec{\mu} \neq \vec{0}} \frac{1 - 3\cos^2\theta_{\vec{\mu}}}{\vec{\mu}^2(\vec{\mu}^2 + 1)} \varphi_{C_{\vec{\mu}}}(\vec{x}) \rho^2 \sin\theta .$$

If $\rho \neq 0$,

$$\lim_{N \to +\infty} h_N(\rho, \theta, \varphi) = \frac{1 - 3\cos^2\theta}{\rho^2(\rho^2 + 1)} \rho^2 \sin\theta .$$

Notations:

$$\vec{x} = x_1 \vec{a}_1 + x_2 \vec{a}_2 + x_3 \vec{a}_3$$

$$|\vec{x}| = \sup(|x_1|, |x_2|, |x_3|)$$

$$\gamma = \sup_{\vec{x} \in C} \|\vec{x}\|$$

$$\gamma' = \sup_{|\vec{x}| \leqslant 1} \|\vec{x}\|$$

$$\varepsilon_0 = \inf_{|\vec{x}| = 1} \|\vec{x}\| .$$

If $\vec{\mu} \neq \vec{0}$ and $\vec{x} \in C_{\vec{\mu}}$, we have

$$\frac{\rho}{\|\vec{\mu}\|} \leqslant \frac{\frac{2\pi}{N}|\vec{m}|\gamma' + \frac{2\pi}{N}\gamma}{\frac{2\pi}{N}|\vec{m}|\varepsilon_0} \leqslant \frac{\gamma' + \gamma}{\varepsilon_0} .$$

Then

$$|h_N(\rho, \theta, \varphi)| \leqslant \frac{4\rho^2}{\vec{\mu}^2(\vec{\mu}^2 + 1)}$$

$$\leqslant \frac{4(\gamma' + \gamma)^2}{\varepsilon_0^2}$$

(which holds for all $\vec{x} \in E$), so that Lebesgue's dominated convergence theorem may be applied:

$$\lim_{N \to +\infty} k_N(\rho) = \int_{\substack{0 \leqslant \theta \leqslant \pi \\ 0 \leqslant \varphi \leqslant 2\pi}} \frac{1 - 3\cos^2\theta}{\rho^2(\rho^2 + 1)} \rho^2 \sin\theta \, d\theta d\varphi$$

if $\rho \neq 0$. According to

$$|k_N(\rho)| \leqslant 2\pi^2 \frac{4(\gamma' + \gamma)^2}{\varepsilon_0^2} \quad \text{for all } \rho ,$$

$$|k_N(\rho)| \leqslant 2\pi^2 \frac{4\rho^2}{(\rho - 2\pi\gamma)^2[(\rho - 2\pi\gamma)^2 + 1]} \quad \text{for} \quad \rho > 2\pi\gamma ,$$

we may apply Lebesgue's dominated convergence theorem:

$$\lim_{N \to +\infty} I_N = \int_0^{+\infty} d\rho \int_{\substack{0 \leqslant \theta \leqslant \pi \\ 0 \leqslant \varphi \leqslant 2\pi}} \frac{1 - 3\cos^2\theta}{\rho^2(\rho^2 + 1)} \rho^2 \sin\theta d\theta d\varphi .$$

Since the function

$$\vec{x} \to \frac{1 - 3\cos^2\theta_{\vec{x}}}{\vec{x}^2(\vec{x}^2 + 1)}$$

is integrable, we may conclude

$$\lim_{N \to +\infty} I_N = \int \frac{1 - 3\cos^2\theta_{\vec{x}}}{\vec{x}^2(\vec{x}^2 + 1)} d\vec{x} .$$

APPENDIX 5

We summarize the method, which is similar with that of appendix 4, and we use the same notations. We have

$$\lim_{N\to+\infty} h_N(\rho, \theta, \varphi) = \frac{(\text{Arctan } \rho)(1 - 3\cos^2\theta)}{\rho^3} \rho^2 \sin\theta \quad \text{if} \quad 0 < \rho < 2\pi\,,$$

$$\lim_{N\to+\infty} h_N(\rho, \theta, \varphi) = 0 \quad \text{if} \quad \rho > 2\pi\,,$$

$$| h_N(\rho, \theta, \varphi) | \leqslant \frac{4\rho^2}{\vec{\mu}^2} \leqslant \frac{4(\gamma' + \gamma)^2}{\varepsilon_0^2}$$

(which holds for all $x \in E$). Then

$$\lim_{N\to+\infty} k_N(\rho) = \int_{\substack{0\leqslant\theta\leqslant\pi\\0\leqslant\varphi\leqslant 2\pi}} \frac{(\text{Arctan } \rho)(1 - 3\cos^2\theta)}{\rho^3} \rho^2 \sin\theta \quad \text{if} \quad 0 < \rho < 2\pi\,,$$

$$\lim_{N\to+\infty} k_N(\rho) = 0 \quad \text{if} \quad \rho > 2\pi\,.$$

If $\| \vec{\mu} \| \leqslant 2\pi$ and $\vec{x} \in C_{\vec{\mu}}$,

$$\rho \leqslant \| \vec{\mu} \| + \frac{2\pi}{N}\gamma \leqslant 2\pi + 2\pi\gamma\,.$$

Then,

$$h_N(\rho, \theta, \varphi) = 0 \qquad \text{and} \qquad k_N(\rho) = 0 \quad \text{if} \quad \rho > 2\pi + 2\pi\gamma\,.$$

Moreover,

$$| k_N(\rho) | \leqslant 2\pi^2 \frac{4(\gamma' + \gamma)^2}{\varepsilon_0^2} \quad \text{for all } \rho\,.$$

We may conclude:

$$\lim_{N\to+\infty} I_N = \int_0^{2\pi} d\rho \int_{\substack{0\leqslant\theta\leqslant\pi\\0\leqslant\varphi\leqslant 2\pi}} \frac{(\text{Arctan } \rho)(1 - 3\cos^2\theta)}{\rho^3} \rho^2 \sin\theta d\theta d\varphi$$

$$= \int_{\|\vec{x}\|\leqslant 2\pi} \frac{(\text{Arctan } \| \vec{x} \|)(1 - 3\cos^2\theta_{\vec{x}})}{\| \vec{x} \|^3} d\vec{x}\,.$$

APPENDIX 6

Notations:

$$\mathrm{C}' = \left[-\frac{1}{2},\frac{1}{2}\right[\vec{a}_1 + \left[-\frac{1}{2},\frac{1}{2}\right[\vec{a}_2 + \left[-\frac{1}{2},\frac{1}{2}\right[\vec{a}_3\,; \quad \mathrm{C}'_{\vec{m}} = \vec{m} + \mathrm{C}'\,; \quad \gamma'' = \sup_{\vec{x}\in\mathrm{C}'} \|\vec{x}\|\,.$$

We define

$$\mathrm{S} = \mathrm{V} \sum_{0<\|\vec{m}\|\leqslant r} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3}$$

$$= \int_{\mathrm{A}} \varphi(\vec{x})d\vec{x}$$

$$\mathrm{S}_1 = \int_{\mathrm{A}_1} \varphi(\vec{x})d\vec{x}$$

$$\mathrm{S}_2 = \int_{\mathrm{A}_1\setminus\mathrm{C}'} f(\vec{x})d\vec{x}\,,$$

where

$$\varphi(\vec{x}) = \sum_{\vec{m}\neq\vec{0}} \frac{1 - 3\cos^2\theta_{\vec{m}}}{\|\vec{m}\|^3}\varphi_{\mathrm{C}'_{\vec{m}}}(\vec{x})\,,$$

$$f(\vec{x}) = \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3}\,,$$

$$\mathrm{A} = \bigcup_{\|\vec{m}\|\leqslant r} \mathrm{C}'_{\vec{m}}\,,$$

$$\mathrm{A}_1 = \{\,\vec{x}\in\mathrm{E}/\,\|\vec{x}\|\leqslant r\,\}\,.$$

According to

$r < \|\vec{x}\| \leqslant r + \gamma''$ and $r - \gamma'' < \|\vec{m}\|$, if $\vec{x}\in\mathrm{A}\setminus\mathrm{A}_1$ and $\vec{x}\in\mathrm{C}'_{\vec{m}}$,

$r - \gamma'' < \|\vec{x}\| \leqslant r$ and $r < \|\vec{m}\|$, if $\vec{x}\in\mathrm{A}_1\setminus\mathrm{A}$ and $\vec{x}\in\mathrm{C}'_{\vec{m}}$,

we may write

$$|\,\mathrm{S} - \mathrm{S}_1\,| = \left|\int_{\mathrm{A}\setminus\mathrm{A}_1} \varphi(\vec{x})d\vec{x} - \int_{\mathrm{A}_1\setminus\mathrm{A}} \varphi(\vec{x})d\vec{x}\right|$$

$$\leqslant \int_{r-\gamma''<\|\vec{x}\|\leqslant r+\gamma''} \frac{4}{(r - \gamma'')^3}\,d\vec{x}$$

$$= \frac{16\pi(6r^2\gamma'' + 2\gamma''^3)}{3(r - y'')^3}\,,$$

which shows that

$$\lim_{r\to+\infty} (\mathrm{S} - \mathrm{S}_1) = 0\,.$$

The integral of f for $\gamma'' \leqslant \|\vec{x}\| \leqslant r$ is equal to 0 (calculated with $\vec{\mathrm{M}}$ as polar axis). Then

$$\mathrm{S}_2 = \int_{\{\vec{x}/\|\vec{x}\|\leqslant\gamma''\}\setminus\mathrm{C}'} f(\vec{x})d\vec{x}$$

does not depend on r.

With orthonormal coordinates and $\vec{M}$ as x_3 axis, Taylor's formula at the first order may be written

$$f(\vec{x}) - f(\vec{m}) = \frac{15x_3'^2}{\|\vec{x}'\|^7}(\vec{x}'\cdot\vec{k}) - \frac{3}{\|\vec{x}'\|^5}(\vec{x}'\cdot\vec{k}) - \frac{6x_3'k_3}{\|\vec{x}'\|^5}$$

where $\vec{k} = \vec{x} - \vec{m}$, $\vec{x}' = \vec{m} + \zeta\vec{k}$, $0 < \zeta < 1$ (if $\vec{0}$ does not belong to the segment joining $\vec{m}$ to $\vec{x}$). With $\vec{m} \neq \vec{0}$ and $\vec{x} \in C'_{\vec{m}}$, we deduce

$$|f(\vec{x}) - \varphi(\vec{x})| \leqslant \frac{24\gamma''}{(\|\vec{x}\| - \gamma'')^4}$$

for $\|\vec{x}\| > \gamma''$, which shows that $f - \varphi$ is integrable on $E\backslash C'$. According to Lebesgue's dominated convergence theorem:

$$\lim_{r\to+\infty}(S_1 - S_2) = \int_{E\backslash C'}(\varphi(\vec{x}) - f(\vec{x}))d\vec{x}\,.$$

In conclusion,

$$\lim_{r\to+\infty} S = \lim_{r\to+\infty}(S - S_1) + \lim_{r\to+\infty}(S_1 - S_2) + S_2$$

exists and is finite.

APPENDIX 7

$$\varphi_{\frac{(B_k \setminus B(r_k)) + C}{f(k)}}(\vec{x}) = \varphi_{\frac{B_k + C}{f(k)}}(\vec{x})\left(1 - \varphi_{\frac{(B(r_k) \cap L) + C}{f(k)}}(\vec{x})\right).$$

We have to prove that

$$\lim_{k \to +\infty} \varphi_{\frac{(B(r_k) \cap L) + C}{f(k)}}(\vec{x}) = \varphi_{B(\varepsilon)}(\vec{x}) \quad \text{almost everywhere}.$$

If $\| \vec{x} \| > \varepsilon$, there is k_0 such that

$$\frac{r_k + \gamma}{f(k)} < \| \vec{x} \| \qquad \text{for all} \quad k \geqslant k_0 .$$

This implies

$$\vec{x} \notin \frac{(B(r_k) \cap L) + C}{f(k)} \qquad \text{for all} \quad k \geqslant k_0 ,$$

i. e.

$$\lim_{k \to +\infty} \varphi_{\frac{(B(r_k) \cap L) + C}{f(k)}}(\vec{x}) = 0 = \varphi_{B(\varepsilon)}(\vec{x}).$$

If $\| \vec{x} \| < \varepsilon$, $\vec{x} \in \dfrac{\vec{m}_k + C}{f(k)}$, we have

$$\| \vec{m}_k \| \leqslant f(k) \| \vec{x} \| + \gamma = r_k \alpha_k$$

with

$$\alpha_k = \frac{f(k) \| \vec{x} \| + \gamma}{r_k}.$$

Since

$$\lim_{k \to +\infty} \alpha_k = \frac{\| \vec{x} \|}{\varepsilon} < 1 ,$$

there is k_0 such that

$$\| \vec{m}_k \| \leqslant r_k \qquad \text{for all} \quad k \geqslant k_0 ,$$

i. e.

$$\vec{x} \in \frac{(B(r_k) \cap L) + C}{f(k)} \qquad \text{for all} \quad k \geqslant k_0 .$$

We deduce:

i)
$$\lim_{k \to +\infty} \varphi_{\frac{(B(r_k) \cap L) + C}{f(k)}}(\vec{x}) = 1 = \varphi_{B(\varepsilon)}(\vec{x}) ;$$

ii)
$$\vec{x} \in \frac{B_k + C}{f(k)} \qquad \text{for all} \quad k \geqslant k_0 ,$$

which implies $\vec{x} \in B$. We may conclude:

$$\lim_{k \to +\infty} \varphi_{\frac{(B(r_k) \cap L) + C}{f(k)}}(\vec{x}) = \varphi_{B(\varepsilon)}(\vec{x}) \qquad \text{if} \quad \| \vec{x} \| \neq \varepsilon ,$$

$$\mathring{B}(\varepsilon) \subset B .$$

APPENDIX 8

$$\mathscr{F}g(\vec{h}) = \int_{B(r)\setminus B(\varepsilon)} \frac{1 - 3\cos^2\theta_{\vec{x}}}{\|\vec{x}\|^3}\cos(2\pi\vec{h}\cdot\vec{x})d\vec{x}$$
$$= I_1 - I_2$$

where

$$I_1 = \int_{B(r)\setminus B(\varepsilon)} \frac{\cos(2\pi\vec{h}\cdot\vec{x})}{\|\vec{x}\|^3}d\vec{x}$$

$$I_2 = \int_{B(r)\setminus B(\varepsilon)} \frac{3(\vec{M}\cdot\vec{x})^2}{\vec{M}^2\|\vec{x}\|^5}\cos(2\pi\vec{h}\cdot\vec{x})d\vec{x}\,.$$

With $\vec{h} \neq \vec{0}$ as polar axis, we obtain:

$$I_1 = 4\pi\int_\varepsilon^r \frac{\sin(2\pi\|\vec{h}\|\rho)}{2\pi\|\vec{h}\|}\frac{d\rho}{\rho^2}$$
$$= 4\pi\left[-\frac{\sin(2\pi\|\vec{h}\|\rho)}{2\pi\|\vec{h}\|\rho}\right]_\varepsilon^r - 4\pi\int_\varepsilon^r -\frac{\cos(2\pi\|\vec{h}\|\rho)}{\rho}d\rho$$
$$= 4\pi\left[-\frac{\sin\sigma}{\sigma}\right]_{\sigma_\varepsilon}^{\sigma_r} + 4\pi J$$

where

$$J = \int_{\sigma_\varepsilon}^{\sigma_r}\frac{\cos\sigma}{\sigma}d\sigma$$
$$\sigma_\zeta = 2\pi\|\vec{h}\|\zeta\,.$$

The same polar coordinates, with $\vec{h}$ along x_3 and $\vec{M}$ in the plane x_1Ox_3, are used for I_2:

$$I_2 = \frac{3}{\vec{M}^2}\int_{\substack{\varepsilon\leq\rho\leq r\\ 0\leq\theta\leq\pi\\ 0\leq\varphi\leq 2\pi}} \frac{(M_1\sin\theta\cos\varphi + M_3\cos\theta)^2}{\rho}\cos(2\pi\|\vec{h}\|\rho\cos\theta)\sin\theta\, d\rho d\theta d\varphi\,.$$

After integration on φ, we obtain, with $u = \cos\theta$ and $\sigma = 2\pi\|\vec{h}\|\rho$:

$$I_2 = \frac{3\pi}{\vec{M}^2}\int_\varepsilon^r\frac{d\rho}{\rho}\int_{-1}^1\cos(\sigma u)[M_1^2 + (2M_3^2 - M_1^2)u^2]du$$
$$= \frac{3\pi}{\vec{M}^2}\int_\varepsilon^r\frac{d\rho}{\rho}\left[M_1^2\frac{\sin(\sigma u)}{\sigma} + (2M_3^2 - M_1^2)\left(\frac{u^2\sin(\sigma u)}{\sigma} + \frac{2u\cos(\sigma u)}{\sigma^2} - \frac{2\sin(\sigma u)}{\sigma^3}\right)\right]_{-1}^1$$
$$= \frac{12\pi}{\vec{M}^2}\int_{\sigma_\varepsilon}^{\sigma_r}\left[M_3^2\frac{\sin\sigma}{\sigma^2} + (2M_3^2 - M_1^2)\left(\frac{\cos\sigma}{\sigma^3} - \frac{\sin\sigma}{\sigma^4}\right)\right]d\sigma\,.$$

With the help of

$$J = \left[\frac{\sin\sigma}{\sigma}\right]_{\sigma_\varepsilon}^{\sigma_r} + \int_{\sigma_\varepsilon}^{\sigma_r}\frac{\sin\sigma}{\sigma^2}d\sigma$$
$$= \left[\frac{\sin\sigma}{\sigma} - \frac{\cos\sigma}{\sigma^2}\right]_{\sigma_\varepsilon}^{\sigma_r} - 2\int_{\sigma_\varepsilon}^{\sigma_r}\frac{\cos\sigma}{\sigma^3}d\sigma$$
$$= \left[\frac{\sin\sigma}{\sigma} - \frac{\cos\sigma}{\sigma^2} - \frac{2\sin\sigma}{\sigma^3}\right]_{\sigma_\varepsilon}^{\sigma_r} - 6\int_{\sigma_\varepsilon}^{\sigma_r}\frac{\sin\sigma}{\sigma^4}d\sigma\,,$$

we may write

$$
I_2 = \begin{cases} 12\pi \cos^2 \theta_{\vec{h}} \left(J - \left[\dfrac{\sin \sigma}{\sigma} \right]_{\sigma_\varepsilon}^{\sigma_r} \right) \\ + 12\pi(3 \cos^2 \theta_{\vec{h}} - 1)\left(-\dfrac{J}{2} + \dfrac{1}{2}\left[\dfrac{\sin \sigma}{\sigma} - \dfrac{\cos \sigma}{\sigma^2} \right]_{\sigma_\varepsilon}^{\sigma_r} \right) \\ + 12\pi(3 \cos^2 \theta_{\vec{h}} - 1)\left(\dfrac{J}{6} - \dfrac{1}{6}\left[\dfrac{\sin \sigma}{\sigma} - \dfrac{\cos \sigma}{\sigma^2} - \dfrac{2 \sin \sigma}{\sigma^3} \right]_{\sigma_\varepsilon}^{\sigma_r} \right) \end{cases}
$$

$$
= \begin{cases} 4\pi J - 4\pi \left[\dfrac{\sin \sigma}{\sigma} \right]_{\sigma_\varepsilon}^{\sigma_r} \\ - 4\pi(1 - 3 \cos^2 \theta_{\vec{h}}) \left[\dfrac{\sin \sigma - \sigma \cos \sigma}{\sigma^3} \right]_{\sigma_\varepsilon}^{\sigma_r} . \end{cases}
$$

Then

$$
\mathscr{F} g(\vec{h}) = 4\pi(1 - 3 \cos^2 \theta_{\vec{h}}) \left[\frac{\sin \sigma - \sigma \cos \sigma}{\sigma^3} \right]_{\sigma_\varepsilon}^{\sigma_r} \quad \text{for all} \quad \vec{h} \neq \vec{0} .
$$

According to

$$
\mathscr{F} \varphi_{B(\zeta)}(\vec{h}) = 4\pi\zeta^3 \frac{\sin \sigma_\zeta - \sigma_\zeta \cos \sigma_\zeta}{\sigma_\zeta^3}
$$

(take $\vec{h} \neq \vec{0}$ as polar axis), we may also write

$$
\mathscr{F} g(\vec{h}) = (1 - 3 \cos^2 \theta_{\vec{h}}) \left[\frac{1}{r^3} \mathscr{F} \varphi_{B(r)}(\vec{h}) - \frac{1}{\varepsilon^3} \mathscr{F} \varphi_{B(\varepsilon)}(\vec{h}) \right].
$$

APPENDIX 9

We define

$$D = \{ \vec{m} \in L / \| \vec{m} \| > \delta \}$$
$$D_k = \{ \vec{m} \in L / \| \vec{m} \| \leqslant d(k) \}$$
$$\Phi(\vec{x}) = \sum_{\| \vec{m} \| > \delta} \frac{\| \vec{m} \|^{\alpha}}{(\| \vec{m} \| - \delta)^4} \varphi_{\vec{m}+C}(\vec{x})$$
$$F(\vec{x}) = \frac{\| \vec{x} \|^{\alpha}}{(\| \vec{x} \| - \delta)^4}.$$

If $\vec{x} \in \vec{m} + C$ is such that $\| \vec{x} \| > \delta + \gamma$ ($\gamma = \sup_{\vec{x} \in C} \| \vec{x} \|$), we may apply Taylor's formula at the first order to F:

$$F(\vec{x}) - \Phi(\vec{x}) = F(\vec{x}) - F(\vec{m})$$
$$= \frac{r'^{\alpha-1}[(\alpha - 4)r' - \alpha\delta]}{(r' - \delta)^5} \frac{\vec{x}' \cdot (\vec{x} - \vec{m})}{r'} \quad ;$$

notations: $\vec{x}' = \vec{x} + \zeta(\vec{m} - \vec{x})$, $0 < \zeta < 1$, $r = \| \vec{x} \|$, $r' = \| \vec{x}' \|$. In the case $\alpha \leqslant 1$, we may deduce

$$| F(\vec{x}) - \Phi(\vec{x}) | \leqslant \frac{[(4 - \alpha)(r + \gamma) + \alpha\delta]\gamma}{(r - \gamma)^{1-\alpha}(r - \delta - \gamma)^5}.$$

Let $\chi > 0$ be fixed. There is k_0 such that, for all $k \geqslant k_0$,

$$B(\delta + \gamma + \chi) \subset D_k + C.$$

Then

$$VS(k) = \int_{(D \cap D_k) + C} \Phi(\vec{x}) d\vec{x}$$
$$= S_1 + I(k)$$

where

$$S_1 = \int_{(D + C) \cap B(\delta + \gamma + \chi)} \Phi(\vec{x}) d\vec{x}$$

and

$$I(k) = \int_{[(D \cap D_k) + C] \cap [E \setminus B(\delta + \gamma + \chi)]} \Phi(\vec{x}) d\vec{x}$$
$$\leqslant \int_{\delta + \gamma + \chi < \| \vec{x} \| \leqslant d(k) + \gamma} | F(\vec{x}) - \Phi(\vec{x}) | d\vec{x} + \int_{\delta + \gamma + \chi < \| \vec{x} \| \leqslant d(k) + \gamma} F(\vec{x}) d\vec{x}.$$

We have

$$\int_{\delta + \gamma + \chi < \| \vec{x} \| \leqslant d(k) + \gamma} | F(\vec{x}) - \Phi(\vec{x}) | d\vec{x} \leqslant \int_{\delta + \gamma + \chi}^{d(k) + \gamma} \frac{[(4 - \alpha)(r + \gamma) + \alpha\delta]\gamma}{(r - \delta - \gamma)^{6-\alpha}} 4\pi r^2 dr$$
$$= S_2 + S_3(k) \quad \text{with} \quad \lim_{k \to +\infty} S_3(k) = 0$$

(by integration with $\rho = r - \delta - \gamma$), and

$$\int_{\delta + \gamma + \chi < \| \vec{x} \| \leqslant d(k) + \gamma} F(\vec{x}) d\vec{x} = \int_{\delta + \gamma + \chi}^{d(k) + \gamma} \frac{r^{\alpha}}{(r - \delta)^4} 4\pi r^2 dr$$
$$\leqslant \int_{\delta + \gamma + \chi}^{d(k) + \gamma} \frac{4\pi r^3}{(r - \delta)^4} dr \qquad \text{(by choosing } \chi \geqslant 1 - \delta - \gamma)$$
$$= 4\pi \operatorname{Log}(d(k) + \gamma - \delta) + S_4 + S_5(k)$$

with $\lim_{k \to +\infty} S_5(k) = 0$ (by integration with $\rho = r - \delta$). We may conclude

$$\lim_{k \to +\infty} \frac{S(k)}{(d(k))^\alpha} = 0 .$$

The case $\alpha > 1$ reduces to the preceding case $\alpha \leqslant 1$, by the following assertion: there is $a' \geqslant 0$ such that for all $\alpha' > 0$, $\alpha' \leqslant \alpha$,

$$1 - c(A_k, \vec{m}) \leqslant a' \left(\frac{\| \vec{m} \|}{f(k)} \right)^{\alpha'} \quad \text{for all } k \quad \text{and} \quad \vec{m} \in B_k . \tag{9.1}$$

Indeed: if $\| \vec{m} \| \leqslant f(k)$, we have

$$1 - c(A_k, \vec{m}) \leqslant a \left(\frac{\| \vec{m} \|}{f(k)} \right)^{\alpha} \leqslant a \left(\frac{\| \vec{m} \|}{f(k)} \right)^{\alpha'} ;$$

and if $\| \vec{m} \| > f(k)$, we have

$$1 - c(A_k, \vec{m}) \leqslant 1 < \left(\frac{\| \vec{m} \|}{f(k)} \right)^{\alpha'} .$$

APPENDIX 10

We summarize the method which is similar with that of appendix 4.

$$E_{6.1}(k) = \frac{\vec{M}^2}{2V} \int_0^{+\infty} g_k(\rho) d\rho$$

with

$$g_k(\rho) = \int_{\substack{0 \leqslant \theta \leqslant \pi \\ 0 \leqslant \varphi \leqslant 2\pi}} h_k(\rho, \theta, \varphi) d\theta d\varphi ,$$

$$h_k(\rho, \theta, \varphi) = \sum_{\vec{\mu} \neq \vec{0}} (1 - c(A_k, \vec{m})) \frac{1 - 3\cos^2 \theta_{\vec{\mu}}}{\| \vec{\mu} \|^3} \varphi_{C\vec{\mu}}(\vec{x}) \varphi_{\frac{B_k + C}{f(k)}}(\vec{x}) \rho^2 \sin \theta .$$

According to

$$| h_k(\rho, \theta, \varphi) | \leqslant \frac{4\rho^2}{\| \vec{\mu} \|^3} \leqslant \frac{4}{\rho} \left(\frac{\gamma' + \gamma}{\varepsilon_0} \right)^3$$

(which holds for all $\rho > 0$), Lebesgue's dominated convergence theorem may be applied:

$$\lim_{k \to +\infty} g_k(\rho) = \int_{\substack{0 \leqslant \theta \leqslant \pi \\ 0 \leqslant \varphi \leqslant 2\pi}} (1 - c(\vec{x})) \frac{1 - 3\cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} \varphi_B(\vec{x}) \rho^2 \sin \theta d\theta d\varphi ,$$

for almost every $\rho > 0$. With the help of (32), we have

$$| h_k(\rho, \theta, \varphi) | \leqslant a \| \vec{\mu} \|^\alpha \frac{4\rho^2}{\| \vec{\mu} \|^3} \leqslant 4a \left(\frac{\gamma' + \gamma}{\varepsilon_0} \right)^{3-\alpha} \frac{1}{\rho^{1-\alpha}}$$

(according to (9.1), we suppose $\alpha < 1$), and $\vec{x} \in \dfrac{B_k + C}{f(k)}$ implies

$$\rho \leqslant b + \frac{\gamma}{\eta}$$

($\eta = \inf\limits_k f(k) > 0$). Hence,

$$| g_k(\rho) | \leqslant 8\pi^2 a \left(\frac{\gamma' + \gamma}{\varepsilon_0} \right)^{3-\alpha} \frac{1}{\rho^{1-\alpha}} \quad \text{if} \quad 0 < \rho \leqslant b + \frac{\gamma}{\eta},$$

$$g_k(\rho) = 0 \quad \text{if} \quad \rho > b + \frac{\gamma}{\eta}.$$

Since $\dfrac{1}{\rho^{1-\alpha}}$ is integrable on $\left[0, b + \dfrac{\gamma}{\eta}\right]$, we may apply Lebesgue's dominated convergence theorem:

$$\lim_{k \to +\infty} E_{6.1}(k) = \frac{\vec{M}^2}{2V} \int_0^{+\infty} d\rho \int_{\substack{0 \leqslant \theta \leqslant \pi \\ 0 \leqslant \varphi \leqslant 2\pi}} (1 - c(\vec{x})) \frac{1 - 3\cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} \varphi_B(\vec{x}) \rho^2 \sin \theta d\theta d\varphi .$$

For almost every $\vec{x} \in B$, there is k_0 such that

$$\vec{x} \in \frac{B_k + C}{f(k)} \quad \text{for all} \quad k \geqslant k_0 .$$

Then

$$\| \vec{x} \| \leqslant b + \frac{\gamma}{\eta},$$

and the inequality

$$1 - c(A_k, \vec{m}_k(\vec{x})) \leqslant a\left(\frac{\| \vec{m}_k(\vec{x}) \|}{f(k)}\right)^\alpha$$

gives, when $k \to +\infty$,

$$1 - c(\vec{x}) \leqslant a \| \vec{x} \|^\alpha.$$

We may then write

$$\left| (1 - c(\vec{x})) \frac{1 - 3\cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} \right| \leqslant \frac{4a}{\| \vec{x} \|^{3-\alpha}}$$

for almost every $\vec{x} \in B$. According to the integrability of $\frac{1}{\rho^{1-\alpha}}$ on $\left[0, b + \frac{\gamma}{\eta}\right]$, the function

$$(1 - c(\vec{x})) \frac{1 - 3\cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} \varphi_B(\vec{x})$$

is then integrable, and we may write

$$\lim_{k \to +\infty} E_{6.1}(k) = \frac{\vec{M}^2}{2V} \int (1 - c(\vec{x})) \frac{1 - 3\cos^2 \theta_{\vec{x}}}{\| \vec{x} \|^3} \varphi_B(\vec{x}) d\vec{x}.$$

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