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Evaluation of angular integrals by harmonic projection*

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Summary. Angular momentum and angular integrations are discussed from the standpoint of the theory of harmonic polynomials. General formulae are developed which provide alternatives to the usual group theoretical approach. These formulae are illustrated by applications to the calculation of molecular electrostatic potentials, Fourier tranforms of charge densities, and multipole expansions.

Key words: Angular integrals – Harmonic projection

1. Introduction

In quantum chemistry and atomic physics, angular momentum has usually been treated from a group theoretical standpoint, i.e. by means of Wigner's Clebsch-Gordon coefficients, Racah coefficients, 6*J*-symbols and so on [10–14]. In this paper we would like to present an alternative method for treating angular momentum and for evaluating angular integrals. This alternative method is based on the theory of harmonic polynomials. By definition, an harmonic polynomial is a homogeneous polynomial h_i which also satisfies the Laplace equation, $\nabla^2 h_i = 0$. Harmonic polynomials are closely related to spherical harmonics; in fact spherical harmonics are nothing but harmonic polynomials, orthonormalized in an appropriate way and divided by appropriate powers of *r*. The theory of harmonic polynomials can easily be generalized to *d*-dimensional spaces; and *d*-dimensional harmonic polynomials are closely related to hyperspherical harmonics [15–25]. In this paper, we shall begin by discussing the general properties of harmonic polynomials in a *d*-dimensional Euclidean space.

^{*} It is a pleasure for us to dedicate this paper to Madame Alberte Pullman, one of the great pioneers of quantum biochemistry. Her work has illuminated many important aspects of chemical reactivity. Among these is the role of excess charge density, and the electrostatic potential which it generates, in determining biochemical reactivity and specificity [1-9]. We are happy to be able to discuss some aspects of this problem in the present paper, using the methods of harmonic projection.

We shall then specialize to 3-dimensional space, and we will show how the theory of harmonic projection can be used to convert angular integrations into problems of differentiation. Finally, we shall give some illustrative examples to show how our angular integration formulae can be used for practical calculations in quantum theory.

2. Harmonic polynomials

Let x_1, x_2, \ldots, x_d be the Cartesian coordinate of a *d*-dimensional space, and let:

$$f_n \equiv \prod_{j=1}^d x_j^{n_j} \tag{1}$$

where the n_i 's are positive integers or zero and:

$$n_1 + n_2 + \dots + n_d = n. \tag{2}$$

Then

$$\sum_{j=1}^{d} x_j \frac{\partial f_n}{\partial x_j} = n f_n.$$
(3)

From Eq. (3) it follows that if Δ is the generalized Laplacian operator:

$$\Delta \equiv \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} \tag{4}$$

and if r is the hypperadius [22]:

$$r^2 \equiv \sum_{j=1}^d x_j^2 \tag{5}$$

then

$$\Delta(r^{\beta}f_{\alpha}) = \beta(\beta + d + 2\alpha - 2)r^{\beta - 2}f_{\alpha} + r^{\beta}\Delta f_{\alpha}.$$
 (6)

Let h_{α} be a homogeneous polynomial of order α satisfying:

$$\Delta h_{\alpha} = 0. \tag{7}$$

Such a homogeneous polynomial is said to be *harmonic*. We would like to resolve f_n into a series of harmonic polynomials of the form:

$$f_n = h_n + r^2 h_{n-2} + r^4 h_{n-4} + \cdots.$$
(8)

Since h_{α} is a linear combination of terms of the form shown in Eq. (1), it follows from Eq. (6) that [22]:

$$\Delta(r^{\beta}h_{\alpha}) = \beta(\beta + d + 2\alpha - 2)r^{\beta - 2}h_{\alpha}.$$
(9)

Applying \varDelta repeatedly to both sides of Eq. (8) we obtain:

$$\Delta f_n = 2(d+2n-4)h_{n-2} + 4(d+2n-6)r^2h_{n-4} + \cdots$$

$$\Delta^2 f_n = 8(d+2n-6)(d+2n-8)h_{n-4} + \cdots$$
(10)

and in general:

$$\Delta^{\nu} f_n = \sum_{k=\nu}^{[1/2n]} \frac{(2k)!!}{(2k-2\nu)!!} \frac{(d+2n-2k-2)!!}{(d+2n-2k-2\nu-2)!!} r^{2k-2\nu} h_{n-2k}.$$
 (11)

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For example, when n is even and v = n/2, we obtain:

$$\Delta^{n/2} f_n = \frac{n!!(d+n-2)!!}{(d-2)!!} h_0 \tag{12}$$

or

$$h_0 = \frac{(d-2)!!}{n!!(d+n-2)!!} \Delta^{n/2} f_n.$$
(13)

Equations (10) or (11) constitute a set of simultaneous equations which can be solved for h_{α} . For n = 2, we obtain:

$$f_{2} = h_{2} + r^{2}h_{0}$$

$$h_{0} = \frac{1}{2d}\Delta f_{2}$$

$$h_{2} = f_{2} - \frac{r^{2}}{2d}\Delta f_{2}$$
(14)

while for n = 3 we have:

$$f_{3} = h_{3} + r^{2}h_{1},$$

$$h_{1} = \frac{1}{2(d+2)}\Delta f_{3}$$

$$h_{3} = f_{3} - \frac{r^{2}}{2(d+2)}\Delta f_{3}.$$
(15)

As exemplified by Eqs. (14) and (15), the harmonic polynomials in the decomposition of f_n (Eq. (8)) are given by:

$$h_n = f_n - \frac{r^2}{2(d+2n-4)} \Delta f_n + \frac{r^4}{8(d+2n-4)(d+2n-6)} \Delta^2 f_n - \cdots$$
 (16)

$$h_{n-2} = \frac{1}{2(d+2n-4)} \left[\Delta f_n - \frac{r^2}{2(d+2n-8)} \Delta^2 f_n + \cdots \right]$$
(17)

and in general:

$$h_{n-2\nu} = \frac{(d+2n-4\nu-2)!!}{(2\nu)!!(d+2n-2\nu-2)!!} \times \sum_{k=0}^{[n/2-\nu]} \frac{(-1)^k (d+2n-4\nu-2k-4)!!}{(2k)!!(d+2n-4\nu-4)!!} r^{2k} \Delta^{k+\nu} f_n.$$
(18)

3. 3-Dimensional space

When d = 3, the generalized Laplacian operator becomes the ordinary Laplacian:

$$\Delta \to \nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$
(19)

and Eqs. (14) and (15) reduce to:

$$f_{2} = h_{2} + r^{2}h_{0}$$

$$h_{0} = \frac{1}{6}\nabla^{2}f_{2}$$

$$h_{2} = f_{2} - \frac{r^{2}}{6}\nabla^{2}f_{2}$$
(20)

and

$$f_{3} = h_{3} + r^{2}h_{1}$$

$$h_{1} = \frac{1}{10}\nabla^{2}f_{3}$$

$$h_{3} = f_{3} - \frac{r^{2}}{10}\nabla^{2}f_{3}$$
(21)

while in the general decomposition of f_n into harmonic polynomials:

$$f_n = h_n + r^2 h_{n-2} + r^2 h_{n-4} + \cdots$$
 (22)

we have:

$$h_n = f_n - \frac{r^2}{2(2n-1)} \nabla^2 f_n + \frac{r^4}{8(2n-1)(2n-3)} \nabla^4 f_n - \cdots$$
 (23)

$$h_{n-2} = \frac{1}{2(2n-1)} \left[\nabla^2 f_n - \frac{r^2}{2(2n-5)} \nabla^4 f_n + \cdots \right]$$
(24)

and so on. Thus, for example, if we wished to decompose $f_3 = x^2 y$ into a series of harmonic polynomials, we would first note that:

$$\nabla^2 x^2 y = 2y. \tag{25}$$

Then from Eq. (21), we obtain:

$$x^{2}y = h_{3} + r^{2}h_{1}$$

$$h_{1} = \frac{y}{5}$$

$$h_{3} = x^{2}y - \frac{r^{2}}{5}y$$
(26)

notice that, apart from the normalization constant, h_1/r is a spherical harmonic with l = 1, while h_3/r^3 is a spherical harmonic with l = 3.

4. Angular momentum eigenfunction

The angular momentum operator:

$$L^{2} = -\sum_{i>j}^{3} \left(x_{i} \frac{\partial}{\partial x_{j}} - x_{j} \frac{\partial}{\partial x_{i}} \right)^{2}$$
(27)

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can be written in the form:

$$L^{2} = -r^{2} \nabla^{2} + \sum_{i,j=1}^{3} x_{i} x_{j} \frac{\partial^{2}}{\partial x_{i} \partial x_{j}} + 2 \sum_{i=1}^{3} x_{i} \frac{\partial}{\partial x_{i}}.$$
 (28)

In a previous section we saw that if:

$$f_n \equiv \prod_{j=1}^{3} x_j^{n_j} n \equiv n_1 + n_2 + n_3$$
(29)

then:

$$\sum_{i=1}^{3} x_i \frac{\partial}{\partial x_i} f_n = n f_n.$$
(30)

Similarly we can show that:

$$\sum_{i,j=1}^{3} x_i x_j \frac{\partial^2}{\partial x_i \partial x_j} f_n = n(n-1) f_n.$$
(31)

Combining Eqs. (30), (31) and (28), we obtain

$$L^{2}f_{n} = -r^{2} \nabla^{2}f_{n} + n(n+1)f_{n}.$$
(32)

Now let h_l be an harmonic polynomial of order *l*. Then from Eq. (32) and from the fact that $\nabla^2 h_l = 0$, it follows that:

$$L^2 h_l = l(l+1)h_l. ag{33}$$

In other words, harmonic polynomials are eigenfunctions of angular momentum. (An analogous argument can be used to show that harmonic polynomials in a d dimensional space are eigenfunctions of generalized angular momentum). It follows from Eq. (33) that harmonic polynomials are closely related to spherical harmonics. As we remarked, spherical harmonics are just harmonic polynomials, orthonormalized in an appropriate way, and divided by an appropriate power of the radius:

$$Y_{lm}(\Omega) = r^{-l}h_{lm} \tag{34}$$

where the index m has been added to distinguish between the different linearly independent harmonic polynomials belonging to the eigenvalue l(l + 1). We can choose the set of harmonic polynomials in such a way that the orthonormality conditions:

$$\int d\Omega Y^*_{I'm'}(\Omega) Y_{Im}(\Omega) = \delta_{II'} \delta_{mm'}$$
(35)

are obeyed. Thus, the decomposition of f_n into a series of harmonic polynomials is, in fact, a decomposition into angular momentum eigenfunctions. In other words, if O_l is a projection operator corresponding to the *l*'th eigenvalue of L^2 :

$$O_{l}[f_{n}] = r^{n-1}h_{l}.$$
(36)

5. Angular integrations

Because of the hermiticity of L^2 , it follows that two harmonic polynomials belonging to different eigenvalues of L^2 are orthogonal:

$$\int d\Omega h_1 h_{l'} = 0 \quad \text{if } l \neq l'. \tag{37}$$

Since h_0 is just a constant, Eq. (36) implies that:

$$d\Omega h_l = 0 \quad \text{if } l \neq 0. \tag{38}$$

Therefore, if n is even:

$$\int d\Omega f_n = \int d\Omega (h_n + r^2 h_{n-2} + \dots + r^n h_0) = 4\pi r^n h_0.$$
(39)

From Eq. (13), and from the definition of f_n (Eq. (1)), we have:

$$h_0 = \frac{1}{(n+1)!} \nabla^n f_n = \frac{1}{(n+1)!!} \prod_{j=1}^3 (n_j - 1)!!.$$
(40)

Thus we obtain the powerful angular integration formula:

$$I(\mathbf{n}) \equiv \int d\Omega x^{n_1} y^{n_2} z^{n_3} = \frac{4\pi r^n}{(n+1)!!} \prod_{j=1}^3 (n_j 1)!!.$$
(41)

6. Harmonic projection

The spherical harmonics obey the sum rule:

$$\sum_{m} Y_{lm}^{*}(\Omega') Y_{lm}(\Omega) = \frac{2l+1}{4\pi} P_{l}(\boldsymbol{u} \cdot \boldsymbol{u}')$$
(42)

where

$$u = \frac{1}{r} (x, y, z)$$

$$u' \equiv \frac{1}{r'} (x', y', z')$$
(43)

and where P_i is a Legendre polynomial. From Eq. (42) it follows that if $F(\Omega)$ is some angular function, then:

$$O_{l}[F(\Omega)] = \sum_{m} Y_{lm}(\Omega) \int d\Omega' Y_{lm}^{*}(\Omega')F(\Omega')$$
$$= \frac{2l+1}{4\pi} \int d\Omega' P_{l}(\boldsymbol{u} \cdot \boldsymbol{u}')F(\Omega').$$
(44)

In a previous section we resolved an angular function into eigenfunctions of L^2 by differentiating. Here we perform the same operation by integrating. The equivalence of the two projections makes it possible to perform angular integrations by differentiation!

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7. Applications of harmonic projection

In order to illustrate the way in which our angular integration formulae can be applied, it may be useful to consider some simple examples. Suppose, for example, that we wish to calculate the potential produced by a charge distribution of the form:

$$\varrho_n(\mathbf{x}) = \varrho(r)\chi_n(\Omega) \tag{45}$$

where

$$\chi_n(\Omega) = \prod_{j=1}^3 \left(\frac{x_j}{r}\right)^{n_j}.$$
(46)

A more general charge distribution can be represented as a superposition of terms this form, centered on each of the atoms of the system. Therefore, if we are able to find the potential produced by such a term, we will also be able to find a potential produced by a more general charge distribution. The potential produced by $\varrho_n(x)$ will be given by:

$$\phi(\mathbf{x}) = \int d^3 x' \frac{1}{|\mathbf{x} - \mathbf{x}'|} \varrho_n(\mathbf{x}'). \tag{47}$$

Expanding 1/|x - x'| in terms of Legendre polynomials

$$\frac{1}{|\boldsymbol{x} - \boldsymbol{x}'|} = \sum_{l=0}^{\infty} \frac{r'_{<}}{r_{>}^{l+1}} P_l(\boldsymbol{u} \cdot \boldsymbol{u}')$$
(48)

we obtain:

$$\phi(\mathbf{x}) = \sum_{l=0}^{\infty} \int_{0}^{\infty} dr' r'^{2} \frac{r_{<}^{l}}{r_{>}^{l+1}} \int d\Omega' P_{l}(\mathbf{u} \cdot \mathbf{u}') \varrho_{n}(\mathbf{x}')$$

=
$$\sum_{l=0}^{\infty} \frac{4\pi}{2l+1} O_{l}[\chi_{n}(\Omega)] \int_{0}^{\infty} dr' r'^{2} \frac{r_{<}^{l}}{r_{>}^{l+1}} \varrho(r').$$
(49)

From Eqs. (1) and (46) it follows that:

$$O_{l}[\chi_{n}(\Omega)] = r^{-n}O_{l}[f_{n}] = r^{-l}h_{l}.$$
(50)

Thus, the angular integrations needed for calculating the potential produced by the charge distribution can be performed by decomposing f_n into harmonic polynomials by the methods discussed above. Since the highest *l*-value in this decomposition is l = n, it follows that higher terms in this series for $\phi(\mathbf{x})$ must vanish. If *n* is even, only even values of *l* will contribute to the series, while if *n* is odd, only odd terms will occur. For example, if n = 2 and $f_2 = x_i x_j$ where $i \neq j$, then:

$$O_2[\chi_n(\Omega)] = \frac{x_i x_j}{r^2}$$
(51)

while all other harmonic projections of $\chi_n(\Omega)$ will vanish. Thus, in this example:

$$\phi(\mathbf{x}) = \frac{4\pi}{5} \frac{x_i x_j}{r^2} \int_0^\infty dr' r'^2 \frac{r_<^2}{r_>^3} \varrho(r').$$
(52)

A very similar type of angular integration must be performed if we wish to calculate the Fourier transform of a charge distribution; and again the integration can be carried out by means of harmonic projections. The Fourier transform

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of the charge distribution $\rho_n(\mathbf{x})$ is given by:

$$\varrho_n^i(k) = \frac{1}{(2\pi)^{3/2}} \int d^3x \, e^{ik \cdot x} \varrho_n(x).$$
 (53)

We now expand $e^{ik \cdot x}$ in terms of Legendre polynomials and spherical Bessel functions:

$$e^{i\boldsymbol{k}\cdot\boldsymbol{x}} = \sum_{l=0}^{\infty} i^{l}(2l+1)j_{l}(\boldsymbol{k}\boldsymbol{r})P_{l}(\boldsymbol{u}\cdot\boldsymbol{u}').$$
(54)

Substituting this expansion into the Fourier transform, we have:

$$\varrho_n^{t}(\boldsymbol{k}) = \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} i^l (2l+1) \int_0^\infty dr r^2 j_l(kr) \varrho(r) \int d\Omega P_l(\boldsymbol{u}_k \cdot \boldsymbol{u}) \chi_n(\Omega)$$
(55)

where u_k is a unit vector in the direction of k, and where we have assumed that the charge density has the form shown in Eq. (45). Making use of Eq. (44) we can rewrite Eq. (55) in the form:

$$\varrho_n^t(k) = \sqrt{\frac{2}{\pi}} \sum_{l=0}^{\infty} i^l O_l[\chi_n(\Omega_k)] \int_0^\infty dr j_l(kr) \varrho(r).$$
(56)

As before:

$$O_l[\chi_n(\Omega_k)] = k^{-n} O_l[f_n(\boldsymbol{k})] = k^{-l} h_l(\boldsymbol{k})$$
(57)

can be evaluated by means of harmonic projection. For example, if $\chi_n(\Omega) = x_i^2/r^2$:

$$O_{2}[\chi_{n}(\Omega_{k})] = \frac{k_{i}^{2}}{k^{2}} - \frac{1}{3}$$

$$O_{0}[\chi_{n}(\Omega_{k})] = \frac{1}{3}$$
(58)

all other projections being zero. The Fourier transform of $\rho_n(\mathbf{x})$ thus becomes:

$$\varrho_n^t(\mathbf{k}) = \frac{1}{(2\pi)^{3/2}} \int d^3x \ e^{i\mathbf{k}\cdot\mathbf{x}} \varrho(r) \frac{x_i^2}{r^2} \\ = \frac{1}{3} \sqrt{\frac{2}{\pi}} \int_0^\infty dr j_0(kr) \varrho(r) - \left(\frac{k_i^2}{k^2} - \frac{1}{3}\right) \sqrt{\frac{2}{\pi}} \int_0^\infty dr j_2(kr) \varrho(r).$$
(59)

As a third application of harmonic projection we can consider the problem of decomposing the product of two spherical harmonics into a sum of angular momentum eigenfunctions. If we let:

$$r^{l}Y_{lm}(\Omega) \equiv h_{l}$$

$$r^{l'}Y_{l'm'}(\Omega) \equiv h_{l'}$$
(60)

then

$$O_{l''}[Y_{lm}(\Omega)Y_{l'm'}(\Omega)] = r^{-l-l'}O_{l''}[h_lh_{l'}].$$
(61)

To evaluate $O_{l''}[h_l h_{l'}]$ we first notice that:

$$\nabla^{2}(h_{l}h_{l'}) = h_{l} \nabla^{2}h_{l'} + h_{l'} \nabla^{2}h_{l} + 2\sum_{i=1}^{3} \frac{\partial h_{l}}{\partial x_{i}} \frac{\partial h_{l'}}{\partial x_{i}}.$$
 (62)

Since $\nabla^2 h_l = \nabla^2 h_{l'} = 0$, only the cross terms survive; and we can write:

$$\nabla^2(h_i h_{i'}) = 2 \sum_{i=1}^3 \frac{\partial h_i}{\partial x_i} \frac{\partial h_{i'}}{\partial x_i}.$$
(63)

Similarly:

$$\nabla^4(h_l h_{l'}) = 4 \sum_{i,j=1}^3 \frac{\partial^2 h_l}{\partial x_i \partial x_j} \frac{\partial^2 h_{l'}}{\partial x_i \partial x_j}$$
(64)

and so on. Notice that the highest power of the Laplacian operator which can be applied to the product $h_l h_{l'}$ without a vanishing result is the smaller of the two quantum numbers l or l'. Thus, for example, if l' = 1 we know that:

$$\nabla^4(h_l h_1) = \nabla^6(h_l h_1) = \dots = 0.$$
(65)

Then, from Eqs. (23), (24) and (63) we have:

$$O_{l+1}[h_{l}h_{1}] = h_{l}h_{1} - \frac{r^{2}}{2l+1} \sum_{i=1}^{3} \frac{\partial h_{l}}{\partial x_{i}} \frac{\partial h_{1}}{\partial x_{i}}$$

$$O_{l-1}[h_{l}h_{1}] = \frac{r^{2}}{2l+1} \sum_{i=1}^{3} \frac{\partial h_{l}}{\partial x_{i}} \frac{\partial h_{1}}{\partial x_{i}}$$
(66)

all other projections being zero.

8. Multipole expansions

As an example of the way in which our angular integration Eq. (41) can be applied, we can consider the interaction between two charge distributions, located respectively on atoms at positions R_a and R_b . This interaction energy will be given by:

$$J = \int d^3x \int d^3x' \varrho_a(\boldsymbol{x} - \boldsymbol{R}_{\alpha}) \frac{1}{|\boldsymbol{x} - \boldsymbol{x}'|} \varrho_b(\boldsymbol{x}' - \boldsymbol{R}_b).$$
(67)

If we introduce a Taylor series expansion of $1/|\mathbf{x} - \mathbf{x}'|$ about the two centers \mathbf{R}_a and \mathbf{R}_b , we obtain:

$$J = \int d^{3}x \varrho_{a}(\mathbf{x} - \mathbf{R}_{a}) \prod_{j=1}^{3} \left[1 + (x_{j} - R_{aj}) \frac{\partial}{\partial R_{aj}} + \cdots \right]$$
$$\times \int d^{3}x' \varrho_{b}(\mathbf{x} - \mathbf{R}_{b}) \prod_{j=1}^{3} \left[1 + (x'_{j} - R_{bj}) \frac{\partial}{\partial R_{bj}} + \cdots \right] \frac{1}{|\mathbf{R}_{a} - \mathbf{R}_{b}|}.$$
(68)

Suppose that:

$$\varrho_a(\mathbf{x}) = \varrho(r)\chi_n(\Omega). \tag{69}$$

(As we remarked above, a more general charge distribution can be represented as a superposition of contributions of this form.) Shifting the origin of our integration we can write:

$$\int d^{3}x \varrho_{a}(\boldsymbol{x} - \boldsymbol{R}_{a}) \prod_{j=1}^{3} \left[1 + (x_{j} - R_{aj}) \frac{\partial}{\partial R_{aj}} + \cdots \right]$$
$$= \int_{0}^{\infty} dr r^{2} \varrho(r) \int d\Omega \chi_{n}(\Omega) \prod_{j=1}^{3} \left[1 + x_{j} \frac{\partial}{\partial R_{aj}} + \cdots \right]. \quad (70)$$

The integrals which must be evaluated in the multipole expansion thus have the form:

$$\int_{0}^{\infty} dr r^{2} \varrho(r) \int d\Omega \chi_{n}(\Omega) \prod_{j=1}^{3} x_{j}^{n_{j}} = \int_{0}^{\infty} dr r^{n'+2} \varrho(r) \int d\Omega \chi_{n}(\Omega) \chi_{n'}(\Omega)$$
(71)

where $n' \equiv n'_1 + n'_2 + n'_3$. The angular functions, $\chi_n(\Omega)$, have the convenient composition property:

$$\chi_n(\Omega)\chi_{n'}(\Omega) = \chi_{n+n'}(\Omega)$$
(72)

so that

$$\int d\Omega \chi_n(\Omega) \chi_{n'}(\Omega) = \int d\Omega \chi_{n+n'}(\Omega) = \frac{4\pi}{(n+n'+1)!!} \prod_{j=1}^3 (n_j + n'_j - 1)!!.$$
(73)

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