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Termo Tensorial Geral para Expansão Multipolar

General Tensorial Term for Multipole Expansion

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Resumo

Neste trabalho estamos interessados em obter uma expressão geral para todos os termos de uma expansão multipolar do potencial elétrico. Isso deve ser visto como mais do que um simples exercício matemático, uma vez que muitos cálculos, principalmente aqueles relacionados a sistemas eletrônicos em Mecânica Quântica, podem se beneficiar dos resultados aqui obtidos.

Primeiramente, no entanto, faremos uma breve introdução à expansão multipolar derivando a expressão usual em termos dos polinômios de Legendre. Na seção seguinte, nós chegamos a uma expressão geral para um multipolo qualquer. A seção três é focada em mostrar que tal expressão se reduz aos casos simples dos multipolos comumente tratados (monopolo, dipolo, quadrupolo e octopolo). Por fim, fazemos uma breve conclusão dos resultados e suas implicações.

Palavras-chave: *Física. Eletrostática. Expansão Multipolar. Tensor de Multipolo.*

Abstract

In this work we are interested in obtaining a general expression for all terms of a multipole expansion of the electric potential[1]. This should be seen as more than a mathematical exercise, since many calculations, mainly those in the realm of electronic systems in Quantum Mechanics, can profit from the results to be shown.

Before anything, we will make a brief introduction to multipole expansion deriving the usual expression in terms of the Legendre polynomials. In the next section we find the general expression for any multipole term. Section three is devoted to the show that this general expression reduces to the usually known multipole terms (monopole, dipole, quadrupole and octopole). We then make a brief conclusion of our results and their implications.

Keywords: *Physics. Electrostatics. Multipole Expansion. Multipole Tensor.*

[1]This problem was suggested in a class on Electromagnetic Theory, at Universidade de Brasília, UnB, by professor L.S.F. Olavo

I. Introduction

Consider a continuous arbitrary charge distribution. If each infinitesimal charge element is in figure a position given by the vector $\mathbf{r}'$, as illustrated in figure 1,

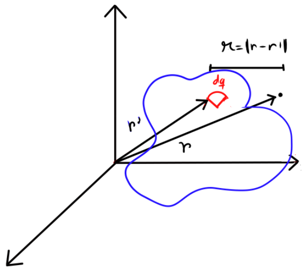

Figure 1

the potential it attributes to a point defined by $\mathbf{r}$ is given by Gauss's law as:

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\int \frac{\rho(\mathbf{r}')}{r}dv', \tag{1}$$

where $\rho(\mathbf{r}')$ is the position dependent charge density, and r is the distance between the charge element and the point where the potential is evaluated. By definition

$$r^2 = |\mathbf{r}|^2 + |\mathbf{r}'|^2 - 2|\mathbf{r}'||\mathbf{r}|cos\theta = r^2\left(1 + t^2 - 2tcos\theta\right), \tag{2}$$

where $t = \frac{|\mathbf{r}'|}{|\mathbf{r}|}$, we have then

$$r = |\mathbf{r}|\sqrt{1 + t^2 - 2tcos\theta}. \tag{3}$$

Considering now that, by the definition of the generating function of the Legendre polynomials

$$\frac{1}{\sqrt{1 + t^2 - 2tx}} = \sum_{n=0}^{\infty} P_n(x)t^n, \tag{4}$$

where $P_n(x)$ are the Legendre polynomials, making $x = cos\theta$ we then have

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\epsilon_0}\sum_{n=0}^{\infty}\frac{1}{r^{n+1}}\int (r')^n P_n(cos\theta)\rho(r')dv'. \tag{5}$$

II. Multipole Tensor

Beginning with the Rodrigues' formula for the Legendre polynomials

$$P_n(cos(\theta)) = P_n(x) = \frac{1}{2^n n!}\frac{d^n[(x^2 - 1)^n]}{dx^n}, \tag{6}$$

we can find the following expression for the nth polynomial

$$P_n(x) = \frac{1}{2^n n!} \sum_{k=0}^{n/2} C_k x^{n-2k}, \tag{7}$$

where we define

$$C_k = (-1)^k \binom{n}{k} \frac{[2(n-k)]!}{(n-2k)!}. \tag{8}$$

Considering the vector r' associated with the position of each element of charge dq, we can write down it's components as

$$r^{i'} = |r'| u^{i'}, \tag{9}$$

where we define, using Einstein index notation,

$$|r'|^2 = r^{i'} r_{i'}. \tag{10}$$

As the modulus of the vector r' and $u^{i'}$ are the components of the unit vector parallel to $r^{i'}$.

Since the space treated here is simply the continous 3-D Euclidean space we can define its metric as follows.

$$\eta_{ij} = u_i \otimes u_j = u_i u_j, \tag{11}$$

where $\otimes$ denotes the tensor product between the bases (which in here are the components of u_i in the adopted coordinate system), and u_i is the 1-form associated with the unit vector in the direction of r^i, which is the position vector of the point in which the potential is evaluated.

Since x was defined as the cosine between the position vector of the charge element and r^i, it can be written as[2]

$$x = u_i u^{i'}, \tag{12}$$

we then have

$$\sum_{k=0}^{n/2} C_k x^{n-2k} = \sum_{k=0}^{n/2} (u_i r^{i'})^n C_k x^{-2k}, \tag{13}$$

and considering that

$$\frac{1}{x} = \frac{|r'|}{u_i r^{i'}}, \tag{14}$$

it is possible to write 8 as

$$\sum_{k=0}^{n/2} (u_i r^{i'})^n C_k x^{-2k} = \sum (u_i r^{i'})^{n-2k} |r'|^{2k}. \tag{15}$$

[2]Although i and i' are different symbols they denote components with respect to the same basis, the only difference being one represents the components of the position vector of the point analyzed and other the position of the charge element

Using 5 and 6 we can deduce the following:

$$\begin{aligned} |r'|^2 =& r^{i'} r_{i'} = r^i r_i = r^i u_i \eta_{ij} \eta^{ij} r^j u_j \\ =& u_i r^i r_i \eta^{ij} u_j = u_i |r'|^2 \eta^{ij} u_j, \end{aligned} \tag{16}$$

Now, using (9), (10) and (11) we arrive at

$$\sum C_k x^{n-2k} = \sum C_k (u_i r^{i'})^{n-2k} (u_i |r'|^2 \eta^{ij} u_j)^k. \tag{17}$$

Noting that

$$(u_i)^n = u_{i_1} \otimes ... \otimes u_{i_n}, \tag{18}$$

we can write the sum in (13) in terms of a tensor. Therefore defining the Generalized Multipole Tensor

$$\mathbf{L} = L^{i_1...i_n} \otimes u_{i_1} ... \otimes u_{i_n}, \tag{19}$$

where the components

$$L^{i_1...i_n} = \frac{(-1)^k}{2^n n!} \int \rho(r') \sum_{k=0}^{\frac{n}{2}} C_k (r^{i'})^{n-2k} (|r'|^2 \eta^{ij})^k dv', \tag{20}$$

are the nth term of the expansion and

$$(\eta^{ij})^k = \eta^{i_1 i_2} ... \eta^{i_{k-1} i_k}, \tag{21}$$

with (15) and (16) we then can write down the general term for the potential expansion.

$$\phi(r) = \frac{1}{4\pi\epsilon_0} \sum_{n=0}^{\infty} \frac{1}{r^{n+1}} L^{i_1...i_n} e_{i_1} ... e_{i_n}. \tag{22}$$

III. Some Specific Cases

III.1. Monopole Potential

The derivation of the monopole contribution for the total potential is trivial. In this case **L** is simply a scalar for which $n = 0$, we then have from (20) and (22).

$$\phi_0(r) = \frac{1}{4\pi\epsilon_0 r} \int \rho(r') dv' = \frac{Q}{4\pi\epsilon_0 r} \tag{23}$$

III.2. Dipole Potential

For the dipole we have $n = 1$, therefore **L** is a (1,0) tensor. We still have a single term in the sum on (20). From (8) we have

$$\frac{C_0}{2^n n!} = \frac{2}{2} = 1 \tag{24}$$

and, from (20)

$$L^i = \int \rho(r')r^{i'}dv' = p^i \tag{25}$$

and therefore

$$\phi_1(r) = \frac{1}{4\pi\epsilon_0 r^2}p^i e_i \tag{26}$$

Where p^i is the dipole momentum vector.

III.3. Quadrupole Potential

For this case we have something more interesting, this part of the contribution is a (2,0) tensor field for which n=2, the coefficients C_k are.

$$C_0 = \binom{2}{0}\frac{4!}{2!} = 12 \tag{27}$$

$$C_1 = \binom{2}{1}\frac{2!}{0!} = 4 \tag{28}$$

Therefore, **L** takes the form

$$L^{ij} = \frac{1}{2}\int \rho(r')\left[3r^{i'}r^{j'} - (|r'|^2\eta^{ij})\right]dv' = Q^{ij} \tag{29}$$

We then can write the potential as

$$\phi_2(r) = \frac{1}{4\pi\epsilon_0 r^2}Q^{ij}e_i e_j \tag{30}$$

III.4. Octopole Potential

At last, the deduction of the octopole contribution is similar to the past ones. For this case

$$C_0 = 120, \tag{31}$$

$$C_1 = -72, \tag{32}$$

$$L^{ijk} = \frac{1}{2}\int \rho(r')\left[5r^{i'}r^{j'}r^{k'} - 3|r'|^2 r^{i'}\eta^{jk}dv'\right], \tag{33}$$

the potential is therefore

$$\phi_3(r) = \frac{1}{4\pi\epsilon r^3}L^{ijk}e_i e_j e_k, \tag{34}$$

reproducing, as expected, the tensors associated with such multipoles

IV. Conclusions

In this paper we have shown how one can arrive at a general tensorial term that enables a quick derivation of the nth order tensor associated with the 2^nth multipole of a charge distribution. This demonstration can be extended to any inverse square force law whose potential can be obtained from the Legendre equation and, as expected, shows that such multipoles fall at a rate proportional to d^n, meaning that at short distances their influence must be taken into account.

Referências

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References

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