Basic mathematics for nano-engineers (II)

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1 Vector calculus

We will prove several important differential identities involving *div*, *curl* and *grad*. Let us first fix some notation. We work with three dimensional vectors, denoted by $\vec{x} = [x_1, x_2, x_3]$. The elements of the standard basis in $\mathbb{R}^3$ are denoted by $\vec{e}_j$, $j = 1, 2, 3$, and we can write

$$\vec{x} = \sum_{j=1}^{3} x_j \vec{e}_j. \tag{1.1}$$

1.1 Kronecker's and Levi-Civita's tensors

The Kronecker delta tensor is denoted by $\delta_{jk} = 1$ if $j = k$ and $\delta_{jk} = 0$ if $j \neq k$. An important sum rule is the following:

$$\sum_{i,j=1}^{3} \delta_{ij} A_i B_j = \sum_{i=1}^{3} A_i B_i = \vec{A} \cdot \vec{B}. \tag{1.2}$$

The Levi-Civita tensor ϵ_{ijk} equals 0 if any of the two indexes are identical, equals 1 is the permutation $123 \to ijk$ is even, and -1 otherwise. How can one decide whether a permutation is even? One counts how many transpositions are necessary in order to bring the permutation back to the identical one $123 \to 123$. If this number is even, then the permutation is even. Otherwise is odd. For example, $123 \to 312$ can be brought back to the identical permutation by first interchanging 3 with 1 obtaining $123 \to 132$, and then changing 3 with 2. Therefore $\epsilon_{312} = 1$. In a similar way, $\epsilon_{231} = \epsilon_{123} = 1$. And $\epsilon_{213} = \epsilon_{132} = \epsilon_{321} = -1$.

This definition implies the following important facts:

$$\epsilon_{ijk} = -\epsilon_{jik} = \epsilon_{jki}. \tag{1.3}$$

This comes from the fact that by swapping two neighboring indexes, we change by 1 the number of transpositions needed to go back to $123 \to 123$. We also say that the Levi-Civita tensor is completely antisymmetric.

An important relationship between Levi-Civita's and Kronecker's tensors is:

$$\sum_{i=1}^{3} \epsilon_{jki}\epsilon_{mni} = \sum_{i=1}^{3} \epsilon_{ijk}\epsilon_{imn} = \delta_{jm}\delta_{kn} - \delta_{jn}\delta_{km}. \tag{1.4}$$

For more things about this subject, follow the link:

$http://planetmath.org/encyclopedia/LeviCivitaPermutationSymbol3.html$

1.2 grad, div, and curl

We work in three dimensions. Let us remind some relevant definitions:

1. For every smooth scalar field $\phi : \mathbb{R}^3 \to \mathbb{R}$ we define its gradient vector as the vector field given by:

$$(grad\ \phi)(\vec{x}) = \nabla\phi(\vec{x}) = \sum_{j=1}^{3} (\partial_j \phi)(\vec{x})\ \vec{e}_j. \tag{1.5}$$

2. For every smooth vector field $\vec{F} = [F_1, F_2, F_3] : \mathbb{R}^3 \to \mathbb{R}^3$ we define its divergence as the scalar field given by:

$$(div\ \vec{F})(\vec{x}) = (\nabla \cdot \vec{F})(\vec{x}) = \sum_{j=1}^{3} (\partial_j F_j)(\vec{x}). \tag{1.6}$$

3. For every smooth vector field $\vec{G} = [G_1, G_2, G_3] : \mathbb{R}^3 \to \mathbb{R}^3$ we define its curl as the vector field given by:

$$(curl\ \vec{G})(\vec{x}) = (\nabla \times \vec{G})(\vec{x}) = \sum_{i=1}^{3} \{curl\ \vec{G}(\vec{x})\}_i \vec{e}_i, \tag{1.7}$$

$$\{curl\ \vec{G}(\vec{x})\}_i = \sum_{j,k=1}^{3} \epsilon_{ijk} (\partial_j G_k)(\vec{x}). \tag{1.8}$$

Exercise 1.1. *Show the identity*

$$div\ (\phi\vec{F}) = \phi(div\ \vec{F}) + (grad\ \phi) \cdot \vec{F}.$$

Hint. The vector field $\phi\vec{F}$ has the components ϕF_j. Then according to (1.6) we have

$$div\ (\phi\vec{F}) = \sum_{j=1}^{3} \partial_j(\phi F_j) = \sum_{j=1}^{3} \{(\partial_j\phi)F_j + \phi(\partial_j F_j)\} = \sum_{j=1}^{3} (\partial_j\phi)F_j + \phi\sum_{j=1}^{3}(\partial_j F_j).$$

□

The Laplace operator is defined as

$$\Delta f = \nabla^2 f = \sum_{j=1}^{3}(\partial_j^2 f) = div[grad(f)]. \tag{1.9}$$

When it acts on vectors, it acts on each component separately.

Exercise 1.2. *(The same as exercise 19 in McQuarrie.) Show the identity*

$$curl(curl\ \vec{G}) = \nabla \times \nabla \times \vec{G} = grad(div\ \vec{G}) - \nabla^2 \vec{G}.$$

Hint. Both sides of the above equality are vectors, hence it is enough to show the equality of the i-th component. We have from the definition of $curl$:

$$\{curl(curl\ \vec{G})\}_i = \sum_{j,k=1}^{3} \epsilon_{ijk}[\partial_j \{curl\ \vec{G}\}_k].$$

Using (1.8), we have $\{curl\ \vec{G}\}_k = \sum_{m,n=1}^{3} \epsilon_{kmn}(\partial_m G_n)$, and thus:

$$\partial_j \{curl\ \vec{G}\}_k = \sum_{m,n=1}^{3} \epsilon_{kmn}(\partial_{mj}^2 G_n).$$

Introduce this in the previous identity and get:

$$\{curl(curl\ \vec{G})\}_i = \sum_{j,k=1}^{3} \epsilon_{ijk} \sum_{m,n=1}^{3} \epsilon_{kmn}(\partial_{mj}^2 G_n) = \sum_{j,k,m,n=1}^{3} \epsilon_{ijk}\epsilon_{kmn}(\partial_{mj}^2 G_n). \tag{1.10}$$

We first perform the sum with respect to k, using the fact that $\epsilon_{kmn} = \epsilon_{mnk}$, and the identity (see (1.4)):

$$\sum_{k=1}^{3} \epsilon_{ijk}\epsilon_{mnk} = \delta_{im}\delta_{jn} - \delta_{in}\delta_{jm}.$$

Introducing this in (1.10) we get:

$$\begin{aligned} \{curl(curl\ \vec{G})\}_i &= \sum_{j,m,n=1}^{3} (\delta_{im}\delta_{jn} - \delta_{in}\delta_{jm})(\partial_{mj}^2 G_n) \\ &= \sum_{j,m,n=1}^{3} \delta_{im}\delta_{jn}(\partial_{mj}^2 G_n) - \sum_{j,m,n=1}^{3} \delta_{in}\delta_{jm}(\partial_{mj}^2 G_n). \end{aligned} \tag{1.11}$$

Now let us concentrate on the first term $\sum_{j,m,n=1}^{3} \delta_{im}\delta_{jn}(\partial_{mj}^2 G_n)$. If we first perform the sum with respect to j, we get:

$$\sum_{j,m,n=1}^{3} \delta_{im}\delta_{jn}(\partial_{mj}^2 G_n) = \sum_{m,n=1}^{3} \delta_{im}(\partial_{mn}^2 G_n),$$

because the only case in which $\delta_{jn} \neq 0$ is when $j = n$. If we do the sum over m, the only nonzero term comes from $m = i$. We get:

$$\sum_{m,n=1}^{3} \delta_{im}(\partial^2_{mn} G_n) = \sum_{n=1}^{3}(\partial^2_{in} G_n) = \partial_i(div\ \vec{G}).$$

In a similar way, we get:

$$\sum_{j,m,n=1}^{3} \delta_{in}\delta_{jm}(\partial^2_{mj} G_n) = \sum_{j,m=1}^{3} \delta_{jm}(\partial^2_{mj} G_i) = \sum_{j}^{3}(\partial^2_{jj} G_i) = \nabla^2 G_i.$$

Putting this back into (1.11) we obtain

$$\{curl(curl\ \vec{G})\}_i = \partial_i(div\ \vec{G}) - \nabla^2 G_i,$$

and the exercise is solved. □

1.3 Applications to electrodynamics

Consider a given scalar field $g(\vec{x}) \in \mathbb{R}$. By the notation $\nabla\nabla g$ we understand the Hessian matrix of g, given by its components $\{\partial^2_{ij} g\}^3_{i,j=1}$. If $\vec{A}$ is an arbitrary constant vector, we see that we can write:

$$[\nabla\nabla g(\vec{x})]\vec{A} = \sum_{i=1}^{3} \vec{e}_i \left(\sum_{j=1}^{3} \partial^2_{ij} g(\vec{x})\ A_j \right) = \sum_{i=1}^{3} \vec{e}_i \partial_i \left(\sum_{j=1}^{3} \partial_j g(\vec{x})\ A_j \right) \quad (1.12)$$

$$= grad[grad(g) \cdot \vec{A}]. \quad (1.13)$$

Note that this identity is only true if $\vec{A}$ does not depend on the variables. Also note the differnece between the Hessian matrix and the Laplace operator (the later is the trace of the Hessian matrix).

Now let us solve a project related exercise:

Exercise 1.3. *Choose an arbitrary constant vector $\vec{A}$. Denote by I the 3×3 identity matrix. If k is a constant real number, denote by $g(\vec{x})$ an arbitrary solution of the Helmholtz equation:*

$$(\nabla^2 + k^2)g(\vec{x}) = 0. \quad (1.14)$$

Define

$$\vec{F}(\vec{x}) = \left[\frac{1}{k^2} \left(\nabla\nabla g(\vec{x}) + \ k^2 g(\vec{x}) I \right) \right] \vec{A}.$$

Then show that $\vec{F}$ solves the vectorial stationary wave equation:

$$-\nabla \times (\nabla \times \vec{F}) + k^2 \vec{F} = 0. \quad (1.15)$$

Hint. Since $\vec{A}$ is constant, we have (use ((1.13))):

$$\vec{F}(\vec{x}) = \frac{1}{k^2} grad[grad(g(\vec{x})) \cdot \vec{A}] + g(\vec{x})\vec{A}. \tag{1.16}$$

Now Exercise 1.2 says that

$$-\nabla \times (\nabla \times \vec{F}) + k^2\vec{F} = -grad(div\vec{F}) + \Delta\vec{F} + k^2\vec{F}. \tag{1.17}$$

It is not difficult to show that $\Delta\vec{F} + k^2\vec{F} = 0$. This is because the only dependence on $\vec{x}$ in (1.16) is the one from g, which already solves the Helmholtz equation (1.14), and because Δ commutes with all other derivatives. Therefore the exercise would be solved if we could prove that $div\vec{F} \equiv 0$.

Let us do that. First, using (1.16), we get

$$div\vec{F} = \frac{1}{k^2} div\ grad[grad(g(\vec{x})) \cdot \vec{A}] + div[g(\vec{x})\vec{A}].$$

But $div\ grad = \Delta$ (see (1.9)), and $div[g\vec{A}] = grad(g) \cdot \vec{A}$ (see (27), page 309 in McQuarrie in the case of constant **v**). Hence we have

$$div\vec{F} = \frac{1}{k^2}\Delta[grad(g) \cdot \vec{A}] + [grad(g) \cdot \vec{A}].$$

But Δ commutes again with *grad* and we have

$$div\vec{F} = \frac{1}{k^2}[grad(\Delta g) \cdot \vec{A}] + [grad(g) \cdot \vec{A}].$$

Now use the linearity of *grad* and dot product, and write

$$div\vec{F} = \frac{1}{k^2}[grad(\Delta g + k^2 g) \cdot \vec{A}].$$

Use (1.14) and the execise is solved. □