

PHY481 - Lecture 9

Sections 3.7-3.8 of PS

A. The electric potential energy of a charge distribution

Potential energy

The potential energy of a charge q at position \vec{r} is $U = qV(\vec{r})$. In the case of a continuum this becomes $\int \rho(\vec{r})V(\vec{r})d\vec{r}$. However in using this continuum equation it is assumed that the potential is unaltered by the added charge $\int \rho(\vec{r})d\vec{r}$.

Potential energy stored in a charge distribution

A different question is: What is the potential energy of a distribution of charges, that is, what is the potential energy stored in a distribution of charges. In this case we must take into account the way in which the electrostatic potential changes as charge is added to the system. The potential energy stored in a distribution of charges is equal to the work done in setting up the distribution of charges, provided there is no dissipation and no kinetic energy is generated. To set up a distribution of charges Q_i at positions \vec{r}_i , we need to bring each of the charges in from infinity and place it at its allocated position. The work required to place the first charge is zero (no other charges are there yet). The work required to place the second charge is Q_2V_{21} , where $V_{21} = kQ_1/r_{21}$ is the electric potential at position \vec{r}_2 due to charge Q_1 . Note that $r_{21} = r_{12} = |\vec{r}_2 - \vec{r}_1|$. The work required to place charge 3 at its position is equal to $Q_3V_{31} + Q_3V_{32}$, and so on, once all of the n charges are in position, we have,

$$U_n = \frac{1}{2} \sum_{i \neq j}^{n,n} \frac{kQ_i Q_j}{r_{ij}} = \sum_{i < j}^{n,n} \frac{kQ_i Q_j}{r_{ij}} \quad (1)$$

In these expressions each pair interaction is counted once and the total potential energy is the sum of the potential energies of all pairs. Note: in writing this energy we have ignored the self-energy of each charge. The self-energy is $n * E_{self}$ and is the same regardless of where the charges are placed. U_n is the interaction energy between the charges. Taking the continuum limit the electric potential due to a charge distribution is,

$$U = \frac{1}{2} \int \frac{\rho(\vec{r})\rho(\vec{r}')d\vec{r}d\vec{r}'}{4\pi\epsilon_0|\vec{r} - \vec{r}'|} = \frac{1}{2} \int \rho(\vec{r})V(\vec{r})d\vec{r} \quad (2)$$

Note that this is 1/2 the value which would be true if the potential were fixed and when the charge $\int \rho(\vec{r})$ is added. This factor of two is thus quite fundamental - it is also a source of considerable confusion.

The energy stored in the electric field

Using the relations,

$$\rho V = -\epsilon_0(\nabla^2 V)V \quad (3)$$

Using the vector identity $\vec{\nabla} \cdot (V\vec{E}) = \vec{\nabla}V \cdot \vec{E} + V\vec{\nabla} \cdot \vec{E}$ and $E = -\vec{\nabla}V$, this may be rewritten as.

$$-\epsilon_0(\nabla^2 V)V = -\epsilon_0\vec{\nabla} \cdot (V\vec{\nabla}V) + \epsilon_0(\vec{\nabla}V)^2 \quad (4)$$

Using Gauss's theorem the first term on the RHS becomes $\oint V\vec{\nabla}V \cdot d\vec{A}$ which goes to zero at $r \rightarrow \text{infinity}$. The only surviving term is the last term on the RHS, so that the energy density in the electric field may then be written as,

$$u(\vec{r}) = \frac{1}{2}\epsilon_0\vec{E}^2 \quad (5)$$

where we used the fact that $\vec{E} = -\vec{\nabla}V$. This is the energy density in the electric field and is the energy required to set up the charge distribution. Problem 3.28 can be solved by integrating this energy density over the volume of interest.

Note that if we integrate the field due to an isolated charge we get infinity!. However we are interested in changes in potential energy due to changing the charge configuration. The infinite self energy of each charge is there no matter what the charge arrangement is, so it plays no role in the physics of the problem. However it is important in trying to formulate a quantum version of EM.

B. The multipole expansion

The multipole expansion is a systematic perturbation theory of the general expressions for the potential due to a charge distribution,

$$V(\vec{r}) = \sum_i \frac{kq_i}{|\vec{r} - \vec{r}_i|} \quad \text{or} \quad \int \frac{k\rho(\vec{r}')d\vec{r}'}{|\vec{r} - \vec{r}'|}. \quad (6)$$

The perturbation expansion requires that the locations of the charges \vec{r}_i are all significantly less than the position at which we plan to find the electrostatic potential and the electric field, i.e. $\vec{r} \gg \vec{r}_i$. In the case of the continuum integral, the charge density $\rho(\vec{r}')$ must have a maximum extent which is much less than \vec{r} .

The result of the expansion for the potential is,

$$V(\vec{r}) = \frac{A}{r} + \frac{B}{r^2} + \frac{C}{r^3} + \dots \quad (7)$$

where A, B, C in general depend on \hat{r} leading to an important angle dependence for the second two terms. Finding A, B, C is where the hard work in the multipole expansion resides. The first term is called the monopole term because it looks like a point charge term, while the second is the dipole term and the third the quadrupole term. All of them have very important applications in physics, chemistry and medicine (e.g. MRI, NMR etc). When the electric field is found by taking a gradient of the terms in this expansion, the first term which results is again the monopole term, while the second and third terms are again the dipole and quadrupole terms respectively. The dependence on r for the electric field multipole expansion is $1/r^2$ for the monopole $1/r^3$ for the dipole and $1/r^4$ for the quadrupole.

The multipole expansion is carried out by expanding the denominator of Eq. (6) by using the cosine rule to write,

$$|\vec{r} - \vec{r}_i| = (r^2 + r_i^2 - 2rr_i \cos\theta)^{1/2} \quad (8)$$

Therefore,

$$\frac{1}{|\vec{r} - \vec{r}_i|} = \frac{1}{[r^2 + r_i^2 - 2rr_i \cos\theta]^{1/2}} = \frac{1}{r[1 - 2\frac{\vec{r}_i \cdot \hat{r}}{r} + (\frac{r_i}{r})^2]^{1/2}} \quad (9)$$

Now we use the expansion,

$$\frac{1}{(1 + \delta)^{1/2}} = 1 - \frac{1}{2}\delta + \frac{3}{8}\delta^2 + \dots \quad (10)$$

with $\delta = -2\frac{\vec{r}_i \cdot \hat{r}}{r} + (\frac{r_i}{r})^2$. We then have,

$$\frac{1}{|\vec{r} - \vec{r}_i|} = \frac{1}{r} - \frac{1}{2r}[-2\frac{\vec{r}_i \cdot \hat{r}}{r} + (\frac{r_i}{r})^2] + \frac{3}{8r}[-2\frac{\vec{r}_i \cdot \hat{r}}{r} + (\frac{r_i}{r})^2]^2 + \dots \quad (11)$$

Which may be written in the form,

$$\frac{1}{|\vec{r} - \vec{r}_i|} = \frac{1}{r} + \frac{\vec{r}_i \cdot \hat{r}}{r^2} + [\frac{3}{2}(\frac{\vec{r}_i \cdot \hat{r}}{r})^2 - \frac{1}{2r}(\frac{r_i}{r})^2] + \dots \quad (12)$$

This may also be written in terms of the angle between \vec{r}_i and \vec{r} ,

$$\frac{1}{|\vec{r} - \vec{r}_i|} = \frac{1}{r} + \frac{r_i \cos\theta_i}{r^2} + \frac{r_i^2}{2r^3}[3\cos^2\theta_i - 1] + \dots \quad (13)$$

This is the basis of the multipole expansion to quadrupole order and shows the angular dependence characteristic of the dipole and quadrupole terms. To complete the expansion we substitute this expansion in Eq. (6) to find,

$$\sum_i \frac{kq_i}{|\vec{r} - \vec{r}_i|} = \sum_i \frac{kq_i}{r} + \sum_i \frac{kq_i r_i \cos\theta_i}{r^2} + \sum_i \frac{kq_i r_i^2}{2r^3}[3\cos^2\theta_i - 1] + O(\frac{1}{r^4}) \quad (14)$$

It is then natural to define the quantities,

$$Q = \sum_i q_i; \quad \vec{p} = \sum_i q_i \vec{r}_i \quad (15)$$

which are the total charge and the total dipole moment of the charge distribution. The definition of the quadrupole term is more subtle, however a matrix form is convenient so that, we finally have,

$$\sum_i \frac{kq_i}{|\vec{r} - \vec{r}_i|} = \frac{kQ}{r} + \frac{k\vec{p} \cdot \hat{r}}{r^2} + \frac{k\hat{r} \cdot \tilde{Q}_2 \cdot \hat{r}}{r^3} + O(1/r^4) \quad (16)$$

where the quadrupole matrix is given by,

$$\tilde{Q}_2 = \sum_i \frac{1}{2} q_i (3\vec{r}_i \otimes \vec{r}_i - r_i^2 \tilde{I}) \quad (17)$$

where \otimes is the outer product and \tilde{I} is a 3×3 identity matrix. It is tedious but straightforward to show that the quadrupole term defined in this way is the same as the more natural forms of Eq. (12,13).

In the continuum limit we have,

$$Q = \int \rho(\vec{r}') d\vec{r}'; \quad \vec{p} = \int \vec{r}' \rho(\vec{r}') d\vec{r}' \quad \tilde{Q}_2 = \frac{1}{2} \int (3\vec{r}' \otimes \vec{r}' - r'^2 \tilde{I}) \rho(\vec{r}') d\vec{r}' \quad (18)$$

In general the dipole and higher order terms depend on the choice of origin for the coordinate system. However if the monopole term is zero it is easy to show that the dipole term is independent of the co-ordinate system.