Jackson Chapter 4 Notes PhL 1.29.03

Chapter 4: The Scalar Multipole Expansion, and Dielectrics

It is a little odd that these two subjects are mixed in one chapter. It is true, however, that dielectric is really based on one of the multipole moments (dipole), so it is good for the reader to at least know what these moments are! Jackson treats the usual set of dielectric problems, but also delves into models for χ and for the microscopic χ which he calls γ. This latter is treated for both polar and non-polar substances. This is a very good and useful chapter.

4.1 The Multipole Expansion. Finally we are getting where we want to be. We already know from 3.61 what the most general form of a potential is in spherical coordinates. You can pick whatever coefficients you want here, and the result will formally satisfy the Laplace Equation. Notice in 3.61 that we have the two characteristic radial functions r^{ℓ} and $r^{-\ell-1}$.

Now, we imagine some ρ distribution that is all contained within some mathematical bounding sphere. Then we know that *outside* that sphere, we cannot have r^{ℓ} terms in the potential because they will diverge at ∞ , so we only have the $r^{-\ell-1}$ terms, so we write 4.1 as shown. This equation is THE MULTIPOLE EXPANSION of the (scalar) potential. That is, you are expanding it onto eigenfunctions of the Laplace equation in spherical coordinates. We know this is a complete expansion, nothing is left out, and it is just a question of finding the coefficients which are here called $q_{\ell m}$. No surprise, these are given in 4.3 and you see that you are just integrating your friendly $Y_{\ell m}$ with r^{ℓ} against ρ over the sphere that contains all the action. For $\ell = 0$ we get the charge. For $\ell=1$ we get the electric dipole as shown, although the p things appear as raising and lowering operator type things due to the way sphericals work. As for the $\ell=2$, the Q_{ij} are what you get from a certain cartesian Taylor expansion of ϕ shown in 4.10. To get this result, you first expand 1/R as (1/r) [1 - r•r'/r^2 + etc] where R = $|\mathbf{r} - \mathbf{r'}|$ and we treat r' as small and just do a regular Taylor series. Then insert this into $\phi = \int \rho/R \, dV$ and you have it.

So that is really all there is to it! The idea is then to think of the specific ℓ,m terms in the expansion by themselves, call these things $\phi_{\ell m}$. Each one implies its own electric field $\mathbf{E}_{\ell m}$ as in 4.11. For $\ell=1$ we get the usual dipole result shown in 4.13, not quoted yet in this text.

4.2. Multipole Expansion of Interaction Energy. The potential energy of a charge q in an external potential Φ is just $q\Phi$. This would be the work needed to bring in q from infinity to some location r. The work to bring in two charges would be $(q1 + q2)\Phi$. Note that this does not include the "self energy", the work needed to assemble q1 and q2 near each other without Φ present, which is certainly non-zero. I think then that $\int \rho\Phi \, dV$ is the energy of some charges just due to the external field, and if you wanted the total energy you would have to compute $\int \rho(\Phi+\phi) \, dV$ where ϕ was the potential just due to ρ with no external Φ. Jackson is thinking of this $\int \rho\Phi \, dV$ as the "interaction energy" between an existing ρ and some externally generated ϕ, a sort of interaction Hamiltonian or Lagrangian type thing. If this integral is broken into multipole terms, you get 4.17 which shows how each moment of ρ interacts with the Φ field. As the moments go up, the derivatives of ϕ go up. Thus, you could rule out a quadrupole interaction if you knew that your external E field had no gradient. Note that this is not the case in a plane wave in the z direction, but we really haven't done waves yet, so let's hold off on this idea.

Page 102 then gives a nuclear physics application. A nucleus has a quantum state and is expected to have a q_{20} moment. A nucleus in a crystal is expected to see a macroscopic ϕ which has first and second order gradients, so there is expected to be an interaction between the crystal field and the nuclear Q moment. In QM we know that this interaction will split the otherwise degenerate m levels, akin to the Zeeman effect for electrons as I dimly recall. So RF techniques can then be used to measure the Q moments in this way, given a knowledge of the local E field.

Jackson's last gasp in this section is to comment on the interaction between an external dipole field and an acted-upon dipole field, we get 4.19. I am not sure why we care about this but OK, maybe he will need it later for something. He might have said something about the dipoles of water molecules here, but he did not.

4.3 Dielectric Materials. This is certainly a change in topic within this chapter, but it is also something I want to know about, since I am thinking of floaters as dielectric spheres.

This discussion is VERY carefully constructed. We start with some microscopic Maxwell equations 4.20 where ε and ρ' are the detailed microfield and charge distributions, a total mess. We know that we have to get into average fields to work at a macroscopic scale. We are going to average the micro field and the micro ρ as shown in 4.22. The starting point is 4.23, standard E from ρ, a superposition of point charges if you like. We then do our multipole expansion of the ε field. This just means do an expansion of 1/R and put it in 4.23. We did this in 4.10, the cartesian Taylor expansion through quadrupole. Jackson leaves ∇ on 1/R, there is not reason to evaluate it right now. Here, he drops quadrupole and above, with the claim that since field variations are larger than atomic size (5000 A larger than 1 A), you won't be doing much quadrupole action. This claim is not supported very well, but it must be true, because you don't see anyone talking about some kind of Q polarization tensor on a footing with P as being important in a dielectric. So things are simplified a lot, we only have two terms as in 4.26. Here Jackson is summing over distinct charges e_j . He replaces those with a fake integration in 4.28 by using delta function ρ and π, where now π is a microscopic level sea of little dipoles as in 4.27, just as I would do this. The subscript "mol" is just to remind us that these are not the macroscopic ρ and P. Jackson likes to think of "molecules" instead of "atoms" which is fine. We now take 4.28 and apply the averaging operation over a volume as shown in 4.22. He treats the ρ term, and says the p term works exactly the same way. In 4.30 the averaging is applied and we move it to the right, where of course it just gives the "average charge" in the volume due to the delta. But then you can write this as the molecule density N times the average charge per molecule in 4.31, all just words, nothing tricky is happening here. The net result is that in 4.28 we get to replace ρ_{mol} with <N><e> as shown in 4.33. Similarly, we replace π_{mol} with <N><p>, so the average polarization in a volume is N times the average polarization per molecule. Then the big step is coming. After all, we want to know what $\nabla \bullet \varepsilon$ is going to be [don't confuse Jackson's choice of $\boldsymbol{\varepsilon}$ as microfield with ε as dielectric constant soon to come!] Applying ∇ gives us a ∇^2 in each term applied to 1/R and we know that gives delta -- THIS is why Jackson just left the ∇ operators sitting. The final result is the very simple 4.34. Jackson interprets the "extra" term on the right as an effective polarization charge density that is getting crunched around as in figure 4.2, affecting the E field divergence. But the next step is to rewrite as 4.35 and identify the pieces as I have marked. And so we end up with the final facts that P = Np and ρ he writes as Ne + ρ_{ext} . All throughout, this <e> thing has been present to account for the average charge, but normally this is going to be exactly 0, and then you only want to worry about the "external to atoms" charge, the free charge that can move around and that is $\rho_{ext.}$ So this I think is a very clear explanation of what P is, and what D is, and why there is no Q or higher term to worry about! I will be interested to see if we really ignore Q in Mie Scattering theory.

Finally, we get the traditional restatement of the two Maxwell equations for E, and the divergence one shows that D sees only the free charge, so that it will be D_{normal} that will see the free surface charge σ. So this is going to be the one big difference at a boundary!

A very good section.

4.4 Dielectric Boundary Conditions. Here the fact that $\mathbf{P} = \chi\mathbf{E}$ is quoted as an experimental fact that has very little error in most substances, ie, there is no tensor aspect to it, see graph of some evidence on this on page 109. The formal boundary conditions are as in 4.45. I remember being confused about this on a final exam in some simple problem they gave, ouch, it really is stupidly simple.

4.5 Dielectric boundary problems. Our first problem is the traditional point charge near a plane interface. Earlier we might have done this with a conductor, but Jackson skipped that traditional problem and went right to the sphere. Looking from the right, the solution is to have a point charge at the image point on the left with a special magic charge q'. Looking from the left, we see a single charge at the q location but with magic charge q". The boundary conditions are as in 4.48, and these are then used to find the sizes of q' and q". You have to differentiate the potentials on both sides in the right directions and apply your BC's. The answer is in 4.51, so the complete problem is solved. There is a σ_{pol} on the interface as in 4.53 that you compute with a pill box, knowing P1 and P2 on the two sides.

Our second problem is another traditional one that has a very simple answer. The dielectric sphere in the constant z direction E field. I might imagine that if this E-field were in a plane wave, it might somehow interact with the overall dipole appearance that the sphere has looking from the outside, as we shall soon see and cause some dipole radiation. To solve this problem, we assume appropriate expansions for ϕ on the two sides in our spherical coords, as in 4.54. We apply the dielectric BC's at the surface (well suited certainly to spherical coordinates!) and do some shuffle to conclude that only the A_1, B_1 and C_1 coefficients are non-zero. The final answer is in 4.60 and is very interesting. Inside, we have a perfectly parallel E field that is along the original field but reduced by $3/(\varepsilon+2)$. Outside, we have our original field plus the field of what appears to be a point-dipole located at sphere center. This dipole points along the original field and has the strength shown in 4.62. , so P is as in 4.63 inside the sphere. Finally, we compute the σ_{pol} .

The third problem is a spherical cavity in a dielectric. The trick here is to look at the second equation in 4.56 and move the ε to the other side, which is like doing $\varepsilon \to 1/\varepsilon$. The answer is then the same except the dipole direction is now reversed against the original field and has a different magnitude as shown in 4.66.

So I think I get the basic idea here and I think I can solve any problem of this type.

Here is a fourth problem we will need right away. Imagine a cavity in an infinite dielectric. What is the E field at the center of the hole? We know how P sits in the dielectric, and we know the σ_{pol} charge sits on the boundary, and the E field sees this charge as well as free charge. The charge is $P\cos\theta$ and the z component of the field it makes at the center makes another $\cos\theta$, so we get 4.68 where the r^2 factors of the dA and the field $1/r^2$ cancel and we get $1/3x^3$ at 1 and -1 which is 2/3, then 2π from azimuth and we get our answer $4\pi P/3$.

4.6. The Clausius-Mossotti Model for χ. Another excellent section. First, we ask: in a dielectric with uniform macroscopic (average) field E, what field does a particular molecule actually see? In section 4.3, we did not ask this question. There we just computed E as an average value of the micro E and computed the divergence of this average E. We did not ask the question that is asked here. The answer is quite

amazing I think. The answer is that a particular molecules *sees* $E' = E + (4\pi/3) P$, where E is the macroscopic field we always use. If from some other model you can compute that $p = \gamma E_i$ on the microscale for your molecules, then $P = Np = N\gamma E_i$ and you combine to get $P/N\gamma = E + (4\pi/3) P$, and you can then solve for $\chi = P/E$ and you get 4.74. The idea is that this relates the macroscopic χ parameter to the microscopic γ parameter. The result is Clausius-Mossotti and is OK for gases, roughly true for liquids and gases. I think for water the result is off by 50% or so. Comment that the static ε for water is 80, obviously not true at optical frequencies!

So, how do we arrive at the fact that a molecule sees $E' = E + (4\pi/3) P$? The E part is because we assume it is present from some source, so it is the extra correction term that is interesting. If you carve out a spherical cavity around your test molecule, the distance P bulk creates the $(4\pi/3) P$ field at the center. For this part, we are not surprised to find that this extra field is in the same direction as E since E is making it. This result is consistent with our solution of the cavity problem in the last section, where the field in a cavity is stronger than the field in the enclosing dielectric.

The real mystery is this: obviously you should now add the effect of a carved out sphere. Jackson shows that for a cubic lattice, the effect is exactly 0, just because you are in the midst of a symmetric environment. (We have already added the external field E, so don't want to add it here again) Well, you must ask, what happens if we take our little cavity to be huge, it will always give 0. Suppose our entire dielectric were a larger sphere. I guess the answer is that eventually you get some dielectric surface charge to deal with. Jackson then argues that this local contribution is roughly zero in any normal material.

4.7 Models for γ. We skipped this section in the course, I read it now.

First, we get a model for γ for non-polar objects (molecules) just from a toy electron model of a harmonic oscillator and we get $\gamma = e^2/m\omega_0^2$ where ω_0 is our resonant HO frequency which we would set to $h\upsilon$ = optical levels. For a mixture of molecule types, we get 4.78. Jackson argues that this effect can only make dielectric constants on the order of 1.00XX and he gives examples of air, helium, etc. That is, his examples are non-polar gases.

Jackson wonders whether thermal agitation affects this result. Intuition says no since the molecules ought to self-polarize regardless of jiggling around, the E field is not much different in non-relativistic action. Jackson proves this is in fact true using a stat mech trick that I unfortunately have forgotten but know at one time. You weight things with the Boltzmann factor in computing a thermal average. So the answer here really is it makes no difference.

The more significant situation is when you have fixed dipole moments as in water or CO gas. Here the Hamiltonian term is $-p \bullet E$ and when be Boltzmanize this one we get that $\gamma = p^2/(3kT)$. Obviously thermal fights the line up, and larger kT relative to $p \bullet E$ energy is going to cost you and reduce γ. Sadly, Jackson does not quote ε values for polar substances, but I think water at DC frequencies has $\varepsilon = 80$, so this completely swamps the non-polar effect.

So, a very clear and to the point section!

4.8 Electrostatic Energy in a Dielectric. I have only skimmed this section today, it is not of direct interest to me right now. The question is this: is 4.86 still true in terms of macroscopic quantities if you assemble charges in a dielectric environment? Jackson concludes that yes it is, provided the dielectric is "linear" so 4.91 is OK. The total energy density is $E \bullet D/8\pi$ as shown in 4.92. He concludes that the dielectric holds an extra energy density due to P shown in 4.97, and comments on the 1/2.

The next subject here is what happens when you "move in" a dielectric object into some fixed fields, or between some battery-fed electrodes held at constant potential. Since there are energy changes, we can expect forces on the dielectric object and these are discussed. Maybe you can levitate something in this way. That is, an E field with gradient ought to have a force on a neutral chunk of dielectric. We know this is true for a fixed dipole moment, etc etc. Have to keep it from rotating.

Nine problems, I did only 3 in the course it would appear.