Magnetization of Matter

Paramagnetism

The magnetism of matter arises due to the currents generated by electrons. These currents arise due to electron spin and due to the electronic orbits about the nucleus. In order to gain a quantitative understanding of magnetism quantum mechanics is required. However, a qualitative understanding can be obtained from some simple classical arguments. First we will consider paramagnetism. Electrons have a property called spin. This endows electrons with both angular momentum and a magnetic moment. You can think of an electron as a tiny sphere of charge spinning on its axis. As electrons fill up atomic orbitals, two are allowed in each shell, one with spin up and one with spin down. Let's consider what happens to the spin when a magnetic induction field is applied. Again it is useful to think of the forces on a small rectangular circuit. In a uniform field the net force is zero as we have shown previously. However, the net torque is not zero. Consider the moments about the center of our previously defined loop.

$$\begin{aligned}\mathbf{T} &= I\left\{\int_0^a \left(x\mathbf{e}_x\right)\times\left(\mathbf{e}_x\times\mathbf{B}\right)dx + \int_0^b \left(a\mathbf{e}_x + y\mathbf{e}_y\right)\times\left(\mathbf{e}_y\times\mathbf{B}\right)dy \right.\\ &\qquad \left. + \int_a^0 \left(x\mathbf{e}_x + b\mathbf{e}_y\right)\times\left(-\mathbf{e}_x\times\mathbf{B}\right)\left(-dx\right) + \int_b^0 \left(y\mathbf{e}_y\right)\times\left(-\mathbf{e}_y\times\mathbf{B}\right)\left(-dy\right)\right\}\\ &= I\left(abB_x\mathbf{e}_y - abB_y\mathbf{e}_x\right)\\ &= m_z B_x\mathbf{e}_y - m_z B_y\mathbf{e}_x\\ &= \mathbf{m}\times\mathbf{B}\end{aligned}$$

What this tells us is that $\mathbf{B}$ tends to rotate the magnetic moment towards the direction it is applied. In general the electron spins are randomly oriented and frustrated by thermal fluctuations. When a field is applied it tends to rotate these spins towards the same direction. However, quantum mechanics dictates that the spins in a given orbital must come in equal but opposite pairs, so only atoms with an odd number of electrons exhibit this behavior.

Diamagnetism

A second source of magnetism is due to the orbits of the electrons about the nucleus. These orbits will also tend to be rotated toward a plane perpendicular to $\mathbf{B}$, but this turns out to be a relatively small effect. Diamagnetism results from the change of orbital angular momentum due to $\mathbf{B}$. To analyze this consider a circular orbit with a $\mathbf{B}$ field applied perpendicular to the plane of the orbit. The additional force on the electron due to the $\mathbf{B}$ field is,

$$\mathbf{F} = -ev\,\mathbf{e}_\theta\times B\mathbf{e}_z = -evB\mathbf{e}_r$$

So, this electron has a force pulling it in towards the center of its orbit, which causes the electron to speed up (or the radius of the orbit to decrease). Prior to the application of the field the magnetic moment due to the orbit of the electron is in the $-\mathbf{e}_z$ direction. If the electron speeds up then the magnitude of this moment increases. On the other hand, if the orbit of the electron is in the $-\mathbf{e}_\theta$ direction then the centripetal force is in the positive $\mathbf{e}_r$ direction and the electron will slow down. This electron has a positive $\mathbf{e}_z$ magnetic moment which decreases under the application of the z-directed $\mathbf{B}$ field. So in either case, the change in the magnetic moment of the electron orbit is in the opposite direction to the applied field. Hence the magnetization decreases with applied field. This is called diamagnetism and occurs primarily in atoms with an even number of electrons or a large number of core electrons. You will likely notice that this simple model has several flaws, however it is really not worth trying to add details because quantum mechanics is required to properly describe this effect. What you should take from this model is a feel for where diamagnetism comes from and that diamagnetic materials have an induced magnetization opposite to the $\mathbf{B}$ field.

Ferromagnetism

From the qualitative descriptions above you might think that the strength of these magnetic effects is similar to the electrical effects in dielectrics. However, diamagnetic and paramagnetic effects are very, very small. The adjustment to the permeability of free space is on the order of 10^{-5}. Not an increase by a factor of 10 to 1000, but rather by a fraction of a percent. There are other materials, which are usually called magnetic materials, like iron, nickel, cobalt, rare earth oxides, etc. where the dipoles of the unpaired electrons in neighboring atoms tend to align with one another such that regions of material all have a strongly aligned spontaneous magnetization. This effect can be very strong in comparison to para- and dia-magnetism. The reason why every piece of iron is not a strong magnet is due to the domain structure that occurs in the material, where each domain has a single spontaneous magnetization direction but the effect over many domains averages out to zero. We will look at the energetics of domain structures in greater detail at a later time. Also, para-, dia-, and ferro-magnetism do not constitute an exhaustive list of magnetic states of matter, but we will stop with these for now, and you are encouraged to do your own research on this topic.

Fields due to a Magnetized Volume of Material

As with the electrical polarization of matter, we will first determine the magnetic fields produced by a distribution of magnetic dipoles. First, we define the magnetic dipole of a magnetized volume of matter as,

$$\mathbf{m} = \int_V \mathbf{M}\, dV$$

The magnetization $\mathbf{M}$ is simply the magnetic dipole moment per unit volume of the material. The vector potential for some distribution of $\mathbf{M}$ is then,

$$\mathbf{A} = \frac{\mu_0}{4\pi}\int_V \frac{\mathbf{M}(\mathbf{x}')\times(\mathbf{x}-\mathbf{x}')}{|\,\mathbf{x}-\mathbf{x}'\,|^3}\,dV'$$

Taking care to note that the $\mathbf{M}$ within the integrand is a function of the primed coordinates, manipulating this equation with index notation leads to,

$$\begin{aligned}
A_i &= \frac{\mu_0}{4\pi}\int_V \frac{\epsilon_{ijk}M_j(x_k-x_k')}{[(x_p-x_p')(x_p-x_p')]^{3/2}}\,dV' \\
&= \frac{\mu_0}{4\pi}\int_V \epsilon_{ijk}M_j\frac{\partial}{\partial x_k'}\left[\frac{1}{\sqrt{(x_p-x_p')(x_p-x_p')}}\right]dV' \\
&= \frac{\mu_0}{4\pi}\int_V \frac{\partial}{\partial x_k'}\left[\frac{\epsilon_{ijk}M_j}{\sqrt{(x_p-x_p')(x_p-x_p')}}\right] - \frac{\epsilon_{ijk}M_{j,k}}{\sqrt{(x_p-x_p')(x_p-x_p')}}\,dV' \\
&= \frac{\mu_0}{4\pi}\int_S \frac{\epsilon_{ijk}M_j n_k}{\sqrt{(x_p-x_p')(x_p-x_p')}}\,dS' - \frac{\mu_0}{4\pi}\int_V \frac{\epsilon_{ijk}M_{j,k}}{\sqrt{(x_p-x_p')(x_p-x_p')}}\,dV'
\end{aligned}$$

This can be cast once again in vector notation as,

$$\mathbf{A} = \frac{\mu_0}{4\pi}\int_S \frac{\mathbf{M}\times\mathbf{n}}{|\,\mathbf{x}-\mathbf{x}'\,|}\,dS' + \frac{\mu_0}{4\pi}\int_V \frac{\nabla'\times\mathbf{M}}{|\,\mathbf{x}-\mathbf{x}'\,|}\,dV'$$

This can be interpreted as the vector potential due to some distribution of bound surface current density $\mathbf{K}_b = \mathbf{M}\times\mathbf{n}$ and some distribution of bound volume current density $\mathbf{J}_b = \nabla\times\mathbf{M}$.

These definitions of bound current densities can be used to simplify the magnetostatic equations in matter.

$$\begin{aligned}
\nabla\times\mathbf{B} &= \mu_0\mathbf{J} \\
&= \mu_0(\mathbf{J}_f + \mathbf{J}_b) \\
&= \mu_0(\mathbf{J}_f + \nabla\times\mathbf{M})
\end{aligned}$$

This leads to

$$\nabla\times(\mathbf{B}/\mu_0 - \mathbf{M}) = \mathbf{J}_f$$

Just as for electrostatics when we recognized that it was the free charges that were under our control, so it goes for magnetostatics where it is the free currents that we can specify. It now becomes useful to redefine the quantity in parentheses as $\mathbf{H} \equiv \mathbf{B}/\mu_0 - \mathbf{M}$. The field $\mathbf{H}$ happens to be called the magnetic field by almost all engineers and even many physicists. To be honest I find this to be a rather poor choice of name. I would call the $\mathbf{B}$ field the magnetic field and the $\mathbf{H}$ field perhaps the magnetic displacement. However, I am not going to try to rewrite history, so we will refer to $\mathbf{H}$ as the magnetic field and $\mathbf{B}$ as the magnetic induction. So, our magnetostatic equations become,

$$\nabla \cdot \mathbf{B} = 0 \quad \text{and} \quad \nabla \times \mathbf{H} = \mathbf{J}_f \ \text{in} \ V \ \text{and} \quad \mathbf{H} \times \mathbf{n} = \mathbf{K}_f \ \text{on} \ S$$

Finally, we would like to know what the increment of work done is for an incremental change in the magnetization. Here we must take care because magnetic fields do not do work. However, in magnetostatics we are interested in the work done to magnetize an object and we would like to relate this to the magnetic fields. Again, we are interested in the work done by an external source (battery) to maintain the free currents. The power expended in the volume is $\mathbf{E} \cdot \mathbf{J}$, and on the surface it is $\mathbf{E} \cdot \mathbf{K}$. Then the *work done by the external source to maintain the currents* is the opposite of these quantities. Recall that the work that we do to put a charge in place is ϕdQ, and the work done by the field that supplies the reaction force is the opposite of this. We will also need Maxwell's equation $\nabla \times \mathbf{E} = -\dfrac{\partial \mathbf{B}}{\partial t}$.

$$\begin{aligned}
\dot{W} &= -\int_V E_i J_i \, dV - \int_S E_i K_i \, dS \\
&= -\int_V E_i \epsilon_{ipq} H_{q,p} \, dV - \int_S E_i \epsilon_{ipq} H_p n_q \, dS \\
&= -\int_V \epsilon_{ipq} \left(E_i H_q \right)_{,p} - \epsilon_{ipq} E_{i,p} H_q \, dV - \int_S E_i \epsilon_{ipq} H_p n_q \, dS \\
&= -\int_V \epsilon_{qpi} E_{i,p} \, \delta H_q \, dV - \int_S \epsilon_{ipq} n_p E_i H_q \, dS - \int_S E_i \epsilon_{ipq} H_p n_q \, dS \\
&= \int_V \dot{B}_q H_q \, dV + \int_S \epsilon_{ipq} n_q E_i H_p \, dS - \int_S E_i \epsilon_{ipq} H_p n_q \, dS \\
&= \int_V H_i \dot{B}_i \, dV \\
&= \int_V \mathbf{H} \cdot \dot{\mathbf{B}} \, dV \\
&= \int_V H_i \epsilon_{ijk} \dot{A}_{k,j} \, dV = \int_V \epsilon_{ijk} (H_i \dot{A}_k)_{,j} - \epsilon_{ijk} H_{i,j} \dot{A}_k \, dV \\
&= -\int_V \epsilon_{ijk} H_{i,j} \dot{A}_k \, dV + \int_S \epsilon_{ijk} H_i n_j \dot{A}_k \, dS \\
&= \int_V J_k \dot{A}_k \, dV + \int_S K_k \dot{A}_k \, dS \\
&= \int_V \mathbf{J} \cdot \dot{\mathbf{A}} \, dV + \int_S \mathbf{K} \cdot \dot{\mathbf{A}} \, dS
\end{aligned}$$

In summary, our most significant results for the magnetostatic relationships in matter are,

$\nabla \cdot \mathbf{B} = 0 \quad \Rightarrow \quad \mathbf{B} = \nabla \times \mathbf{A}$	$B_{i,i} = 0 \quad \Rightarrow \quad B_i = \epsilon_{ijk} A_{k,j}$
$\nabla \times \mathbf{M} = \mathbf{J}_b$	$\epsilon_{ijk} M_{k,j} = J^b_i$
$\mathbf{M} \times \mathbf{n} = \mathbf{K}_b$	$\epsilon_{ijk} M_j n_k = K^b_i$
$\mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{M})$	$B_i = \mu_0 (H_i + M_i)$
$\nabla \times \mathbf{H} = \mathbf{J}_f$	$\epsilon_{ijk} H_{k,j} = J^f_i$
$\mathbf{H} \times \mathbf{n} = \mathbf{K}_f$	$\epsilon_{ijk} H_j n_k = K^f_i$
$\delta W = \int_V \mathbf{H} \cdot \delta \mathbf{B} \, dV$	$\delta W = \int_V H_i \, \delta B_i \, dV$

As was the case in electrostatics , we still need an additional relationship between **B**, **M** and **H** in order to close the loop on our equations. This is of course a material constitutive relationship and in general must be cast in incremental form for irreversible behavior. Diamagnetism and paramagnetism yield a linear relationship between our field quantities through the *magnetic susceptibility* χ_m .

$$\mathbf{M} = \chi_m \mathbf{H}$$

Then the relationship between **B** and **H** is,

$$\begin{aligned} \mathbf{B} &= \mu_0 (\mathbf{H} + \mathbf{M}) \\ &= \mu_0 (\mathbf{H} + \chi_m \mathbf{H}) \\ &= \underbrace{\mu_0 (1 + \chi_m)}_{\mu} \mathbf{H} \end{aligned}$$

The material property μ is referred to as the *magnetic permeability* of the material. Note that for diamagnetic materials $\chi_m < 0$ and for paramagnetic materials $\chi_m > 0$. Thermodynamic restrictions would require that a *stable* material has $\mu > 0$.

In many circumstances we might be interested in situations where the free current density in the volume is zero. In such cases we have that the curl of the magnetic field **H** is zero. Then we can introduce a scalar magnetic potential φ such that $\mathbf{H} = -\nabla \varphi$. For a linear material our governing equations then become,

$$
\begin{aligned}
B_{i,i} &= 0 \\
(\mu H_i)_{,i} &= 0 \\
-\mu\varphi_{,ii} &= 0 \\
\nabla^2\varphi &= 0
\end{aligned}
$$

So, we are left once again with solving Laplace's equation in the volume. The useful boundary conditions come from the jump conditions at an interface,

$$(\mathbf{H}^- - \mathbf{H}^+)\times\mathbf{n} = \mathbf{K}_f \quad \text{and} \quad (\mathbf{B}^- - \mathbf{B}^+)\cdot\mathbf{n} = 0$$

where the unit normal to the interface points from the "–" side towards the "+" side.

Let's look at an example of the fields around a magnetized object. Specifically, let's look at the problem of a sphere with a uniform spontaneous magnetization M_s embedded in a non-magnetic matrix. Since the magnetic permeability of most non-magnetic materials is very close to μ_0, we will simply make the approximation that it is equal to μ_0. Then, to determine the fields we can simply evaluate the vector potential using the integral representation,

$$\mathbf{A} = \frac{\mu_0}{4\pi}\int_S \frac{\mathbf{M}\times\mathbf{n}}{|\,\mathbf{x}-\mathbf{x}'\,|}\,dS' + \frac{\mu_0}{4\pi}\int_V \frac{\nabla'\times\mathbf{M}}{|\,\mathbf{x}-\mathbf{x}'\,|}\,dV'$$

Since the magnetization is uniform we have $\nabla\times\mathbf{M} = 0$ and the volume integral vanishes. Obviously we will be implementing spherical coordinates to evaluate the surface integral, and at first glance one might think that we should choose the z-axis to be aligned with the magnetization direction. This is one possibility, but it makes the evaluation of the integral more difficult. A more convenient choice is to take the point where we are evaluating the vector potential to be located at $\mathbf{x} = z\,\mathbf{k}$. If we can determine the potential at this point for an arbitrary orientation of the magnetization then we can ultimately make the transformation to determine the potential at any point in space for a fixed magnetization direction. We can take the magnetization direction to be in the x-z plane and be at an angle ψ to the z-axis. This implies that,

$$\mathbf{M} = M_s(\sin\psi\,\mathbf{i} + \cos\psi\,\mathbf{k})$$

$$\mathbf{n} = \sin\theta'\cos\phi'\,\mathbf{i} + \sin\theta'\sin\phi'\,\mathbf{j} + \cos\theta'\,\mathbf{k}$$

$$\mathbf{M}\times\mathbf{n} = M_s[-\cos\psi\sin\theta\sin\phi\,\mathbf{i} + (\cos\psi\sin\theta\cos\phi - \sin\psi\cos\theta)\,\mathbf{j} + \sin\psi\sin\theta\sin\phi\,\mathbf{k}]$$

Finally, we also need to determine $|\,\mathbf{x}-\mathbf{x}'\,|$. Here it should become clear why we have chosen our coordinate system in a somewhat strange manner. The point $\mathbf{x}'$ lies on the sphere, and so $|\,\mathbf{x}-\mathbf{x}'\,|=\sqrt{z^2+a^2-2za\cos\theta'}$. Finally, $dS'=a^2\sin\theta'\,d\theta'\,d\phi'$ and we need to integrate over $\theta'=0,\pi$ and $\phi'=0,2\pi$. Note that ϕ' does not appear in the denominator and so when we integrate any terms with a factor of $\sin\phi'$ or $\cos\phi'$ over the range of $\phi'=0,2\pi$ we get zero. As such only one term remains.

$$\mathbf{A}=\frac{\mu_0}{2}\int_0^{\pi}\frac{-M_s\sin\psi\cos\theta'\,\mathbf{j}}{\sqrt{z^2+a^2-2za\cos\theta'}}a^2\sin\theta'\,d\theta'$$

Using the change of variables $u=-\cos\theta'\rightarrow du=\sin\theta' d\theta'$, the integral becomes,

$$\mathbf{A}=\frac{\mu_0 a^2 M_s\sin\psi\,\mathbf{j}}{2}\int_{-1}^{1}\frac{u}{\sqrt{z^2+a^2+2zau}}\,du$$

This integral can be found in tables and has the solution,

$$\begin{aligned}\mathbf{A}&=\frac{\mu_0 a^2 M_s\sin\psi\,\mathbf{j}}{2}\left[\frac{-z^2-a^2+azu}{3z^2a^2}\sqrt{z^2+a^2+2zau}\right]_{-1}^{1}\\&=-\frac{\mu_0 M_s\sin\psi\,\mathbf{j}}{6z^2}\Big[\Big(z^2+a^2-az\Big)\Big(z+a\Big)-\Big(z^2+a^2+az\Big)\Big|z-a\Big|\Big]\end{aligned}$$

There are two cases to consider corresponding to whether z is inside or outside the sphere. This leads to

$$\mathbf{A}=\begin{cases}-\dfrac{\mu_0 a^3 M_s\sin\psi\,\mathbf{j}}{3z^2} & \text{for } z>a\\[2ex] -\dfrac{\mu_0 M_s\sin\psi\,z\,\mathbf{j}}{3} & \text{for } z<a\end{cases}$$

Next we want to generalize this result, so we must recognize that $z=|\,\mathbf{x}\,|$ and $-M_s\sin\psi\,z\,\mathbf{j}=\mathbf{M}\times\mathbf{x}$, so our final results are,

$$\mathbf{A}=\begin{cases}\dfrac{\mu_0 a^3\,\mathbf{M}\times\mathbf{x}}{3\,|\,\mathbf{x}\,|^3} & \text{for } z>a\\[2ex] \dfrac{\mu_0\,\mathbf{M}\times\mathbf{x}}{3} & \text{for } z<a\end{cases}$$

Notice that the dipole due to the magnetized sphere is $\mathbf{m}=\frac{4}{3}\pi a^3\mathbf{M}$, so the vector potential outside of the sphere is exactly that of a concentrated dipole at the origin.

Inside the sphere the **B** field will be uniform. This is an interesting result, and the general feature of uniform fields within the inclusion actually holds for general (but homogeneous) anisotropy in both of the phases and a general ellipsoidal shape for the inclusion.

Mechanics and Thermodynamics

In this section we will couple together our studies of electrostatics and magnetostatics with mechanics. In general this should be done in a finite deformation setting, but in order to simplify the concepts we will first do this assuming infinitesimal deformations. A supplemental note will be supplied for the corresponding finite deformation derivations. First we will review the equations of mechanics.

Small Deformation Kinematics

Given some displacement field in the material we would like to determine the strain of an oriented line element in the vicinity of a point. In some reference configuration the point has coordinates (x_1, x_2, x_3) and the endpoint of the line element under consideration has coordinates $(x_1 + dx_1, x_2 + dx_2, x_3 + dx_3)$. Hence, the original length of this line element is simply $L_0 = \sqrt{dx_i dx_i}$ and the orientation of the line element can be represented by the unit vector $n_i = dx_i / L_0$. The material is now deformed such that there is the displacement field $u_i(\mathbf{x})$. Therefore, the new locations of the endpoints of our line element become $(x_1 + u_1(\mathbf{x}), x_2 + u_2(\mathbf{x}), x_3 + u_3(\mathbf{x}))$ and $(x_1 + dx_1 + u_1(\mathbf{x} + d\mathbf{x}), x_2 + dx_2 + u_2(\mathbf{x} + d\mathbf{x}), x_3 + dx_3 + u_3(\mathbf{x} + d\mathbf{x}))$. Since we will be considering a line element of differential length, we can expand the displacement components in a Taylor series,

$$x_i + dx_i + u_i(\mathbf{x} + d\mathbf{x}) = x_i + dx_i + u_i + \frac{\partial u_i}{\partial x_j} dx_j + O(dx_i dx_j)$$

Then, the new length of the line element is,

$$\begin{aligned} L &= \sqrt{\left[dx_i + \frac{\partial u_i}{\partial x_j} dx_j + O(dx_i dx_j)\right]\left[dx_i + \frac{\partial u_i}{\partial x_k} dx_k + O(dx_k dx_l)\right]} \\ &= \sqrt{dx_i dx_i + 2\frac{\partial u_i}{\partial x_j} dx_i dx_j + \frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_k} dx_j dx_k + O(dx_i dx_j dx_k)} \\ &= L_0\sqrt{1 + 2\frac{\partial u_i}{\partial x_j} n_i n_j + \frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_k} n_j n_k + O(dx_i)} \end{aligned}$$

Next, we will assume that all terms of the displacement gradient are small in comparison to 1. This assumption implies that both the strains and the rotations in the vicinity of the point must be small.

$$\frac{\partial u_i}{\partial x_j} \ll 1 \rightarrow L \approx L_0 \sqrt{1 + 2\frac{\partial u_i}{\partial x_j} n_i n_j + O(dx_i)}$$

We now define the strain of the line element as, $\varepsilon = L / L_0 - 1$. Letting the length of our line element go to zero, and using the Taylor series expansion in the small displacement gradient limit yields,

$$\varepsilon \approx \sqrt{1 + 2\frac{\partial u_i}{\partial x_j} n_i n_j} - 1 \approx \left(1 + \frac{\partial u_i}{\partial x_j} n_i n_j\right) - 1 = \frac{\partial u_i}{\partial x_j} n_i n_j$$

Finally, we recognize that the displacement gradient contains both strain and rotation, and the rotation will not affect the strain of our line element.

$$\begin{aligned}
\varepsilon &= \frac{\partial u_i}{\partial x_j} n_i n_j \\
&= \underbrace{\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)}_{\varepsilon_{ij}} n_i n_j + \underbrace{\underbrace{\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right)}_{\Omega_{ij}} n_i n_j}_{0} \\
&= \varepsilon_{ij} n_i n_j
\end{aligned}$$

Here we have defined ε_{ij} as the small-strain or linear kinematics strain tensor, and Ω_{ij} as the small-rotation or linear kinematics rotation tensor. As you can see, the strain tensor can be used to give us the strain of a line element of any orientation in the vicinity of some point if we know the displacement field.

Kinetics

Next we will consider the conservation of linear and angular momentum. We will assume that the material is loaded by body forces **b** per unit volume and surface forces/tractions **t** per unit area. Conservation of linear momentum then states that the rate of change of the linear momentum is equal to the net force on the body.

$$\int_V b_i \, dV + \int_S t_i \, dS = \tfrac{d}{dt} \int_V \rho v_i \, dV$$

We assume the existence of the Cauchy stress tensor such that at the surface we have,

$$\sigma_{ji} n_j = t_i \quad \text{on } S$$

Using this relation and applying the divergence theorem to the second term yields,

$$\int_V \sigma_{ji,j} + b_i \, dV = \int_V \rho \frac{dv_i}{dt} dV$$

This equation must hold for any arbitrary volume of material. As such the point-wise linear momentum balance becomes,

$$\sigma_{ji,j} + b_i = \rho \frac{dv_i}{dt}$$

Taking moments about the fixed origin, the angular momentum balance can be manipulated as,

$$\int_V \epsilon_{ijk} x_j b_k \, dV + \int_S \epsilon_{ijk} x_j t_k \, dS = \tfrac{d}{dt} \int_V \rho \epsilon_{ijk} x_j v_k \, dV$$

$$\int_V \epsilon_{ijk} x_j b_k \, dV + \int_S \epsilon_{ijk} x_j \sigma_{lk} n_l \, dS = \int_V \rho \epsilon_{ijk} \frac{dx_j}{dt} v_k + \rho \epsilon_{ijk} x_j \frac{dv_k}{dt} dV$$

$$\int_V \epsilon_{ijk} x_j b_k \, dV + \int_V \epsilon_{ijk} x_j \sigma_{lk,l} + \epsilon_{ijk} x_{j,l} \sigma_{lk} \, dV = \int_V \rho \underbrace{\epsilon_{ijk} v_j v_k}_{0} + \rho \epsilon_{ijk} x_j \frac{dv_k}{dt} dV$$

$$\int_V \epsilon_{ijk} x_j \underbrace{\left(\sigma_{lk,l} + b_k - \rho \frac{dv_k}{dt} \right)}_{0} dV + \int_V \epsilon_{ijk} \delta_{jl} \sigma_{lk} \, dV = 0$$

$$\int_V \epsilon_{ijk} \sigma_{jk} \, dV = 0$$

Point-wise this last equation becomes,

$$\epsilon_{ijk} \sigma_{jk} = 0 \rightarrow \sigma_{ji} = \sigma_{ij}$$

Then, collecting our basic mechanics relationships we have,

$$\sigma_{ji,j} + b_i = \rho \frac{dv_i}{dt} \quad \text{and} \quad \sigma_{ji} = \sigma_{ij} \quad \text{in } V$$

$$\sigma_{ji} n_j = t_i \quad \text{on } S$$

$$\varepsilon_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}) \text{ in } V$$

Thermodynamics

At this point we have in hand a set of fundamental balance laws governing electrostatic, magnetostatic, and mechanical fields. These equations are applicable to any material (under the appropriate assumptions allowing for the approximations that have been made). However, this set of equations cannot be solved at this point because it is not complete. In order to close the loop on these equations we need the material constitutive relationships. These relationships must be required to satisfy the first and second laws of thermodynamics.

The first law of thermodynamics states that energy is conserved. Specifically, the amount of work and heat put into a system is balanced by that system's change in kinetic and internal energy. In integral form this can be stated as

$$\tfrac{d}{dt}\int_V \tfrac{1}{2}\rho v_i v_i \, dV + \tfrac{d}{dt}\int_V \tilde{u}\, dV = \int_V b_i v_i + \phi\dot{q} + J_i\dot{A}_i + r\, dV + \int_S t_i v_i + \phi\dot{\omega} + K_i\dot{A}_i - \tilde{q}_i n_i \, dS$$

Here, $\tilde{u}$ is the internal energy of the material and the right hand side of this equation represents the external work done by mechanical, electrical and magnetic sources. Under the assumptions of small strains and rotations where we can neglect the rates of changes of the volume elements, surface elements and surface normals, this equation is manipulated as follows.

$$\tfrac{d}{dt}\int_V \tfrac{1}{2}\rho v_i v_i \, dV + \tfrac{d}{dt}\int_V \tilde{u}\, dV = \int_V b_i v_i + \phi\dot{q} + J_i\dot{A}_i + r\, dV + \int_S t_i v_i + \phi\dot{\omega} + K_i\dot{A}_i - \tilde{q}_i n_i \, dS$$

$$\int_V \rho v_i \dot{v}_i \, dV + \int_V \frac{d\tilde{u}}{dt} dV = \int_V b_i v_i + \phi\dot{q} + J_i\dot{A}_i + r\, dV + \int_S \sigma_{ji} n_j v_i - \phi\dot{D}_i n_i + \epsilon_{ijk} H_j n_k \dot{A}_i - \tilde{q}_i n_i \, dS$$

$$\int_V \rho v_i \dot{v}_i \, dV + \int_V \frac{d\tilde{u}}{dt} dV = \int_V b_i v_i + \phi\dot{q} + J_i\dot{A}_i + r\, dV + \int_V \sigma_{ji,j} v_i + \underbrace{\sigma_{ji} v_{i,j}}_{\sigma_{ji}\dot{\varepsilon}_{ij}} - \phi\dot{D}_{i,i} - \underbrace{\phi_{,i}}_{-E_i}\dot{D}_i + \epsilon_{ijk}\dot{A}_i\dot{H}_{j,k} + \underbrace{\epsilon_{ijk}\dot{A}_{i,k}}_{\dot{B}_j} H_j - \tilde{q}_{i,i}\, dV$$

$$\int_V \frac{d\tilde{u}}{dt} dV = \int_V \underbrace{\left(\sigma_{ji,j} + b_i - \rho\dot{v}_i\right)}_{0} v_i + \phi\underbrace{\left(-\dot{D}_{i,i} + \dot{q}\right)}_{0} + \underbrace{\left(J_i - \epsilon_{ijk}H_{k,j}\right)}_{0}\dot{A}_i \, dV + \int_V \sigma_{ji}\dot{\varepsilon}_{ij} + E_i\dot{D}_i + H_i\dot{B}_i + r - \tilde{q}_{i,i}\, dV$$

$$\rightarrow \frac{d\tilde{u}}{dt} = \sigma_{ji}\dot{\varepsilon}_{ij} + E_i\dot{D}_i + H_i\dot{B}_i + r - \tilde{q}_{i,i}$$

This last line is the point-wise form of the energy balance equation. Note that we have defined r as the heat (energy) input per unit volume per unit of time, and $\tilde{q}_i$ are the components of the heat flux vector with dimensions of heat (energy) flow per unit area per unit of time.

We must also satisfy the second law of thermodynamics which states that the internal entropy of a system must at least increase in the same amount as the entropy input to the system. The entropy input is defined as the heat input divided by the absolute temperature θ. This entropy (im)balance statement is written and manipulated as,

$$\frac{d}{dt}\int_V s\,dV \geq \int_V \frac{r}{\theta}dV - \int_S \frac{\tilde{q}_i n_i}{\theta}dS$$
$$\int_V \dot{s}\,dV \geq \int_V \frac{r}{\theta}dV - \int_V \frac{\tilde{q}_{i,i}}{\theta} - \frac{\tilde{q}_i\theta_{,i}}{\theta^2}dV$$
$$\rightarrow \quad \theta\dot{s} \geq r - \tilde{q}_{i,i} + \frac{1}{\theta}\tilde{q}_i\theta_{,i}$$

This point-wise entropy inequality can now be further manipulated,

$$\theta\dot{s} \geq r - \tilde{q}_{i,i} + \frac{1}{\theta}\tilde{q}_i\theta_{,i}$$
$$\theta\dot{s} \geq \frac{d\tilde{u}}{dt} - \sigma_{ji}\dot{\varepsilon}_{ij} - E_i\dot{D}_i - H_i\dot{B}_i + \frac{1}{\theta}\tilde{q}_i\theta_{,i}$$
$$\frac{d\tilde{u}}{dt} \leq \sigma_{ji}\dot{\varepsilon}_{ij} + E_i\dot{D}_i + H_i\dot{B}_i + \theta\dot{s} - \frac{1}{\theta}\tilde{q}_i\theta_{,i}$$

Next, we define the Helmholtz free energy as, $\psi = \tilde{u} - \theta s$, which leads to,

$$\frac{d\psi}{dt} \leq \sigma_{ji}\dot{\varepsilon}_{ij} + E_i\dot{D}_i + H_i\dot{B}_i - s\dot{\theta} - \frac{1}{\theta}\tilde{q}_i\theta_{,i}$$

To analyze this inequality we must describe the free energy by postulating what ψ is dependent upon. Note that the *principle of equi-presence* states that if we allow one quantity to depend upon a given independent variable then all other quantities must also be allowed to depend upon this variable as well. The second law inequality suggest some minimum set of independent variables, specifically $(\varepsilon_{ij}, D_i, B_i, \theta, \theta_{,j}, ...)$. Then the other dependent quantities in our equation ψ, σ_{ij}, E_i, H_i, s, and $\tilde{q}_i$ must be allowed to depend on *all* of these dependent variables, including those not listed explicitly. The second law inequality now becomes,

$$\frac{\partial\psi}{\partial\varepsilon_{ij}}\dot{\varepsilon}_{ij} + \frac{\partial\psi}{\partial D_i}\dot{D}_i + \frac{\partial\psi}{\partial B_i}\dot{B}_i + \frac{\partial\psi}{\partial\theta}\dot{\theta} + \frac{\partial\psi}{\partial\theta_{,i}}\dot{\theta}_{,i} + \frac{\partial\psi}{\partial(\cdot)}\frac{d(\cdot)}{dt} \leq \sigma_{ji}\dot{\varepsilon}_{ij} + E_i\dot{D}_i + H_i\dot{B}_i - s\dot{\theta} - \frac{1}{\theta}\tilde{q}_i\theta_{,i}$$

Grouping terms,

$$\left(\frac{\partial\psi}{\partial\varepsilon_{ij}} - \sigma_{ji}\right)\dot{\varepsilon}_{ij} + \left(\frac{\partial\psi}{\partial D_i} - E_i\right)\dot{D}_i + \left(\frac{\partial\psi}{\partial B_i} - H_i\right)\dot{B}_i + \left(\frac{\partial\psi}{\partial\theta} + s\right)\dot{\theta} + \frac{\partial\psi}{\partial\theta_{,i}}\dot{\theta}_{,i} + \frac{1}{\theta}\tilde{q}_i\theta_{,i} + \frac{\partial\psi}{\partial(\cdot)}\frac{d(\cdot)}{dt} \leq 0$$

To analyze this inequality we take an approach proposed by Coleman and Noll in 1963. They postulated that this inequality must be valid for every *admissible process* that may occur in the material. An admissible process is any process that we can impose on the material through the associated control of the external sources available to us. Up to this point those sources include the mechanical body force $\mathbf{b}$, the electrical free charge density q, the free body currents $\mathbf{J}$, and the heat source r. We are allowed to manipulated these sources in space and time to create any spatial and temporal dependence of the associated independent variables, $\mathbf{b} \to \varepsilon_{ij}$, $q \to D_i$, $\mathbf{J} \to B_i$, and $r \to \theta$. In this sense we can think of any independent variable, its spatial gradients, and its rates of change, as arbitrary so long as it has an associated source capable of controlling it.

Now we proceed to the mathematical analysis of the second law inequality. Fist note that the second law inequality applies to any material and as such will admit a wide range of responses. Hence, any physical arguments to further constrain the types of material behaviors you are interested in are always welcomed and useful. For the materials we are interested in we will assume that there are several zero stress, electric field, magnetic field, and temperature change states that differ in their configuration due to differences in some set of internal variable, e.g. plastic strain, remanent polarization, spontaneous magnetization, etc. Therefore, let's consider the case where the $(\cdot)$ are some set of internal variables c, their rates of change $\dot{c}$, and their gradients $c_{,i}$. The inequality then becomes,

$$\left(\frac{\partial\psi}{\partial\varepsilon_{ij}} - \sigma_{ji}\right)\dot{\varepsilon}_{ij} + \left(\frac{\partial\psi}{\partial D_i} - E_i\right)\dot{D}_i + \left(\frac{\partial\psi}{\partial B_i} - H_i\right)\dot{B}_i + \left(\frac{\partial\psi}{\partial\theta} + s\right)\dot{\theta} + \frac{\partial\psi}{\partial\theta_{,i}}\dot{\theta}_{,i} + \frac{1}{\theta}\tilde{q}_i\theta_{,i}$$
$$+ \frac{\partial\psi}{\partial c}\dot{c} + \frac{\partial\psi}{\partial c_{,i}}\dot{c}_{,i} + \frac{\partial\psi}{\partial\dot{c}}\ddot{c} \leq 0$$

Now, let's consider admissible processes. Immediately we are confronted with a dilemma. How can we control the internal variables, their rates, and their gradients if we do not have an independent source available to do so? One appealing procedure is to introduce a system of micro-forces that do work on the changes in the internal variables and act as the sources forcing their changes. Let's assume that we have some external source of micro-force f that does work on changes in c in the volume and another external surface micro-force $g = \xi_i n_i$ that does work on changes in c on the surface. The quantity $\xi_i n_i$ represents a balance to g on the surface. These external sources will have some contribution to the external work done on the system. We will postulate that the micro-force power per unit volume is $f\dot{c}$ and on the surface is $g\dot{c}$. We should also expect that there is some material resistance to changes in c. We will

postulate that this internal micro-force π acts to balance the external micro-forces such that,

$$\int_V f\ dV + \int_S g\ dS + \int_V \pi\ dV = 0$$
$$\int_V f\ dV + \int_S \xi_i n_i\ dS + \int_V \pi\ dV = 0$$
$$\int_V f\ dV + \int_V \xi_{i,i}\ dS + \int_V \pi\ dV = 0$$
$$\rightarrow \quad \xi_{i,i} + f + \pi = 0 \ \text{ in } V$$

This is one possibility. There are other systems where a micro-torque balance may be more appropriate, and it also might be appropriate to consider a micro-inertia term. Neglecting these other possibilities, we must now include the external power terms $\int_V f\dot{c}\, dV$ and $\int_S g\dot{c}\, dS$ in the energy balance. The point-wise version of the first law now becomes

$$\frac{d\tilde{u}}{dt} = \sigma_{ji}\dot{\varepsilon}_{ij} + E_i\dot{D}_i + H_i\dot{B}_i + \xi_i\dot{c}_{,i} - \pi\dot{c} + r - \tilde{q}_{i,i}$$

The second law inequality is also modified and becomes,

$$\left(\frac{\partial\psi}{\partial\varepsilon_{ij}} - \sigma_{ji}\right)\dot{\varepsilon}_{ij} + \left(\frac{\partial\psi}{\partial D_i} - E_i\right)\dot{D}_i + \left(\frac{\partial\psi}{\partial B_i} - H_i\right)\dot{B}_i + \left(\frac{\partial\psi}{\partial\theta} + s\right)\dot{\theta} + \frac{1}{\theta}\tilde{q}_i\theta_{,i}$$
$$+\left(\frac{\partial\psi}{\partial c} + \pi\right)\dot{c} + \left(\frac{\partial\psi}{\partial c_{,i}} - \xi_i\right)\dot{c}_{,i} + \frac{\partial\psi}{\partial\dot{c}}\ddot{c} + \frac{\partial\psi}{\partial\theta_{,i}}\dot{\theta}_{,i} \le 0$$

Now, we are able to rely on the arguments that the $\left(\varepsilon_{ij}, D_i, B_i, \theta, c\right)$, their rates and gradients can each be arbitrarily controlled through the application of the available sources. Next, recognize that the first four and the last three terms on the left-hand side of the inequality are linear in $\dot{\varepsilon}_{ij}$, $\dot{D}_i$, $\dot{B}_i$, $\dot{\theta}$, $\dot{c}_{,i}$, $\ddot{c}$, and $\dot{\theta}_{,i}$. Under these conditions we will always be able to find some $\dot{\varepsilon}_{ij}$, $\dot{D}_i$, $\dot{B}_i$, $\dot{\theta}$, $\dot{c}_{,i}$, $\ddot{c}$, and $\dot{\theta}_{,i}$ that violate the inequality unless the coefficients contracted with these terms vanish. This implies that,

$$\sigma_{ij} = \frac{\partial\psi}{\partial\varepsilon_{ji}}, \quad E_i = \frac{\partial\psi}{\partial D_i}, \quad H_i = \frac{\partial\psi}{\partial B_i}, \quad s = -\frac{\partial\psi}{\partial\theta}, \quad \frac{\partial\psi}{\partial c_{,i}} = \xi_{,i}, \ \frac{\partial\psi}{\partial\dot{c}} = 0, \text{ and } \frac{\partial\psi}{\partial\theta_{,i}} = 0.$$

The reduced form of the inequality now becomes,

$$\left(\frac{\partial\psi}{\partial c}+\pi\right)\dot{c}+\frac{1}{\theta}\tilde{q}_{i}\theta_{,i}\leq 0$$

We must be cautious to recognize that since π and $\tilde{q}_{i}$ are functions of $(\varepsilon_{ij},D_{i},B_{i},\theta,\theta_{,i},c,c_{,i},\dot{c})$, the left-hand side is *not* necessarily linear in $\dot{c}$ and $\theta_{,i}$. To generally satisfy this inequality we take,

$$\pi=-\frac{\partial\psi}{\partial c}-\beta\dot{c}-\eta_{i}\theta_{,i}\quad\text{and}\quad\tilde{q}_{i}=-\lambda_{i}\dot{c}-k_{ij}\theta_{,j}$$

where $\beta\dot{c}^{2}+(\eta_{i}+\frac{1}{\theta}\lambda_{i})\dot{c}\theta_{,i}+\frac{1}{\theta}k_{ij}\theta_{,i}\theta_{,j}\geq 0$. Notice that $\beta\dot{c}^{2}+(\eta_{i}+\frac{1}{\theta}\lambda_{i})\dot{c}\theta_{,i}+\frac{1}{\theta}k_{ij}\theta_{,i}\theta_{,j}$ is the rate of dissipation of energy in the material due to changes in the internal variable and heat flow. The tensor k_{ij} is the thermal conductivity of the material.

The micro-force and energy balances can be re-written as,

$$\left(\frac{\partial\psi}{\partial c_{,i}}\right)_{,i}-\frac{\partial\psi}{\partial c}+f=\beta\dot{c}+\eta_{i}\theta_{,i}$$

$$\theta\dot{s}=\beta\dot{c}^{2}+\eta_{i}\theta_{,i}\dot{c}+(\lambda_{i}\dot{c})_{,i}+(k_{ij}\theta_{,j})_{,i}+r$$

The first equation is sometimes referred to as a time-dependent Landau-Ginzburg equation for the evolution of the internal variable (also called the *order parameter*). The second equation is the generalization of the heat equation. This is readily seen using a description for a *simple* material as, $\beta=\eta_{i}=\lambda_{i}=0$, and *no thermal coupling to the other fields*, and the definition of specific heat $C=\dfrac{\partial\tilde{u}}{\partial\theta}=\dfrac{\partial\tilde{u}}{\partial s}\dfrac{\partial s}{\partial\theta}=-\theta\dfrac{\partial^{2}\psi}{\partial\theta^{2}}$,

$$\begin{aligned}\theta\dot{s}&=(k_{ij}\theta_{,j})_{,i}+r\\ \theta\frac{d}{dt}\left(-\frac{\partial\psi}{\partial\theta}\right)&=(k_{ij}\theta_{,j})_{,i}+r\\ -\theta\frac{\partial^{2}\psi}{\partial\theta^{2}}\dot{\theta}&=(k_{ij}\theta_{,j})_{,i}+r\\ C\dot{\theta}&=(k_{ij}\theta_{,j})_{,i}+r\end{aligned}$$

Note that the definition of C can also come from the incremental description of the entropy temperature relation, $ds=C\,d\theta\,/\,\theta$.

Reversible Material Behavior

For the case of linear reversible material behavior we assume that there is no dissipation due to changes in internal variables or due to heat flow. Hence the values of the internal variables are "frozen" and the temperature gradient vanishes (this does not mean that the temperature cannot change, only that it is homogeneous). When dealing with active materials, the linear response is actually a linear response about some reference state. That state is best described by a remanent (i.e. plastic) strain, remanent polarization, remanent magnetization, and remanent entropy. When considering these quantities at the crystal lattice level the term spontaneous is used instead of remanent. The Helmholtz free energy for such a linear response can be written as,

$$\begin{aligned}\psi = {} & \tfrac{1}{2} c_{ijkl}(\varepsilon_{ij} - \varepsilon^r_{ij})(\varepsilon_{kl} - \varepsilon^r_{kl}) + \tfrac{1}{2}\beta_{ij}(D_i - P^r_i)(D_j - P^r_j) + \tfrac{1}{2}\chi_{ij}(\tfrac{1}{\mu_0}B_i - M^r_i)(\tfrac{1}{\mu_0}B_j - M^r_j) + \\ & - h_{kij}(D_k - P^r_k)(\varepsilon_{ij} - \varepsilon^r_{ij}) - j_{kij}(\tfrac{1}{\mu_0}B_k - M^r_k)(\varepsilon_{ij} - \varepsilon^r_{ij}) - f_{ij}(\varepsilon_{ij} - \varepsilon^r_{ij})(\theta - \theta_0) \\ & - q_i(D_i - P^r_i)(\theta - \theta_0) - r_i(\tfrac{1}{\mu_0}B_i - M^r_i)(\theta - \theta_0) - l_{ij}(\tfrac{1}{\mu_0}B_i - M^r_i)(D_j - P^r_j) \\ & + C[(\theta - \theta_0) - \theta \ln(\theta / \theta_0)] - \theta s^r\end{aligned}$$

Also of some interest are the higher order nonlinear effects of *magnetostriction* and *electrostriction*. These effects are more important in non-polar materials and in such cases contribute terms to the free energy as,

$$\psi = \tfrac{1}{2} b_{ijkl}\varepsilon_{ij}D_k D_l + \tfrac{1}{2} g_{ijkl}\varepsilon_{ij}B_k B_l$$

In most cases we will not be interested in this very general fully coupled description of a material. Usually we will be concerned with one type of coupling and will reduce the free energy to account only for the effects of interest.

Linear Piezoelectricity

Linear piezoelectric response is one of the most widely studied "smart" material responses. This behavior is applied in both sensors (the production of an electrical signal from a mechanical stimulus as in sonar) and actuators (the production of an actuating displacement from an electrical input as in the vibrating element in your cell phone). The Helmholtz free energy for a linear piezoelectric material is written as,

$$\begin{aligned}\psi = {} & \tfrac{1}{2} c^D_{ijkl}(\varepsilon_{ij} - \varepsilon^r_{ij})(\varepsilon_{kl} - \varepsilon^r_{kl}) - h_{kij}(D_k - P^r_k)(\varepsilon_{ij} - \varepsilon^r_{ij}) + \tfrac{1}{2}\beta^{\varepsilon}_{ij}(D_i - P^r_i)(D_j - P^r_j) \\ & - f_{ij}(\varepsilon_{ij} - \varepsilon^r_{ij})(\theta - \theta_0) - q_i(D_i - P^r_i)(\theta - \theta_0) + C^{\varepsilon,D}[(\theta - \theta_0) - \theta \ln(\theta / \theta_0)] - \theta s^r\end{aligned}$$

A more commonly used form of the constitutive law is derived from the *Gibbs free energy*, $g = \psi - \sigma_{ij}\varepsilon_{ij} - E_i D_i$,

$$g = -\tfrac{1}{2} s^E_{ijkl}\sigma_{ij}\sigma_{kl} - d_{kij}E_k\sigma_{ij} - \tfrac{1}{2}\kappa^\sigma_{ij}E_iE_j - \alpha_{ij}\sigma_{ij}(\theta-\theta_0) - p_iE_i(\theta-\theta_0)$$
$$+ C^{\sigma,E}[(\theta-\theta_0) - \theta\ln(\theta/\theta_0)] - \theta s^r - \sigma_{ij}\varepsilon^r_{ij} - E_iP^r_i$$

The derivation of the strain, electric displacement and entropy follow as,

$$\varepsilon_{ij} = -\frac{\partial g}{\partial \varepsilon_{ij}} = s^E_{ijkl}\sigma_{kl} + d_{kij}E_k + \alpha_{ij}(\theta-\theta_0) + \varepsilon^r_{ij}$$

$$D_i = -\frac{\partial g}{\partial E_i} = d_{ikl}\sigma_{kl} + \kappa^\sigma_{ij}E_i + p_i(\theta-\theta_0) + P^r_i$$

$$s = -\frac{\partial g}{\partial \theta} = \alpha_{ij}\sigma_{ij} + p_iE_i + C^{\sigma,E}\ln(\theta/\theta_0) + s^r$$

With these forms each term can be thought of as an independent contribution to the left-hand side quantity. In other words, $s^E_{ijkl}\sigma_{kl}$ is the elastic strain, $d_{kij}E_k$ is the piezoelectric strain, $\alpha_{ij}(\theta-\theta_0)$ is the thermal strain, and ε^r_{ij} is the remanent strain. Similarly, $d_{ikl}\sigma_{kl}$, $\kappa^\sigma_{ij}E_i$, $p_i(\theta-\theta_0)$, and P^r_i are the piezoelectric, dielectric, pyroelectric, and remanent contributions to the electric displacement.

Material Symmetry

The structure of each of the material property tensors is dictated by the symmetry of the material itself. Mathematically, the material property tensors must satisfy the relations,

$$A_{ij\ldots kl} = a_{im}a_{jn}\ldots a_{kp}a_{lq}A_{mn\ldots pq}$$

where $A_{ij\ldots kl}$ is some material property tensor of arbitrary rank, and a_{ij} is any orthogonal rotation tensor that leaves the appearance of the material unchanged. (Note that for simplicity we will only consider proper rotations, however the analysis of structures with mirror and rotoinversion symmetries requires improper rotations as well. See the solutions for Homework #5 for brief discussions of these symmetries.) For example, the relevant rotation matrices for a centrosymmetric cubic crystal are,

$$a^{1,2,3}_{ij} = \delta_{i1}\delta_{j1} + \epsilon_{1ij}, \quad \delta_{i2}\delta_{j2} + \epsilon_{2ij}, \quad \delta_{i3}\delta_{j3} + \epsilon_{3ij}$$

For a tetragonal crystal with its c-axis aligned in the x_3-direction, we would only have $a_{ij} = \delta_{i3}\delta_{j3} + \epsilon_{3ij}$ (and perhaps a 180° rotation if the crystal is centrosymmetric).

If a material is isotropic then the equation must hold for all possible rotations. Analyzing this case would seem to be a daunting task, but it turns out that it is sufficient to analyze the equation for any possible *infinitesimal* rotation given by $a_{ij} = \delta_{ij} + \epsilon_{kij}\theta_k$ where θ_k is the arbitrary small rotation vector. Let's investigate how this can be applied to the pyroelectric and thermal expansion tensors.

$$
\begin{aligned}
&p_i = a_{ij}p_j \\
&p_i = (\delta_{ij} + \epsilon_{kij}\theta_k)p_j \\
&p_i = \delta_{ij}p_j + \epsilon_{kij}\theta_k p_j \\
&0 = \epsilon_{kij}\theta_k p_j \quad \rightarrow \quad p_i = 0 \text{ since } \theta_k \text{ is arbitrary}
\end{aligned}
$$

$$
\begin{aligned}
&\alpha_{ij} = a_{ik}a_{jl}\alpha_{kl} \\
&\alpha_{ij} = (\delta_{ik} + \epsilon_{pik}\theta_p)(\delta_{jl} + \epsilon_{qjl}\theta_q)\alpha_{kl} \\
&\alpha_{ij} = \delta_{ik}\delta_{jl}\alpha_{kl} + \delta_{ik}\epsilon_{qjl}\theta_q\alpha_{kl} + \delta_{jl}\epsilon_{pik}\theta_p\alpha_{kl} + \underbrace{\epsilon_{pik}\theta_p\epsilon_{qjl}\theta_q}_{\text{higher order term}}\alpha_{kl} \\
&0 = \theta_p(\epsilon_{pjk}\alpha_{ik} + \epsilon_{pik}\alpha_{kj}) \quad \rightarrow \quad \alpha_{11} = \alpha_{22} = \alpha_{33}, \quad \alpha_{12} = \alpha_{21} = \alpha_{13} = \alpha_{31} = \alpha_{23} = \alpha_{32} = 0
\end{aligned}
$$

Since θ_p is arbitrary, it can be "factored out" of the last equation. This last tensor equation represents 27 different scalar equation, which I have not written out, but I have given the consequences of them.

For the sake of comparison, let's take a look at what these tensors look like for a tetragonal material without a center of symmetry.

$$
\begin{aligned}
&p_i = a_{ij}p_j \\
&p_i = (\delta_{i3}\delta_{j3} + \epsilon_{3ij})p_j \\
&p_i = \delta_{i3}p_3 + \epsilon_{3ij}p_j \\
&\left.\begin{aligned} i = 1 \rightarrow p_1 &= 0 + p_2 \\ i = 2 \rightarrow p_2 &= 0 - p_1 \end{aligned}\right\} \rightarrow p_1 = p_2 = 0 \\
&i = 3 \rightarrow p_3 = p_3 + 0
\end{aligned}
$$

Therefore, the general form for the pryoelectric vector for a tetragonal material aligned in the x_3-direction looks like $p_i = p\delta_{i3}$.

$$\alpha_{ij} = a_{ik}a_{jl}\alpha_{kl}$$
$$\alpha_{ij} = (\delta_{i3}\delta_{k3} + \epsilon_{3ik})(\delta_{j3}\delta_{l3} + \epsilon_{3jl})\alpha_{kl}$$
$$\alpha_{ij} = \delta_{i3}\delta_{k3}\delta_{j3}\delta_{l3}\alpha_{kl} + \delta_{i3}\delta_{k3}\epsilon_{3jl}\alpha_{kl} + \delta_{j3}\delta_{l3}\epsilon_{3ik}\alpha_{kl} + \epsilon_{3ik}\epsilon_{3jl}\alpha_{kl}$$
$$\alpha_{ij} = \delta_{i3}\delta_{j3}\alpha_{33} + \delta_{i3}\epsilon_{3jl}\alpha_{3l} + \delta_{j3}\epsilon_{3ik}\alpha_{k3} + \epsilon_{3ik}\epsilon_{3jl}\alpha_{kl}$$

This represents 9 equations,

$$\alpha_{ij} = \delta_{i3}\delta_{j3}\alpha_{33} + \delta_{i3}\epsilon_{3jl}\alpha_{3l} + \delta_{j3}\epsilon_{3ik}\alpha_{k3} + \epsilon_{3ik}\epsilon_{3jl}\alpha_{kl}$$
$$ij = 11 \rightarrow \alpha_{11} = 0 + 0 + 0 + \alpha_{22}$$
$$ij = 12 \rightarrow \alpha_{12} = 0 + 0 + 0 - \alpha_{21}$$
$$ij = 13 \rightarrow \alpha_{13} = 0 + 0 + \alpha_{23} + 0$$
$$ij = 21 \rightarrow \alpha_{21} = 0 + 0 + 0 - \alpha_{12}$$
$$ij = 22 \rightarrow \alpha_{22} = 0 + 0 + 0 + \alpha_{11}$$
$$ij = 23 \rightarrow \alpha_{23} = 0 + 0 - \alpha_{13} + 0$$
$$ij = 31 \rightarrow \alpha_{31} = 0 + \alpha_{32} + 0 + 0$$
$$ij = 32 \rightarrow \alpha_{32} = 0 - \alpha_{31} + 0 + 0$$
$$ij = 33 \rightarrow \alpha_{33} = \alpha_{33} + 0 + 0 + 0$$
$$\rightarrow \alpha_{31} = \alpha_{13} = \alpha_{23} = \alpha_{32} = 0, \quad \alpha_{12} = -\alpha_{21}, \quad \alpha_{11} = \alpha_{22}$$

Hence, a general second rank tensor for a tetragonal material aligned in the x_3-direction can be written as $\alpha_{ij} = \alpha_{11}\delta_{ij} + (\alpha_{33} - \alpha_{11})\delta_{i3}\delta_{j3} + \alpha_{12}\epsilon_{3ij}$. However, the thermal expansion tensor relates a *symmetric* second rank tensor to a scalar, so the skew-symmetric part of the thermal expansion tensor must be zero, i.e. $\alpha_{12} = -\alpha_{21} = 0$.

Two-dimensional Linear Piezoelectric Boundary Value Problems

Here we will investigate how to solve two-dimensional (independent of the x_3-direction) problems in homogeneous, linear, piezoelectric materials with no body forces or charges under non-inertial conditions. The governing equations for this problem are,

$$E_1 = -\frac{\partial \phi}{\partial x_1} \quad \text{and} \quad E_2 = -\frac{\partial \phi}{\partial x_2}$$

$$\varepsilon_{11} = \frac{\partial u_1}{\partial x_1}, \quad \varepsilon_{22} = \frac{\partial u_2}{\partial x_2}, \quad 2\varepsilon_{12} = \frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1}, \quad 2\varepsilon_{31} = \frac{\partial u_3}{\partial x_1}, \text{ and } \quad 2\varepsilon_{32} = \frac{\partial u_3}{\partial x_2}$$

$$\frac{\partial D_1}{\partial x_1}+\frac{\partial D_2}{\partial x_2}=0$$

$$\frac{\partial \sigma_{11}}{\partial x_1}+\frac{\partial \sigma_{21}}{\partial x_2}=0\,,\quad \frac{\partial \sigma_{12}}{\partial x_1}+\frac{\partial \sigma_{22}}{\partial x_2}=0\,,\ \text{and}\quad \frac{\partial \sigma_{31}}{\partial x_1}+\frac{\partial \sigma_{32}}{\partial x_2}=0\quad \text{with}\quad \sigma_{ij}=\sigma_{ji}$$

Finally, we need the appropriate form of the constitutive equations. Our process of deriving the governing equations will be as follows. Ultimately we will state the equilibrium equations in terms of the mechanical displacements and the electrical potential, so we need the stresses and electric displacements in terms of the strain and electric field from the constitutive response, then the stresses and electric displacements can be written in terms of the displacement and potential, and finally these relationships will be placed into the equilibrium equations and Gauss' law to get three governing partial differential equations for the displacements and potential. The first step is that the constitutive response needs to yield the stress and electric displacement as a function of the strain and electric field. This can be obtained from the *electrical enthalphy* which is defined as $h=\psi-E_iD_i$, and then $\sigma_{ij}=\partial h/\partial\varepsilon_{ij}$ and $D_i=-\partial h/\partial E_i$. For a linear piezoelectric material the electrical enthalpy about a fixed remanent state is,

$$h=\tfrac{1}{2}c^E_{ijkl}\varepsilon_{ij}\varepsilon_{kl}-e_{kij}E_k\varepsilon_{ij}-\tfrac{1}{2}\kappa^\varepsilon_{ij}E_iE_j$$

Then the changes in the stress and electric displacement are,

$$\sigma_{ij}=c^E_{ijkl}\varepsilon_{kl}-e_{kij}E_k$$

$$D_i=e_{ikl}\varepsilon_{kl}+\kappa^\varepsilon_{ij}E_j$$

We are interested in generalized plane strain and electric field conditions such that none of the field quantities depend on the x_3 coordinate. Therefore, $\varepsilon_{33}=E_3=0$. Our governing equations now become,

$$\left.\begin{aligned}c^E_{i\beta j\delta}u_{j,\delta\beta}+e_{\gamma i\delta}\phi_{,\gamma\delta}=0\\ e_{\alpha j\delta}u_{j,\delta\alpha}-\kappa^\varepsilon_{\alpha\beta}\phi_{,\beta\alpha}=0\end{aligned}\right\}\rightarrow\begin{bmatrix}c^E_{i\delta j\gamma} & e_{\gamma i\delta}\\ e_{\delta j\gamma} & -\kappa^\varepsilon_{\delta\gamma}\end{bmatrix}\begin{pmatrix}u_j\\ \phi\end{pmatrix}_{,\gamma\delta}=0$$

where the Greek subscripts are only allowed to take on the values 1 and 2, and summation over repeated indices is still assumed. The first equations are the equilibrium equations and the second line is Gauss' law, each in terms of the displacements and the electric potential.

Before tackling these equations, let's look at a simpler situation in order to get a feel for the solution procedure for anisotropic material problems. Let's consider uncoupled but anisotropic two-dimensional dielectric behavior. In this case Gauss' law in terms of the electric potential becomes,

$$\kappa_{11}\frac{\partial^2\phi}{\partial x_1^2}+2\kappa_{12}\frac{\partial^2\phi}{\partial x_1\partial x_2}+\kappa_{22}\frac{\partial^2\phi}{\partial x_2^2}=0$$

To solve this equation let's make a change of variables, $x_1=x_1(z_1,z_2)$ and $x_2=x_2(z_1,z_2)$. Note that z_1 and z_2 are not necessarily real and should not be interpreted as orthogonal directions. Also, we will assume that these transformations are linear and we can invert the transformation such that $z_1=z_1(x_1,x_2)$ and $z_2=z_2(x_1,x_2)$. This then implies that,

$$\frac{\partial}{\partial x_\alpha}=\frac{\partial}{\partial z_\beta}\frac{\partial z_\beta}{\partial x_\alpha}\quad\text{and}\quad\frac{\partial^2}{\partial x_\alpha\partial x_\beta}=\frac{\partial^2}{\partial z_\gamma\partial z_\delta}\frac{\partial z_\gamma}{\partial x_\alpha}\frac{\partial z_\delta}{\partial x_\beta}$$

Summation over Greek subscripts is assumed over 1 to 2. Now our equation can be written as,

$$\kappa_{\alpha\beta}\frac{\partial z_\gamma}{\partial x_\alpha}\frac{\partial z_\delta}{\partial x_\beta}\frac{\partial^2\phi}{\partial z_\gamma\partial z_\delta}=0$$

or

$$\kappa_{\alpha\beta}\left[\frac{\partial z_1}{\partial x_\alpha}\frac{\partial z_1}{\partial x_\beta}\frac{\partial^2\phi}{\partial z_1\partial z_1}+\left(\frac{\partial z_1}{\partial x_\beta}\frac{\partial z_2}{\partial x_\alpha}+\frac{\partial z_1}{\partial x_\alpha}\frac{\partial z_2}{\partial x_\beta}\right)\frac{\partial^2\phi}{\partial z_1\partial z_2}+\frac{\partial z_2}{\partial x_\alpha}\frac{\partial z_2}{\partial x_\beta}\frac{\partial^2\phi}{\partial z_2\partial z_2}\right]=0$$

Let's now attempt to simplify this equation by looking for transformations where

$$\kappa_{\alpha\beta}\frac{\partial z}{\partial x_\alpha}\frac{\partial z}{\partial x_\beta}=0$$

Since the transformations are linear, we can assume without loss of generality that $z=x_1+px_2$. Then our equation becomes,

$$\kappa_{\alpha\beta}\frac{\partial z}{\partial x_\alpha}\frac{\partial z}{\partial x_\beta}=0\quad\rightarrow\quad\kappa_{11}+2p\kappa_{12}+p^2\kappa_{22}=0\quad\rightarrow\quad p_{1,2}=-\frac{\kappa_{12}}{\kappa_{22}}\pm i\frac{\sqrt{\kappa_{11}\kappa_{22}-\kappa_{12}^2}}{\kappa_{22}}$$

We have used the fact that the dielectric permittivity is positive definite to ensure that the radicand is positive. Note that the solutions for the transformation factors are a

complex conjugate pair. Now, if we take $z_1 = x_1 + p_1 x_2$ and $z_2 = x_1 + p_2 x_2$ we find that our original equation reduces to,

$$\left[\kappa_{11} + \kappa_{12}(p_1 + p_2) + p_1 p_2 \kappa_{22}\right] \frac{\partial^2 \phi}{\partial z_1 \partial z_2} = 0$$

Fortunately, (actually by our judicious choice of the coordinate transformations) this is a very simple equation to solve. Specifically, we have,

$$\phi = f_1(z_1) + f_2(z_2)$$

Since the electric potential must be real and $z_2 = \overline{z}_1$ the general solution for real ϕ has the form,

$$\phi = f_1(z_1) + \overline{f_1(z_1)} = 2\,\mathrm{Re}[f(z)]$$

So our solutions for ϕ can be represented by a general function of a single complex variable, and for the sake of simplicity we can drop the subscripts on z and p. Next, the electric field and electric displacement components are given as,

$$\begin{Bmatrix} E_1 \\ E_2 \end{Bmatrix} = -\begin{bmatrix} 1 & 1 \\ p & \overline{p} \end{bmatrix} \begin{Bmatrix} f'(z) \\ \overline{f}'(\overline{z}) \end{Bmatrix} \quad \text{and} \quad \begin{Bmatrix} D_1 \\ D_2 \end{Bmatrix} = -\begin{bmatrix} \kappa_{11} & \kappa_{12} \\ \kappa_{12} & \kappa_{22} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ p & \overline{p} \end{bmatrix} \begin{Bmatrix} f'(z) \\ \overline{f}'(\overline{z}) \end{Bmatrix}$$

Noting that $\kappa_{11} + 2p\kappa_{12} + p^2\kappa_{22} = 0$ define $b \equiv (\kappa_{11} + p\kappa_{12}) / p = -\kappa_{12} - p\kappa_{22}$. Then it is possible to define an electric displacement potential ψ such that $D_1 = -\psi_{,2}$ and $D_2 = \psi_{,1}$. Specifically, $\psi = b\, f(z) + \overline{b\, f(z)}$. Then,

$$\begin{aligned} \begin{Bmatrix} -\psi_{,2} \\ \psi_{,1} \end{Bmatrix} &= b \begin{Bmatrix} -p \\ 1 \end{Bmatrix} f'(z) + \overline{b} \begin{Bmatrix} -\overline{p} \\ 1 \end{Bmatrix} \overline{f'(z)} \\ &= -\begin{Bmatrix} \kappa_{11} + p\kappa_{12} \\ \kappa_{12} + p\kappa_{22} \end{Bmatrix} f'(z) - \begin{Bmatrix} \kappa_{11} + \overline{p}\kappa_{12} \\ \kappa_{12} + \overline{p}\kappa_{22} \end{Bmatrix} \overline{f'(z)} = \begin{Bmatrix} D_1 \\ D_2 \end{Bmatrix} \end{aligned}$$

Finally, we would like to present a formula for the net charge on an arc, since such a formula can be of use when applying boundary conditions. The net charge per unit thickness on and arbitrary arc is,

$$Q = -\int_A^B D_1 n_1 + D_2 n_2 \, ds$$

Where A and B are the endpoints of the arc, ds is the increment of arc-length and $\mathbf{n}$ is the unit normal pointing to the right of the arc as it is traversed in the positive direction. The components of the unit normal are related to the geometry of the arc as,

$$n_1 = \frac{dx_2}{ds} \quad \text{and} \quad n_2 = -\frac{dx_1}{ds}$$

Then, using these results and the electric displacement potential, the charge per unit thickness on the arc is,

$$Q = -\int_A^B -\frac{\partial \psi}{\partial x_2}\frac{dx_2}{ds} - \frac{\partial \psi}{\partial x_1}\frac{dx_1}{ds} ds = \int_A^B \frac{d\psi}{ds}\, ds = \psi_B - \psi_A = 2\,\mathrm{Re}[bf(z_B) - bf(z_A)]$$

So both Dirichlet and Neumann boundary conditions can be related to the complex function $f(z)$. We will stop with this example here and move on to the seemingly more complicated fully coupled piezoelectric case. However, it is important to not get too bogged down in all of the details. These are certainly necessary when solving an actual problem with numerical values of the material parameters, but in the general formulation we will use the compact notation of vectors and matrices to aid in the manipulation of the equations.

One last comment about the coordinate transformation before we move on to the piezoelectric case. Note that the dielectric permittivity tensor has principal directions that will make $\kappa_{12} = 0$. In such a coordinate system $p = i\sqrt{\kappa_{11}/\kappa_{22}}$. Then we can interpret the coordinate transformation as $z = x_1 + i\tilde{x}_2$, where $\tilde{x}_2 = \sqrt{\kappa_{11}/\kappa_{22}}x_2$. This then looks like an isotropic problem but with the $\tilde{x}_2$-direction stretched by the factor $\sqrt{\kappa_{11}/\kappa_{22}}$. Hence, the solution for a circular hole problem in an anisotropic material looks like the solution to an elliptical hole problem in an isotropic material.

Returning to the piezoelectric case, we will start directly from the assumption that the solution can be represented as a function of one complex variable. Since we have four second order PDEs we should expect eight solutions and eight complex variables. We restate our governing equations as,

$$c^E_{i\beta j\delta} u_{j,\delta\beta} + e_{\gamma i\beta}\phi_{,\gamma\beta} = 0$$
$$e_{\alpha j\delta} u_{j,\delta\alpha} - \kappa^{\varepsilon}_{\alpha\beta}\phi_{,\beta\alpha} = 0$$

To solve these equations we will assume a solution of the form,

$$\begin{pmatrix} u_i \\ \phi \end{pmatrix} = \begin{pmatrix} a_i \\ a_4 \end{pmatrix} f(z) = \mathbf{a} f(z)$$

where $z = x_1 + p x_2$ is a complex variable (p is complex with generally both real and imaginary parts). We will deal with the fact that the displacement and electric potential must be real in due course. Therefore,

$$\frac{\partial}{\partial x_1} = \frac{\partial}{\partial z}\frac{\partial z}{\partial x_1} = \frac{\partial}{\partial z}$$

$$\frac{\partial}{\partial x_2} = \frac{\partial}{\partial z}\frac{\partial z}{\partial x_2} = p\frac{\partial}{\partial z}$$

$$\frac{\partial^2}{\partial x_1^2} = \frac{\partial^2}{\partial z^2}, \quad \frac{\partial^2}{\partial x_1 \partial x_2} = p\frac{\partial^2}{\partial z^2}, \quad \frac{\partial^2}{\partial x_2^2} = p^2\frac{\partial^2}{\partial z^2}$$

Plugging this assumed form of the solution into the governing equations we have,

$$[c^E_{i\beta j\delta}(\delta_{\beta 1} + p\delta_{\beta 2})(\delta_{\delta 1} + p\delta_{\delta 2})a_j + e_{\gamma i\beta}(\delta_{\beta 1} + p\delta_{\beta 2})(\delta_{\gamma 1} + p\delta_{\gamma 2})a_4]f''(z) = 0$$
$$[e_{\alpha j\delta}(\delta_{\alpha 1} + p\delta_{\alpha 2})(\delta_{\delta 1} + p\delta_{\delta 2})a_j - \kappa^{\varepsilon}_{\alpha\beta}(\delta_{\alpha 1} + p\delta_{\alpha 2})(\delta_{\beta 1} + p\delta_{\beta 2})a_4]f''(z) = 0$$

$$\{c^E_{i1j1}a_j + e_{1i1}a_4 + p[(c^E_{i1j2} + c^E_{i2j1})a_j + (e_{2i1} + e_{1i2})a_4] + p^2(c^E_{i2j2}a_j + e_{2i2}a_4)\}f''(z) = 0$$
$$\{e_{1j1}a_j - \kappa^{\varepsilon}_{11}a_4 + p[(e_{1j2} + e_{2j1})a_j - (\kappa^{\varepsilon}_{12} + \kappa^{\varepsilon}_{21})a_4] + p^2(e_{2j2}a_j - \kappa^{\varepsilon}_{22}a_4)\}f''(z) = 0$$

This represents an eigenvalue problem with p as the eignevalues and $\mathbf{a}$ as the eignevectors.

It is useful to introduce the contracted Voigt notation. Instead of representing stress and strain as second rank tensors we resort to arranging the stress and strain components into 6-component vectors,

$$\begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{pmatrix} \rightarrow \begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{pmatrix} \rightarrow \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix}$$

So the constitutive relationships can now be written as,

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{bmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix} - \begin{bmatrix} e_{11} & e_{21} & e_{31} \\ e_{12} & e_{22} & e_{32} \\ e_{13} & e_{23} & e_{33} \\ e_{14} & e_{24} & e_{34} \\ e_{15} & e_{25} & e_{35} \\ e_{16} & e_{26} & e_{36} \end{bmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix}$$

$$\begin{pmatrix} D_1 \\ D_2 \\ D_3 \end{pmatrix} = \begin{bmatrix} e_{11} & e_{12} & e_{13} & e_{14} & e_{15} & e_{16} \\ e_{21} & e_{22} & e_{23} & e_{24} & e_{25} & e_{26} \\ e_{31} & e_{32} & e_{33} & e_{34} & e_{35} & e_{36} \end{bmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix} + \begin{bmatrix} \kappa_{11} & \kappa_{12} & \kappa_{13} \\ \kappa_{12} & \kappa_{22} & \kappa_{23} \\ \kappa_{13} & \kappa_{23} & \kappa_{33} \end{bmatrix} \begin{pmatrix} E_1 \\ E_2 \\ E_3 \end{pmatrix}$$

Then our characteristic equation can be written as,

$$\left\{\mathbf{Q} + p(\mathbf{R} + \mathbf{R}^T) + p^2\mathbf{T}\right\}\mathbf{a} = 0$$

Where,

$$\mathbf{Q} = \begin{bmatrix} c_{11} & c_{16} & c_{15} & e_{11} \\ c_{16} & c_{66} & c_{56} & e_{16} \\ c_{15} & c_{56} & c_{55} & e_{15} \\ e_{11} & e_{16} & e_{15} & -\kappa_{11} \end{bmatrix}, \quad \mathbf{R} = \begin{bmatrix} c_{16} & c_{12} & c_{14} & e_{21} \\ c_{66} & c_{26} & c_{46} & e_{26} \\ c_{56} & c_{25} & c_{45} & e_{25} \\ e_{16} & e_{12} & e_{14} & -\kappa_{12} \end{bmatrix}, \quad \mathbf{T} = \begin{bmatrix} c_{66} & c_{26} & c_{46} & e_{26} \\ c_{26} & c_{22} & c_{24} & e_{22} \\ c_{46} & c_{24} & c_{44} & e_{24} \\ e_{26} & e_{22} & e_{24} & -\kappa_{22} \end{bmatrix}$$

Non-trivial solutions to the characteristic equation exist when the determinant of the bracketed matrix is zero.

$$\left|\mathbf{Q} + p(\mathbf{R} + \mathbf{R}^T) + p^2\mathbf{T}\right| = 0$$

This represents an eighth order polynomial for p. First, it is useful to establish that p cannot be real, because if this is the case then, since the coefficients of the octic equation are real, the solutions for p must come in complex conjugate pairs.

Our original set of governing equations is,

$$c^E_{ijkl}(\delta_{1l}+p\delta_{2l})(\delta_{1j}+p\delta_{2j})a_k + e_{lij}(\delta_{1l}+p\delta_{2l})(\delta_{1j}+p\delta_{2j})a_4 = 0$$
$$e_{lkj}(\delta_{1l}+p\delta_{2l})(\delta_{1j}+p\delta_{2j})a_k - \kappa^{\varepsilon}_{lj}(\delta_{1l}+p\delta_{2l})(\delta_{1j}+p\delta_{2j})a_4 = 0$$

Next, take the dot product of these equations with **a**.

$$c^E_{ijkl}(\delta_{1l}+p\delta_{2l})a_i(\delta_{1j}+p\delta_{2j})a_k + e_{lij}(\delta_{1l}+p\delta_{2l})a_i(\delta_{1j}+p\delta_{2j})a_4 = 0$$
$$e_{lkj}(\delta_{1l}+p\delta_{2l})a_4(\delta_{1j}+p\delta_{2j})a_k - \kappa^{\varepsilon}_{lj}(\delta_{1l}+p\delta_{2l})a_4(\delta_{1j}+p\delta_{2j})a_4 = 0$$

If p is real and since the material properties are real, then the eignevector **a** can also be chosen to be real. For clarity define the real quantities $u^s_{i,l} = (\delta_{1l}+p\delta_{2l})a_i$ and $\phi^s_{,l} = (\delta_{1l}+p\delta_{2l})a_4$, and subtract the two equations. Then we have,

$$c^E_{ijkl}u^s_{i,j}u^s_{k,l} + \kappa^{\varepsilon}_{lj}\phi^s_{,l}\phi^s_{,j} = 0$$

We know that the elastic stiffness and the dielectric permittivity tensors must be positive definite for a stable material, so any set of real non-zero fields create a contradiction with this equation, and hence p cannot be real.

So, since the coefficients of the eighth order polynomial are real, the roots appear as complex conjugate pairs. Without loss of generality we can take,

$$p_5 = \overline{p}_1, \quad p_6 = \overline{p}_2, \quad p_7 = \overline{p}_3, \quad p_8 = \overline{p}_4$$

Where $z_I = x + p_I y$, the general solution has the form,

$$\begin{pmatrix} u_i \\ \phi \end{pmatrix} = \sum_{J=1}^{8} \begin{pmatrix} A_{iJ} \\ A_{4J} \end{pmatrix} f_J(z_J)$$

For each eignevalue p_J there is an associated eignevector (A_{iJ}, A_{4J}). The matrix **A** is assembled by placing the components of the eigenvectors **a** in the columns. Since the displacements and the electric potential are real-valued functions, we must have,

$$A_{i(J+4)}f_{(J+4)}(z_{J+4}) = \overline{A_{iJ}f_J(z_J)}$$

and our solution can be written as,

$$\begin{pmatrix} u_i \\ \phi \end{pmatrix} = 2\,\mathrm{Re}\sum_{J=1}^{4} \begin{pmatrix} A_{iJ} \\ A_{4J} \end{pmatrix} f_J(z_J) = \sum_{J=1}^{4} \begin{pmatrix} A_{iJ} \\ A_{4J} \end{pmatrix} f_J(z_J) + \sum_{J=1}^{4} \begin{pmatrix} \overline{A}_{iJ} \\ \overline{A}_{4J} \end{pmatrix} \overline{f_J(z_J)}$$

The stresses and electric displacements are given as,

$$\sigma_{i\alpha} = c^E_{i\alpha j\beta} u_{j,\beta} + e_{\beta i\alpha}\phi_{,\beta}$$
$$D_\alpha = e_{\alpha j\beta} u_{j,\beta} - \kappa^\varepsilon_{\alpha\beta}\phi_{,\beta}$$

$$\sigma_{i\alpha} = \sum_{K=1}^{8}[c^E_{i\alpha j\beta}(\delta_{\beta 1} + p\delta_{\beta 2})a_{jK} + e_{\beta i\alpha}(\delta_{\beta 1} + p\delta_{\beta 2})a_{4K}]f'_K(z_K)$$
$$D_\alpha = \sum_{K=1}^{8}[e_{\alpha j\beta}(\delta_{\beta 1} + p\delta_{\beta 2})a_{jK} - \kappa^\varepsilon_{\alpha\beta}(\delta_{\beta 1} + p\delta_{\beta 2})a_{4K}]f'_K(z_K)$$

$$\sigma_{i\alpha} = \sum_{K=1}^{8}(c^E_{i\alpha j1}A_{jK} + e_{1i\alpha}A_{4K} + pc^E_{i\alpha j2}A_{jK} + pe_{2i\alpha}A_{4K})f'_K(z_K)$$
$$D_\alpha = \sum_{K=1}^{8}(e_{\alpha j1}A_{jK} - \kappa^\varepsilon_{\alpha 1}A_{4K} + pe_{\alpha j2}A_{jK} - p\kappa^\varepsilon_{\alpha 2}A_{4K})f'_K(z_K)$$

Define,

$$b_i = c^E_{i2j1}a_j + e_{1i2}a_4 + pc^E_{i2j2}a_j + pe_{2i2}a_4$$
$$b_4 = e_{2j1}a_j - \kappa^\varepsilon_{21}a_4 + pe_{2j2}a_j - p\kappa^\varepsilon_{22}a_4$$

From,

$$c^E_{i1j1}a_j + e_{1i1}a_4 + p[(c^E_{i1j2} + c^E_{i2j1})a_j + (e_{2i1} + e_{1i2})a_4] + p^2(c^E_{i2j2}a_j + e_{2i2}a_4) = 0$$
$$e_{1j1}a_j - \kappa^\varepsilon_{11}a_4 + p[(e_{1j2} + e_{2j1})a_j - (\kappa^\varepsilon_{12} + \kappa^\varepsilon_{21})a_4] + p^2(e_{2j2}a_j - \kappa^\varepsilon_{22}a_4) = 0$$

$$b_i = c^E_{i2j1}a_j + e_{1i2}a_4 + pc^E_{i2j2}a_j + pe_{2i2}a_4 = -\frac{1}{p}(c^E_{i1j1}a_j + e_{1i1}a_4 + pc^E_{i2j1}a_j + pe_{2i1}a_4)$$
$$b_4 = e_{2j1}a_j - \kappa^\varepsilon_{21}a_4 + pe_{2j2}a_j - p\kappa^\varepsilon_{22}a_4 = -\frac{1}{p}(e_{1j1}a_j - \kappa^\varepsilon_{11}a_4 + pe_{1j2}a_j - p\kappa^\varepsilon_{12}a_4)$$

Then it is possible to write the stresses and electric displacements in vector form as,

$$\begin{pmatrix} \sigma_{i2} \\ D_2 \end{pmatrix} = 2\,\mathrm{Re}\sum_{J=1}^{4}\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} f'_J(z_J) = \sum_{J=1}^{4}\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} f'_J(z_J) + \sum_{J=1}^{4}\begin{pmatrix} \overline{B}_{iJ} \\ \overline{B}_{4J} \end{pmatrix}\overline{f'_J(z_J)}$$
$$\begin{pmatrix} \sigma_{i1} \\ D_1 \end{pmatrix} = -2\,\mathrm{Re}\sum_{J=1}^{4}\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} p_J f'_J(z_J) = -\sum_{J=1}^{4}\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} p_J f'_J(z_J) - \sum_{J=1}^{4}\begin{pmatrix} \overline{B}_{iJ} \\ \overline{B}_{4J} \end{pmatrix}\overline{p_J f'_J(z_J)}$$

The matrix **B** is assembled by placing the **b** vectors in the columns. Finally, note that the stress and electric displacement can be derived from a set of stress and electric displacement potential functions as,

$$\begin{pmatrix} \sigma_{i2} \\ D_2 \end{pmatrix} = \begin{pmatrix} \psi_{i,1} \\ \psi_{4,1} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \sigma_{i1} \\ D_1 \end{pmatrix} = -\begin{pmatrix} \psi_{i,2} \\ \psi_{4,2} \end{pmatrix}$$

The potential functions can then be given in terms of the complex functions as,

$$\begin{pmatrix} \psi_i \\ \psi_4 \end{pmatrix} = 2\,\mathrm{Re}\sum_{J=1}^{4}\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} f_J(z_J) = \sum_{J=1}^{4}\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} f_J(z_J) + \sum_{J=1}^{4}\begin{pmatrix} \overline{B}_{iJ} \\ \overline{B}_{4J} \end{pmatrix}\overline{f_J(z_J)}$$

This set of generalized potentials is then useful for determining the net force and charge on an arc. The net forces and charge on an arc per unit thickness are,

$$F_i = \int_A^B \sigma_{i1} n_1 + \sigma_{i2} n_2 \, ds \qquad Q = -\int_A^B D_1 n_1 + D_2 n_2 \, ds$$

Using our previously derived formulas for the unit normal to the arc and the stress/electric displacement potential functions, these equations simplify to,

$$\begin{aligned} F_i &= \int_A^B -\frac{\partial \psi_i}{\partial x_2}\frac{dx_2}{ds} - \frac{\partial \psi_i}{\partial x_1}\frac{dx_1}{ds}\,ds \\ &= \int_A^B \frac{d\psi_i}{ds}\,ds \\ &= \psi_i(z_B) - \psi_i(z_A) \\ &= 2\sum_{J=1}^{4}\mathrm{Re}[B_{iJ}f_J(z_{JB}) - B_{iJ}f_J(z_{JA})] \end{aligned} \qquad \begin{aligned} Q &= -\int_A^B -\frac{\partial \psi_4}{\partial x_2}\frac{dx_2}{ds} - \frac{\partial \psi_4}{\partial x_1}\frac{dx_1}{ds}\,ds \\ &= \int_A^B \frac{d\psi_4}{ds}\,ds \\ &= \psi_4(z_B) - \psi_4(z_A) \\ &= 2\sum_{J=1}^{4}\mathrm{Re}[B_{4J}f_J(z_{JB}) - B_{4J}f_J(z_{JA})] \end{aligned}$$

We will not go into detail on how to use these results to solve problems on specific geometries and for specific loadings, but we will look at one of my favorite problems, the crack. Take the case of a semi-infinite crack with traction-free and charge-free boundaries. Many linear piezoelectric problems can be solved by assuming that the $f_I(z_I)$ each have the same functional form. The boundary conditions that we are interested in imply that,

$$\begin{pmatrix} F_i \\ Q \end{pmatrix} = \sum_{J=1}^{4}\left[\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} f(z_J) + \begin{pmatrix} \overline{B}_{iJ} \\ \overline{B}_{4J} \end{pmatrix}\overline{f}(\overline{z}_J)\right] = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{on} \quad z = re^{\pm i\pi}$$

Note that r and θ are not the radial and angular coordinates in the standard sense, but are defined through $z_I = x_1 + p_I x_2 = r_I e^{i\theta_I}$. Then the lines $\theta = \pm\pi$ correspond to $\theta_I = \pm\pi$ and $z_I = x_1 = -r$ if and only if $\mathrm{Im}(p_I) > 0$, so we must choose this convention

in order for the remainder of this development to be valid. Next, investigate solutions of the form $f(z_I) = z_I^n = r_I^n e^{in\theta_I}$. Our boundary condition equations become,

$$\sum_{J=1}^{4}\left[\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} r^n(\cos n\pi + i\sin n\pi) + \begin{pmatrix} \bar{B}_{iJ} \\ \bar{B}_{4J} \end{pmatrix} r^n(\cos n\pi - i\sin n\pi)\right] = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\sum_{J=1}^{4}\left[\begin{pmatrix} B_{iJ} + \overline{B_{iJ}} \\ B_{4J} + \overline{B_{4J}} \end{pmatrix} (\cos n\pi) + i\begin{pmatrix} B_{iJ} - \overline{B_{iJ}} \\ B_{4J} - \overline{B_{4J}} \end{pmatrix} (\sin n\pi)\right] = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

The solutions can then have n as integers and the first vector equal to zero, or n as half-integers and the second vector equal to zero. We now constrain the solution further to have bounded displacements and electric potential at the crack tip as $r \to 0$. This condition implies that $n \geq 0$ since $u_i, \phi \sim f(z)$. Hence, the first value of n that satisfies this inequality and still yields singular fields at the crack tip is $n = 1/2$. So, we will take $n = 1/2$ and,

$$\sum_{J=1}^{4}\begin{bmatrix} B_{iJ} - \overline{B_{iJ}} \\ B_{4J} - \overline{B_{4J}} \end{bmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Note, that this equation does not imply that all of the B_{iJ} components are real, but rather that the sum of the rows of **B** is real. Recall that,

$$\begin{aligned} \begin{pmatrix} \sigma_{i2} \\ D_2 \end{pmatrix} &= \sum_{J=1}^{4}\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} f'(z_J) + \sum_{J=1}^{4}\begin{pmatrix} \bar{B}_{iJ} \\ \bar{B}_{4J} \end{pmatrix}\overline{f'(z_J)} \\ &= \frac{1}{2}\sum_{J=1}^{4}\left[\begin{pmatrix} B_{iJ} \\ B_{4J} \end{pmatrix} z_J^{-1/2}\right] + \frac{1}{2}\sum_{J=1}^{4}\left[\begin{pmatrix} \bar{B}_{iJ} \\ \bar{B}_{4J} \end{pmatrix}\overline{z_J^{-1/2}}\right] \end{aligned}$$

So, on the plane ahead of the crack tip, $\theta = 0$ and $z_I = x_1 = r$, we have,

$$\begin{pmatrix} \sigma_{i2} \\ D_2 \end{pmatrix} = \frac{1}{2\sqrt{r}}\sum_{J=1}^{4}\begin{pmatrix} B_{iJ} + \bar{B}_{iJ} \\ B_{4J} + \bar{B}_{4J} \end{pmatrix} \equiv \frac{1}{\sqrt{2\pi r}}\begin{pmatrix} K_{II} \\ K_I \\ K_{III} \\ K_{IV} \end{pmatrix}$$

The last definition is an arbitrary but well-established convention. It states that the stress or electric displacement ahead of the crack tip is equal to its corresponding

intensity factor K divided by the square root of $2\pi r$. Using this convention and our previous conclusion from the boundary conditions we can show,

$$\sum_{J=1}^{4}\begin{Bmatrix} B_{iJ} \\ B_{4J} \end{Bmatrix} = \begin{bmatrix} B_{11} & B_{12} & B_{13} & B_{14} \\ B_{21} & B_{22} & B_{23} & B_{24} \\ B_{31} & B_{32} & B_{33} & B_{34} \\ B_{41} & B_{42} & B_{43} & B_{44} \end{bmatrix}\begin{Bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{Bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ \frac{B_{21}}{B_{11}} & \frac{B_{22}}{B_{12}} & \frac{B_{23}}{B_{13}} & \frac{B_{24}}{B_{14}} \\ \frac{B_{31}}{B_{11}} & \frac{B_{32}}{B_{12}} & \frac{B_{33}}{B_{13}} & \frac{B_{34}}{B_{14}} \\ \frac{B_{41}}{B_{11}} & \frac{B_{42}}{B_{12}} & \frac{B_{43}}{B_{13}} & \frac{B_{44}}{B_{14}} \end{bmatrix}\begin{Bmatrix} B_{11} \\ B_{12} \\ B_{13} \\ B_{14} \end{Bmatrix} = \frac{1}{\sqrt{2\pi}}\begin{Bmatrix} K_{II} \\ K_{I} \\ K_{III} \\ K_{IV} \end{Bmatrix}$$

Note that the second equality recognizes that the **B** matrix is a set of vectors of *unknown* length. Note that this form cannot be used for certain special classes of materials (e.g. when one or more of the $B_{1i} = 0$) and another similar form must be used. The B_{1J} vector can then be solved for from the linear equations represented by the third equality. Finally, our solutions for the stress/electric displacement potentials and the displacements and electric potential are,

$$\begin{Bmatrix} \psi_i \\ \psi_4 \end{Bmatrix} = 2\,\mathrm{Re}\sum_{J=1}^{4}\begin{Bmatrix} B_{iJ} \\ B_{4J} \end{Bmatrix}\sqrt{z_J} \quad \text{and} \quad \begin{Bmatrix} u_i \\ \phi \end{Bmatrix} = 2\,\mathrm{Re}\sum_{J=1}^{4}\begin{Bmatrix} A_{iJ} \\ A_{4J} \end{Bmatrix}\sqrt{z_J}$$

Where,

$$(\mathbf{A})_I = (\mathbf{R}^T + p_I\mathbf{T})^{-1}(\mathbf{B})_I$$

and $(\cdot)_I$ denotes the I^{th} column.

For homework you will be required to go through this procedure and plot the asymptotic stress and electric displacement fields. One last quantity of considerable interest is the energy release rate associated with an incremental advance of the crack tip. This quantity can be computed using a crack closure integral,

$$\mathcal{G}\delta a = \frac{1}{2}\int_0^{\delta a}\begin{Bmatrix} \sigma_{i2}(r) \\ D_2(r) \end{Bmatrix}^T \cdot \begin{Bmatrix} \Delta u_i(r-\delta a) \\ \Delta\phi(r-\delta a) \end{Bmatrix} dr$$

where Δu_i and $\Delta\phi$ are the crack opening/sliding displacements and potential jump. The two vectors appearing in the integrand are given as,

$$\begin{pmatrix} \sigma_{12} \\ \sigma_{22} \\ \sigma_{32} \\ D_2 \end{pmatrix} = \frac{1}{\sqrt{2\pi x_1}} \begin{pmatrix} K_{II} \\ K_I \\ K_{III} \\ K_{IV} \end{pmatrix}$$

and

$$\begin{pmatrix} \Delta u_1 \\ \Delta u_2 \\ \Delta u_3 \\ \Delta\phi \end{pmatrix} = 2\,\mathrm{Re}\left\{ i\mathbf{A}\mathbf{B}^{-1}\mathbf{B} \cdot \begin{pmatrix} \sqrt{r} \\ \sqrt{r} \\ \sqrt{r} \\ \sqrt{r} \end{pmatrix} \right\} = \underbrace{\left[i\mathbf{A}\mathbf{B}^{-1} + \overline{i\mathbf{A}\mathbf{B}^{-1}} \right]}_{\mathbf{H}} \cdot \underbrace{\left[\mathbf{B} + \bar{\mathbf{B}} \right] \cdot \begin{pmatrix} \sqrt{r} \\ \sqrt{r} \\ \sqrt{r} \\ \sqrt{r} \end{pmatrix}}_{\sqrt{\frac{2r}{\pi}}(K_{II}\ K_I\ K_{III}\ K_{IV})^T} = \sqrt{\frac{2r}{\pi}} \mathbf{H} \begin{pmatrix} K_{II} \\ K_I \\ K_{III} \\ K_{IV} \end{pmatrix}$$

So the closure integral becomes,

$$\begin{aligned} \mathcal{G} &= \frac{1}{2\delta a} \int_0^{\delta a} \begin{pmatrix} \sigma_{i2}(r) \\ D_2(r) \end{pmatrix}^T \cdot \begin{pmatrix} \Delta u_i(r - \delta a) \\ \Delta\phi(r - \delta a) \end{pmatrix} dr \\ &= \frac{1}{2\pi\delta a} \begin{pmatrix} K_{II}\, K_I\, K_{III}\, K_{IV} \end{pmatrix} \cdot \mathbf{H} \cdot \begin{pmatrix} K_{II} \\ K_I \\ K_{III} \\ K_{IV} \end{pmatrix} \int_0^{\delta a} \frac{\sqrt{\delta a - r}}{\sqrt{r}} dr = \frac{1}{4} \begin{pmatrix} K_{II}\, K_I\, K_{III}\, K_{IV} \end{pmatrix} \cdot \mathbf{H} \cdot \begin{pmatrix} K_{II} \\ K_I \\ K_{III} \\ K_{IV} \end{pmatrix} \end{aligned}$$

