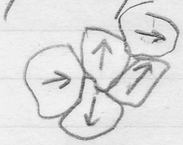
Theory of Inhomogeneous Materials

Examples of inhomogeneous media (we're surrounded by them!):

1. atmosphere : air w/ water droplets or molecules
   air w/ density fluctuations

2. rocks : aggregates of individual grains

3. metals : aggregates of crystals w/ different orientation



polycrystal

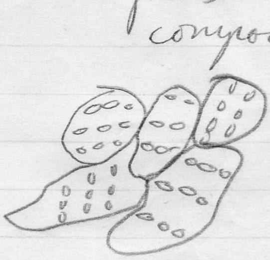
4. composite materials : laminated structures 
   reinforced concrete (w/ steel rods)
   fiber composites (used in skis)
   cermets (metal particles in ceramic)
   bio. materials.

5. porous media : sandstones - composite of air and rock
   or rock air + liquid
   such as oil or brine
   (fractal structure)

6. sea ice : ice, brine + air

   composite on two levels polycrystal

   but the individual crystals are themselves composites



7. doped semiconductors

random impurities

hopping conduction

8. turbulent fluid

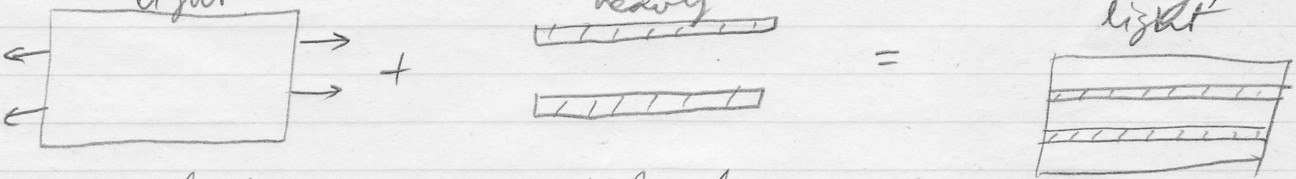
Properties of composites can be different from constituents:

1

weak, cheap
light

strong, expensive
heavy

strong, cheap
light

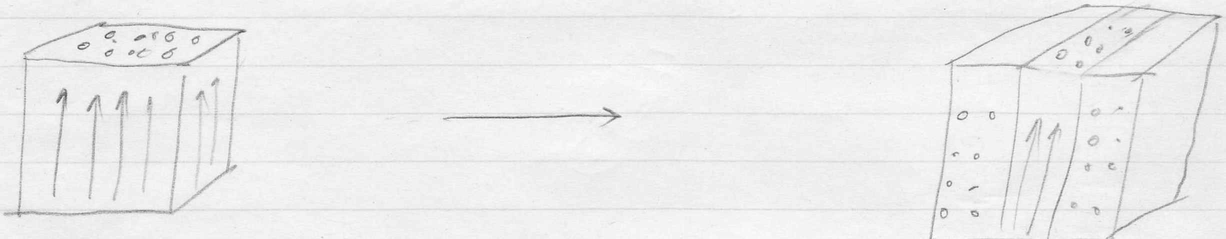


concrete breaks
apart under tension

steel rods

(in skis also)

2

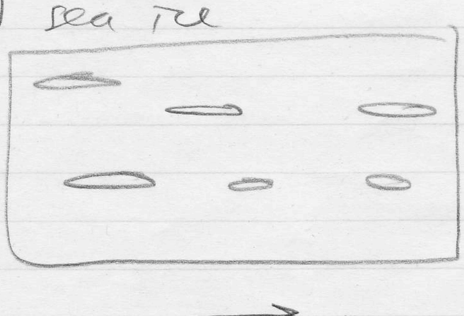


wood, strong in
fibre direction
but fibers can be
pulled apart easily

plywood
strong in two (or all)
directions

introduces problem of interfaces
(also in polycrystals)

3 sea ice



E field

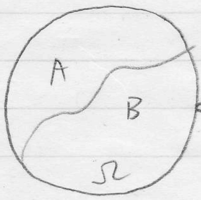
anomolous dielectric effect
effect of interfaces.

Composites arise as solutions in optimization problems:

(1) need to fix relative volume of two materials w/ conductivities σ_1 and σ_2, $\sigma_1 \ll \sigma_2$

maximize conductivity in x-direction

(2) Example of Tartar and Murat



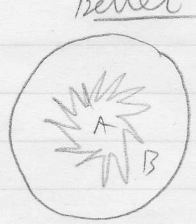
Heat generated uniformly within circle whose ∂B kept at const. T
good cond. A, bad cond. B
w/ fixed vol. fracs.

Which configuration minimizes avg. temp.

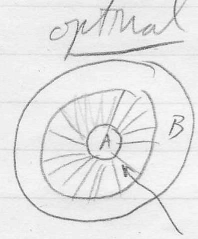
$$\int_\Omega T(x)\,dx$$

Good

Better



optimal



infinitely fine
(problem of existence)

G-closure (Lurie + Cherkaev)

Types of Inhomogeneities

periodic, quasiperiodic, random (translation invariant)

Equations of Interest

$$J = \sigma E \qquad \nabla \cdot J = \rho \qquad E = \nabla u \qquad \nabla \cdot \sigma \nabla u = \rho$$

source

Problem	J	E	σ
elec. cond.	elect. current J	elec. field E	cond. tensor $\underline{\sigma}$
dielectrics	displacement D	" E	permittivity $\underline{\underline{\varepsilon}}$
magnetism	mag. ind. B	mag. field int. H	permeability $\underline{\underline{\mu}}$
thermal cond.	heat current Q	temp grad ∇T	thermal cond K
diffusion	particle current	conc. grad ∇c	diffusivity D
homog. flow. in porous media	fluid current v	pressure grad ∇p	permeability

Homog. eqs.

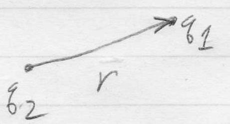
$$J = \sigma E$$
$$\downarrow$$
$$\langle J \rangle = \sigma^* \langle E \rangle$$

Material Properties

We are interested in response of materials subjected to the application of electromagnetic, elastic, and other fields.

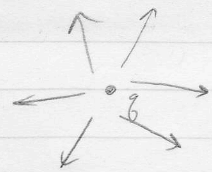
Focus on electromagnetic fields:

Force on q_1 due to q_2 $\qquad \underset{q_2}{F} = \dfrac{q_1 q_2}{4\pi\varepsilon_0} \dfrac{r}{|r|^3}$ $\qquad$ Coulomb



Electric field $\quad E = \lim_{q \to 0} \dfrac{F_q}{q}$

E due to point charge



$$E(\vec{r}) = \frac{q}{4\pi\varepsilon} \frac{r}{|r|^3}$$

$$E = -\nabla\varphi \quad , \quad \varphi(\vec{r}) = \frac{1}{4\pi\varepsilon_0} \frac{q}{|r|} \qquad (\nabla \times E = 0)$$

materials are
- conductors
- insulators (dielectrics)

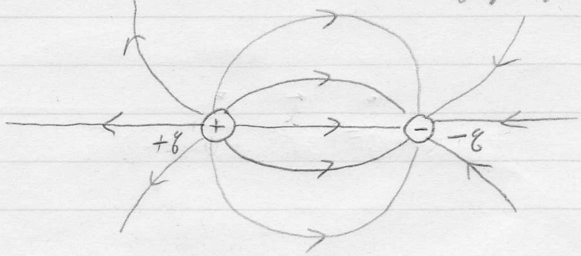
conductors : have large numbers of free charge carriers (like metals)
they move (and carry current) when subjected to E field

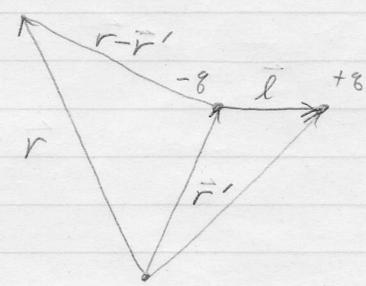
dielectrics: all charged particles are bound to constituent molecules
charged particles shift slightly in response to E field
(real dielectrics show some cond., but 10^{20} times smaller than real conductors)

some materials, such as semiconductors and electrolytes, have properties intermediate between dielectric + conductor.

example : brine solution

Let's examine dielectric media, aggregates of dipoles





to leading order, $\varphi(r) = \frac{1}{4\pi\varepsilon_0} \frac{p\cdot(r-r')}{|r-r'|^3}$, $\bar{p} = q l$

in dielectric media, when field is applied, get displacement of pos. charge relative to neg. charge.

consider small element Δv of dielectric medium, which as whole is electrically neutral

$$\Delta p = \int_{\Delta v} r \, dq$$

electric dipole moment per unit volume

$$P = \lim_{\Delta v \to 0} \frac{\Delta p}{\Delta v} \quad \text{electric polarization}$$

$$\text{or} \quad \bar{P} = \frac{1}{\Delta v} \sum_m \bar{p}_m , \quad p_m = \int_{\text{molecules}} r \, dq$$

For isotropic media

$$P = \chi(E)\, E$$

χ = electric susceptibility

Now define electric displacement

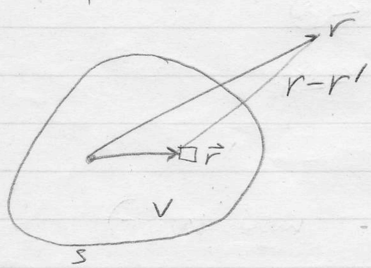
$$D = \varepsilon_0 E + P \qquad \text{so that} \qquad \varepsilon_0 E = D - P$$

$$= \varepsilon_0 E + \chi E$$

$$\boxed{D = \varepsilon E}, \qquad \varepsilon = \varepsilon_0 + \chi = \text{permittivity}$$

<u>equation for D :</u>

potential due to dielectric medium

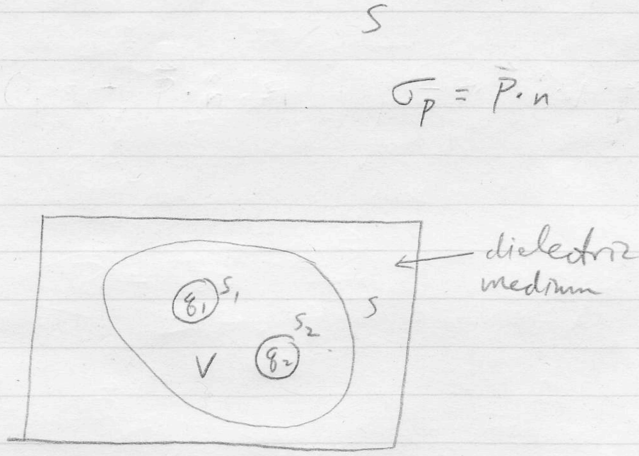


$$\phi(r) = \frac{1}{4\pi\varepsilon_0}\int_V \frac{P(r')\cdot(r-r')}{|r-r'|^3}\,dV$$

$$= \frac{1}{4\pi\varepsilon_0}\int_S \frac{P\cdot n}{|r-r'|}\,dA + \frac{1}{4\pi\varepsilon_0}\int_V \frac{-\nabla\cdot P}{|r-r'|}\,dV$$

$$\sigma_p = P\cdot n \qquad \rho_p = -\nabla\cdot P$$

Now consider



Gauss $\displaystyle\int_S E\cdot n\,dA = \frac{1}{\varepsilon_0}(Q + Q_p)$ $\qquad Q = q_1 + q_2$ free charge

Q_p = polarization charge

$$Q_p = \int_{S_1+S_2} P\cdot n\,dA + \int_V (-\nabla\cdot P)\,dV$$

no contr from S in Q_p since no real boundary in dielectric use divergence thm on vol. int. in Q_p, we get

$$Q_p = -\int_S P \cdot n \, dA$$

thus

$$\varepsilon_0 \int_S E \cdot n \, dA + \int_S P \cdot n \, dA = Q$$

or with $\boxed{D = \varepsilon_0 E + P}$

$$\int_S D \cdot n \, dA = Q \quad \text{or} \quad \int_V \nabla \cdot D \, dV = Q$$

or

$$\boxed{\nabla \cdot D = \rho}, \quad \rho = \text{free charge density (MKS)}$$

thus $D = \varepsilon E = (\varepsilon_0 + \chi) E$

$\varepsilon = K \varepsilon_0$, K is dielectric constant (dimensionless)

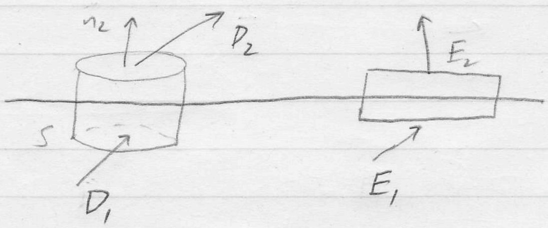
$$K = \frac{\varepsilon}{\varepsilon_0} = 1 + \frac{\chi}{\varepsilon_0}, \quad \varepsilon_0 = \text{permittivity of free space.}$$

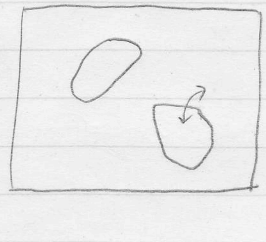
Material	K	E_{max} (volts/m) ← max electric field before material becomes cond.
Glass	5–10	9×10^6
wood	2.5–8	
oil	2.1	12×10^6
Water (0°C)	88.0	
Water (20°C)	80.0	
Air (1 atm)	1.00059	3×10^6

$$\nabla \times E = 0$$

$$\nabla \cdot D = \rho$$

Boundary Conditions





composite

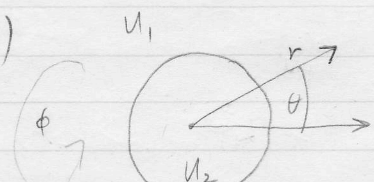
$\nabla \cdot D = \rho \implies D_{2n} - D_{1n} = \sigma$ $\quad$ σ = surface density of free charge

$\nabla \times E = 0 \implies E_{1t} = E_{2t}$

Fundamental Example: Dielectric sphere in uniform electric field

sphere of dielectric const K and radius a in initially uniform field $\vec{E}_0$

(r, θ, ϕ)



$\Delta u = 0$, u indep. of ϕ

two lowest order spherical harmonics are enough

$$u_1(r,\theta) = A_1 r \cos\theta + C_1 r^{-2} \cos\theta$$

$$u_2(r,\theta) = A_2 r \cos\theta + C_2 r^{-2} \cos\theta$$

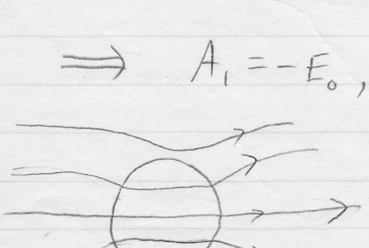
$1/r$ not necessary since it corresponds to net charge on sphere

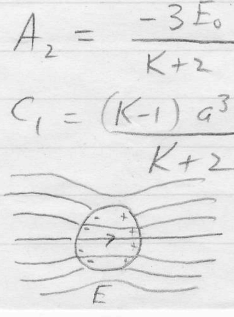
Use following conds to det coeff:
1. $u_1 \to -E_0 r \cos\theta$ as $r \to \infty$
2. cont. of U across interface
3. cont of D_n

$\implies A_1 = -E_0$, $A_2 = \dfrac{-3E_0}{K+2}$, $C_2 = 0$ (otherwise macro dipole, ∞ field)

$C_1 = \dfrac{(K-1)\, a^3 E_0}{K+2}$ $\implies$ $\boxed{E_2 = \dfrac{3}{K+2} E_0}$ $\quad K > 1$

Resonance in K plane at $K = -2$





$|E_2| < |E_0|$

lines of D are cont. (no surface charge)

lines of E are discont. (due to polarization charge caused by dielec. discont.)

polarizability of sphere.

Electric Current

current $I = \frac{dQ}{dt}$, rate at which net charge Q is transported past a given point

$$1 \text{ amp} = 1 \ \frac{\text{coul.}}{\text{sec.}}$$

current passing through surface S is

$$I = \int_S J \cdot n \, dA \quad , \quad J = \text{current density} = N q v$$

N = # charge carriers per unit volume
q = charge
v = drift velocity of each carrier.

if S is closed and contains V, the current entering V is

$$I = -\int_S J \cdot n \, dA = -\int_V \nabla \cdot J \, dV$$

But $\quad I$ = rate at which charge is being transported into V

$$= \frac{dQ}{dt} = \frac{d}{dt}\int_V \rho \, dV = \int_V \frac{\partial \rho}{\partial t} \, dV$$

$$\Longrightarrow \quad \int_V \left(\frac{\partial \rho}{\partial t} + \nabla \cdot J \right) dV = 0 \quad \Longrightarrow \quad \boxed{\frac{\partial \rho}{\partial t} + \nabla \cdot J = 0}$$

Found experimentally that $J = \sigma E$, σ = conductivity (generally $\sigma = \sigma(E)$)

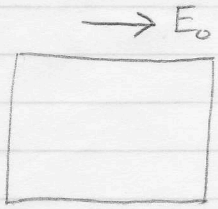
Resistivity $\quad \eta = \frac{1}{\sigma}$

η meas. in $\frac{\text{volt} \cdot \text{m}}{\text{amp}}$ or ohm meters $\qquad 1 \text{ ohm} = \frac{1 \text{ volt}}{1 \text{ amp}}$

$$\sigma = \frac{1}{\text{ohm m.}}$$

Material	Resistance ρ (ohm·m)	
Silver (0°C)	1.5×10^{-8}	
Copper	1.7×10^{-8}	
Aluminum	2.8×10^{-8}	
Iron	8.9×10^{-8}	
Silicon (pure)	640.0	(doped semiconductors have complicated $\rho(T)$.)
Silicon (10^{-4}% As)	0.003	
Glass	$10^{10} - 10^{14}$	
Fused quartz	7.5×10^{17}	
Wood	$10^{8} - 10^{11}$	

Dielectrics in Oscillating Fields



when place dielectric in field, polarization doesn't attain max instantaneously

delay due to viscosity of medium and inertia of electric charges

Now consider

$$E = E_0 e^{i\omega t}$$

Then P may be unable to keep pace with E, may be shifted

$$P = P_0 e^{i(\omega t - \varphi)}$$

but $P = \chi E \Rightarrow P_0 e^{i(\omega t - \varphi)} = \chi E_0 e^{i\omega t}$

$$P_0 e^{i\omega t} = \underbrace{\chi e^{i\varphi}} E_0 e^{i\omega t}$$

replace $\chi e^{i\varphi}$ with complex $\chi = \chi' + i\chi''$

Similarly if $D = D_0 e^{i(\omega t-\delta)}$ then $D = (1+\frac{\chi}{\varepsilon_0})\varepsilon_0 E$

can be written as $D = \varepsilon\varepsilon_0 E$, $\varepsilon = \varepsilon' + i\varepsilon''$, $\varepsilon_{space} = 1 + i0$

Thus, when the "response" is out of phase with applied field, the material parameters may be considered to be <u>complex</u>. ☆

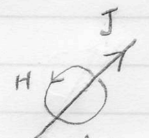
To understand the physical meaning of ε' and ε'', we must examine <u>Maxwell's</u> <u>Equations</u>.

We will derive them from the experimentally determined laws of electricity and magnetism:

(Written in Gaussian units: $D = E + 4\pi P$, $H = B - 4\pi M$, $\varepsilon_0 = \mu_0 = 1$)

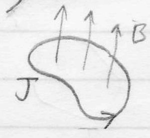
Coulomb's law : $\nabla \cdot D = 4\pi\rho$

Ampere's law : $\nabla \times H = \frac{4\pi}{c} J$



Current causes magnetic field

Faraday's law : $\nabla \times E = -\frac{1}{c}\frac{\partial B}{\partial t}$



current induced in circuit if magnetic flux changed in area enclosed (move magnet in and out) − sign means current is produced so as to oppose change in B (otherwise energy diverges)

Absence of magnetic monopoles : $\nabla \cdot B = 0$

All laws above, except Faraday, were derived from steady state observations! Consequently, from logical point of view, there is no a priori reason to expect that this set of equations holds unchanged for time-dependent fields!

The genius of J.C. Maxwell was that he saw the inconsistency in this set of equations, and modified them into a consistent set which implied new physical phenomena!

For this brilliant stroke in 1865, the new set is known as

Maxwell's equations

The faulty equation is Ampere's law $\nabla \times H = \frac{4\pi}{c} J$

It was derived for steady-state current with $\nabla \cdot J = 0$, which is automatically built into the law:

$$\nabla \cdot (\nabla \times H) \equiv 0 \Rightarrow \nabla \cdot J = 0$$

$\nabla \cdot J = 0$ valid for steady-state, <u>however</u>, in general, we have

$$\nabla \cdot J + \frac{\partial \rho}{\partial t} = 0 \quad , \quad \text{continuity equation}$$

But, since $\rho = \nabla \cdot \frac{1}{4\pi} D$, we have

$$\nabla \cdot J + \frac{\partial \rho}{\partial t} = \nabla \cdot \left(J + \frac{1}{4\pi} \frac{\partial D}{\partial t} \right) = 0$$

Then Maxwell replaced J in Ampere's law with

$$J \longrightarrow J + \frac{1}{4\pi} \frac{\partial D}{\partial t}$$

So that Ampere's law became

$$\nabla \times H = \frac{4\pi}{c} J + \frac{1}{c} \frac{\partial D}{\partial t}$$

Maxwell called $\frac{\partial D}{\partial t}$ the displacement current. It symmetrized the free space versions ($J=0$) to $\nabla \times H = \frac{1}{c}\frac{\partial D}{\partial t}$, $\nabla \times E = -\frac{1}{c}\frac{\partial B}{\partial t}$ suggest mutual production of E and B (waves)

From this insight, Maxwell predicted:
light is E-M wave phenomenon, and should be waves of all frequencies!

Maxwell's Equations:

in Gaussian ($\varepsilon_0=\mu_0=1$)

$$\boxed{\begin{array}{ll} \nabla\cdot D=4\pi\rho & \nabla\times E=-\frac{1}{c}\frac{\partial B}{\partial t} \\ \nabla\cdot B=0 & \nabla\times H=\frac{4\pi}{c}J+\frac{1}{c}\frac{\partial D}{\partial t} \end{array}}$$

in rationalized MKS

$\varepsilon_0=\frac{10^7}{4\pi c^2}\left(I^2t^4m^{-1}l^{-3}\right)$

$\mu_0=4\pi\times10^{-7}\left(mlI^{-2}t^{-2}\right)$

$D=\varepsilon_0E+P, \quad H=\frac{1}{\mu_0}-M$

$$\boxed{\begin{array}{ll} \nabla\cdot D=\rho & \nabla\times E=-\frac{\partial B}{\partial t} \\ \nabla\cdot B=0 & \nabla\times H=J+\frac{\partial D}{\partial t} \end{array}}$$

Plane Waves in Homogeneous, Nonconducting Medium

ε, μ const., non-dispersive (indep of freq.)

$$\nabla\cdot E = 0 \qquad \nabla\times E = -\frac{1}{c}\frac{\partial B}{\partial t}$$
$$\nabla\cdot B = 0 \qquad \nabla\times B = \frac{\mu\varepsilon}{c}\frac{\partial E}{\partial t}$$
(in Gaussian)

By combining two curl equations and using vanishing divergences, each cartesian component of E and B satisfies wave equation:

$$\frac{\partial^2 u}{\partial t^2} = v^2 \Delta u$$

$$v = \frac{c}{\sqrt{\mu\varepsilon}}$$ in freespace $\mu = \varepsilon = 1$ $\Rightarrow v = c$

Wave eq. has well known plane wave solutions

$$u(x,t) = e^{i(k\cdot x - \omega t)}$$

$$|k| = \frac{\omega}{v} = \sqrt{\mu\varepsilon}\,\frac{\omega}{c}$$

For propagation in x-direction, fund. sol. is

$$u(x,t) = A e^{i(kx-\omega t)} + B e^{i(-kx-\omega t)}$$

or

$$u_k(x,t) = A e^{ik(x-vt)} + B e^{-ik(x+vt)}$$

general sol. $\quad u(x,t) = f(x-vt) + g(x+vt) \qquad (\star)$

When medium is dispersive, i.e., if $\mu\varepsilon$ is function of freq.,

Then for <u>each freq. component</u> the plane waves are still solutions,

but reconstructing the (x,t) dep, $\star$ no longer holds, the wave changes shape as it propagates.

Dispersion Characteristics of Dielectrics and Conductors

Simple model of frequency dispersion based on extension of static case:

polarization can arise in two ways: 1. induced dipole moments 2. alignment of randomly oriented permanent dipoles

1. To estimate induced moments, consider harmonically bound charges each charge e bound under restoring force

$$F = -m\omega_0^2 x \qquad (k = m\omega_0^2 \;,\; \omega_0 = \sqrt{\tfrac{k}{m}})$$

x = displacement

Now apply electric field E, with $-F = eE$

$$m\omega_0^2 x = eE$$

Then induced dipole moment is

$$p_{mol} = ex = \frac{e^2}{m\omega_0^2} E = \frac{e^2}{k} E \qquad k = \text{"spring" strength}$$

$\Rightarrow$ polarizibility is $e^2/m\omega_0^2$ or $\sum_j \frac{e_j^2}{m_j \omega_j^2}$

2. For the random case, let Ω be the phase space. For field E applied in z-direction, the Hamiltonian is

$$H = \frac{1}{2m} p^2 + \frac{m}{2}\omega_0^2 x^2 - eEz$$

Then the average dipole moment is

$$\langle p_{mol} \rangle = \frac{\int_\Omega (ez) e^{-\beta H} d\Omega}{\int_\Omega e^{-\beta H} d\Omega} \underset{\uparrow}{=} \frac{e^2}{m\omega_0^2} E \,,$$ same as for induced.

Now consider <u>oscillating</u> case.

For simplicity, neglect difference between applied and local field

$\Longrightarrow$ model only valid for substances of low density.

eg. for electron $(-e)$ bound by harmonic force acted on by $E(x,t)$ is

$$m\left[\ddot{x}+\gamma\dot{x}+\omega_0^2 x\right] = -eE(x,t)$$

γ measures damping force

<u>Assume</u>: (a) amplitude of oscillation small enough so electric field can be eval. at <u>avg</u> pos. of particle.

(b) field varies in time with freq. ω as $e^{-i\omega t}$

Then <u>dipole moment</u> for one electron is

$$p = -ex = \frac{e^2}{m}\left(\omega_0^2-\omega^2-i\omega\gamma\right)^{-1}E$$

Now Spose N mol/unit vol. w/ Z electrons/mol

and there are f_j elec/mol w/ binding freq. ω_j and damping const. γ_j then the diel. const. $\varepsilon = 1+4\pi\chi_e$ is

$$\varepsilon(\omega) = 1+\frac{4\pi N e^2}{m}\sum_j f_j\left(\omega_j^2-\omega^2-i\omega\gamma_j\right)^{-1} \qquad (\star)$$

where $\sum_j f_j = Z$

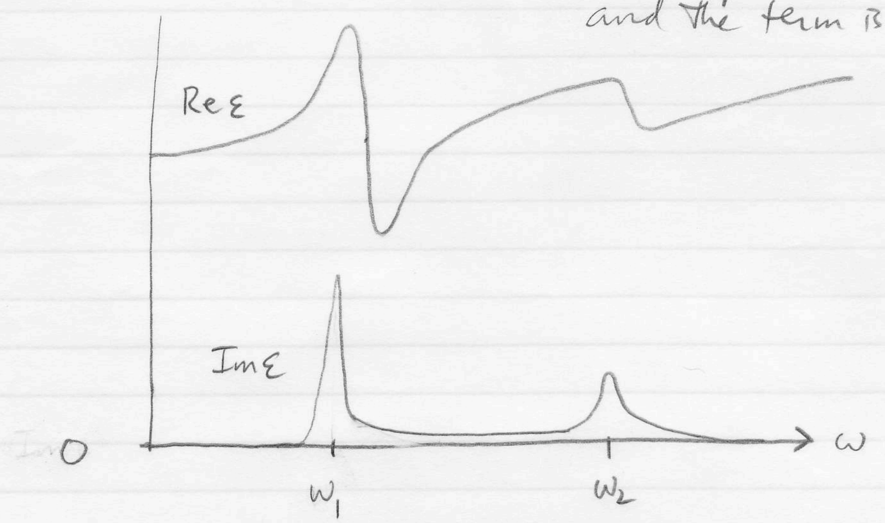
Anomolous Dispersion and Resonant Absorption

Generally $\gamma_j \ll \omega_j \Rightarrow \varepsilon(\omega)$ approx real for most ω

$\frac{1}{\omega_j^2 - \omega^2}$ is pos for $\omega < \omega_j$ and neg for $\omega > \omega_j$

A low freq., below the smallest ω_j, all terms in (★) are pos, and $\varepsilon(\omega) > 1$. As ω incr, and get more and more neg. terms, eventually, $\varepsilon(\omega) < 1$.

Resonance: ω near ω_j Real part of denom in (★) vanishes and the term is large and imaginary



Normal Dispersion: incr. in $\mathrm{Re}\,\varepsilon(\omega)$ with ω (occurs everywhere except in nbhd. of resonance)

Anomolous Dispersion: decr. in $\mathrm{Re}\,\varepsilon(\omega)$ with ω

Resonant Absorption: $\mathrm{Im}\,\varepsilon$ large and pos. — wave loses energy

($\mathrm{Im}\,\varepsilon < 0 \Rightarrow$ energy given to wave by med. — laser)

<u>Attenuation of plane wave</u>. Write wave number as

$$k = \beta + i\frac{\alpha}{2} = \sqrt{\mu\varepsilon}\,\frac{\omega}{c}$$

α = absorption coeff. or attenuation const.

intensity of wave $\sim e^{-\alpha z}$

We have from above (with $\mu = 1$)

$$\beta^2 - \frac{\alpha^2}{4} = \frac{\omega^2}{c^2}\,\mathrm{Re}\,\varepsilon$$

$$\beta\alpha = \frac{\omega^2}{c^2}\,\mathrm{Im}\,\varepsilon$$

If $\alpha \ll \beta$ (weak absorption) then

$$\alpha \approx \frac{\mathrm{Im}\,\varepsilon(\omega)}{\mathrm{R}\,\varepsilon(\omega)}\,\beta\,, \qquad \beta = \sqrt{\mathrm{Re}\,\varepsilon}\;\omega/c$$

<u>Low Frequency Behavior</u>:

As $\omega \to 0$, response depends on whether lowest res. freq. is zero or not.

For insulators, the lowest res. $\neq 0$. Then at $\omega = 0$

the molecular polarizability given by $\sum \frac{e_j^2}{m_j\omega_j^2}$, as before

Now, if some fraction f_0 of electrons/molecule are <u>free</u> $(\omega_0 = 0)$

then $\varepsilon(\omega)$ is singular at $\omega = 0$.

Now separate out free electron behavior, from (★)

$$\varepsilon(\omega) = 1 + C\sum f_j \frac{1}{(\omega_j^2-\omega^2-i\omega\gamma_j)}\ , \quad C = \frac{4\pi Ne^2}{m}$$

$$= \hat{\varepsilon} - C\,\frac{f_0}{\omega(i\gamma_0+\omega)} \qquad \leftarrow \omega_0 = 0\ , \quad \hat{\varepsilon} = \text{contr. from non-zero res.}$$

$$= \hat{\varepsilon} + i\,\frac{Cf_0}{\omega(\gamma_0-i\omega)} \qquad (★★)$$

Lets examine this singular behavior:

$$\nabla\times H = \frac{4\pi}{c}J + \frac{1}{c}\frac{\partial D}{\partial t}$$

Now assume Ohm's Law $J=\sigma E$ and has "normal" dielectric const $\hat{\varepsilon}$ $(D=\hat{\varepsilon}E)$

Assume harmonic time dependence for fields $e^{-i\omega t}$

$$(\nabla\times H)e^{-i\omega t} = \left(\frac{4\pi}{c}\sigma E + \frac{1}{c}(-i\omega)\hat{\varepsilon}E\right)e^{-i\omega t}$$

$$\nabla\times H = -i\frac{\omega}{c}\left(\hat{\varepsilon} + i\frac{4\pi\sigma}{\omega}\right)E$$

Now, if we had not inserted Ohm's law explicitly, but attributed all properties of medium to the dielectric constant, then we would identify

$$\varepsilon(\omega) = \hat{\varepsilon} + i\frac{4\pi\sigma}{\omega}$$

Comparison of this expression with (★★) yields

$$\sigma = \frac{f_0 N e^2}{m(\gamma_0 - i\omega)} ,$$

which is essentially the model of Drude (1900) for electrical cond., w/ $f_0 N$ = # free elec. / unit vol.
(Assume $f_0 = O(1)$)
Measurements of conductivity of copper give $\gamma_0 \sim O(10^{13})$
$\Rightarrow$ At frequencies well beyond microwave region $\omega \lesssim 10^{11}\ \mathrm{sec}^{-1}$, conductivities of metals are essentially real ($\gamma_0 \gg \omega$)
i.e., the current is in phase w/ field and indep. of freq.

At higher frequencies (infrared and beyond) cond. is complex and varies w/ freq., described qualitatively by above Drude-model.

Free electrons actually valence electrons of isolated atoms that become quasi-free and move through lattice (if their energies lie in certain bands)

Damping effects come from collisions involving momentum transfer between electrons and lattice vibrations, imperfections + impurities.

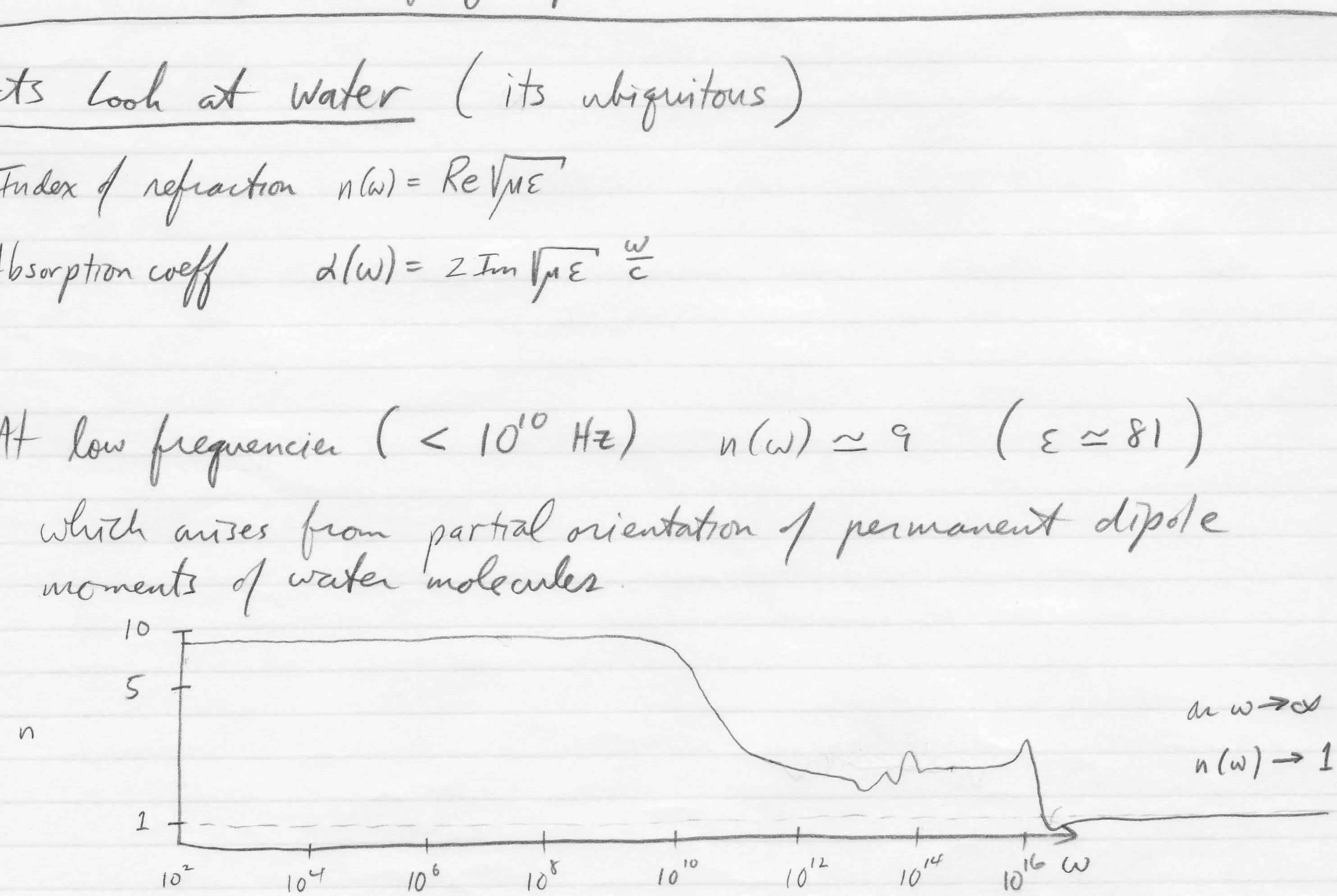
The above shows that distinction between dielectrics and conductors is an artificial one, at least away from $\omega = 0$.
If the medium has free electrons, it is a cond. at low freq., otherwise it is an insulator.
But at non-zero frequencies, the "cond." contribution to (☆) appears as a resonant amplitude.
Thus: the dispersive properties of the medium can be attributed equally well to a complex dielectric constant, as to a freq.-dep. cond. and a dielectric constant.

Lets Look at Water (its ubiquitous)

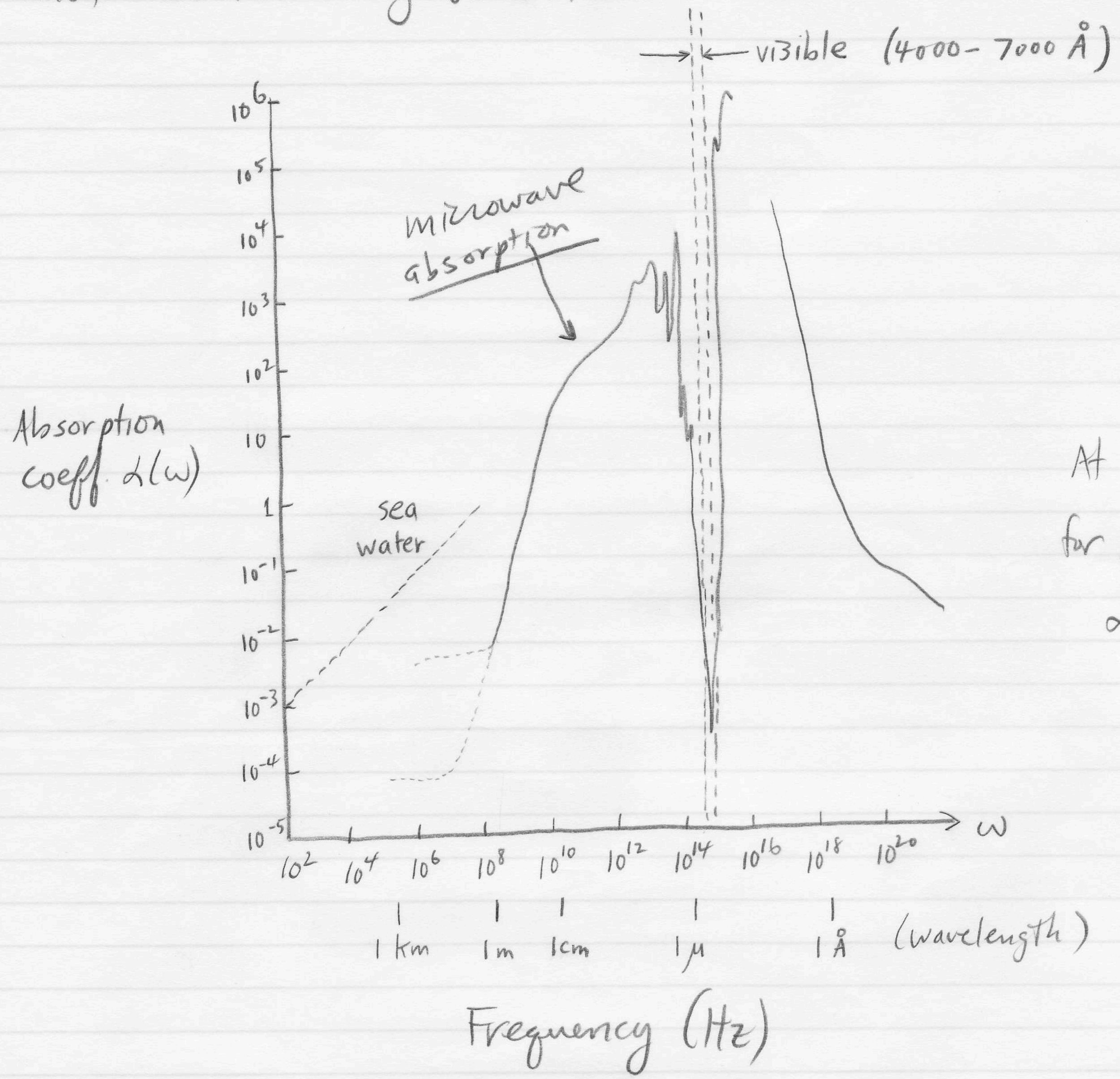
Index of refraction $n(\omega) = \mathrm{Re}\sqrt{\mu\varepsilon}$

Absorption coeff $\alpha(\omega) = 2\,\mathrm{Im}\sqrt{\mu\varepsilon}\ \frac{\omega}{c}$

At low frequencies ($< 10^{10}$ Hz) $n(\omega) \simeq 9$ ($\varepsilon \simeq 81$)
which arises from partial orientation of permanent dipole moments of water molecules



$\alpha(\omega)$ has fascinating behavior



At low freq. for sea water $\alpha \sim \sqrt{\omega}$

visible window (4000-7000 Å)

water is transparent in this freq. regime.

(origins in energy level structure of atoms and molecules)

animals see in this spectrum regime!

Nature has exploited this window !

Homogenization on Molecular Scale

Goal: Find macroscopic or effective properties (ε) from molecular properties.

Induced dipole p_i of molecule i induced by field E_{local} (field seen by i, which is function of applied field and all other dipoles)

$$p_i = \alpha E_{local}$$

α = molecular, atomic, or ionic polarizability

Polarization field P arising from induced dipoles, if all identical and n_0 per unit volume is (with $p_i \parallel E_{local}$)

$$P = n_0 \alpha E_{local}$$

Remarks: E = macroscopic field strength
= avg of vector sum of all dipoles in medium

E_{local} = actual field seen by i, which is E, excluding the effect of dipole i, which does not act on itself.

We may then write

$$E_{local} = E + E_{corr}.$$

<u>Note</u>: even though $E_{dipole} \sim \frac{1}{r^3}$, sums do not converge rapidly

there are larger numbers of dipoles far away, so their contr. is as important as nearby dipoles

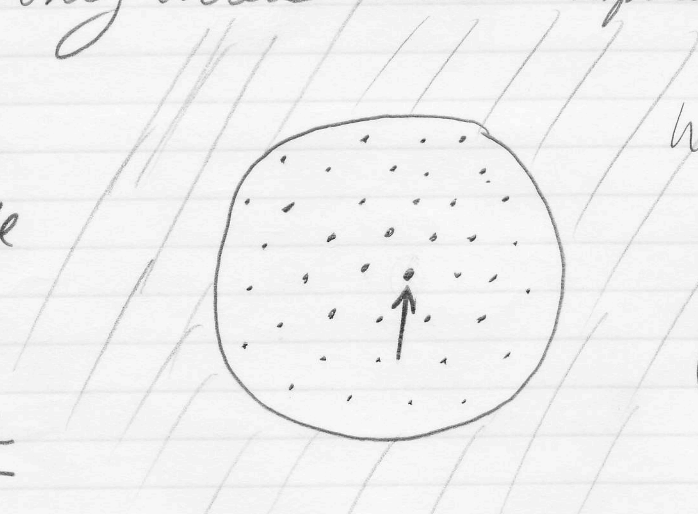
$\Rightarrow$ dipole field is "long-range"

The Lorentz Correction and Clausius-Mossotti Relation

Get approx sol. to E_{corr} (Lorentz)

applies only when induced dipoles parallel to appl. E

<u>calculate E_{local} at center of sphere</u>



homog medium with polarization P

(effective medium)

homog med. produces contribution $= E'$

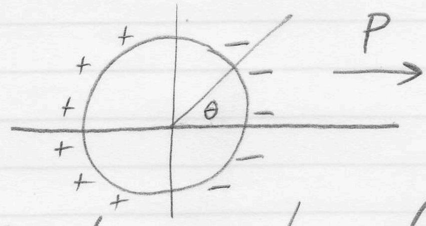
net field strength of "nearby" dipoles $= E''$

(radius of sphere is large compared to intermolecular distances so get representative average)

Then write

$$E' + E'' = E_{corr}$$

To calculate E'



only contribution is from bound surface charge density (with − sign since we want contr. from <u>outside</u> sphere)

$$\sigma_p = -P \cdot n = -P\cos\theta$$

Integrating,

$$E' = \frac{1}{3\varepsilon_0} P,$$

where P is actual polarization in medium.

For E'', Lorentz showed that for cubic array of parallel dipoles, $\underline{E'' = 0}$

result valid for induced dipoles which are parallel to applied field, but <u>not</u> for randomly oriented permanent dipoles (such as water)

Now, with $E'' = 0$, we have

$$E_{corr} = E' = \frac{1}{3\varepsilon_0} P$$

$\Longrightarrow$

$$E_{local} = E + E_{corr} = E + P/3\varepsilon_0$$

But $\quad P = n_0 \alpha E_{local}$

$\varepsilon =$ diel. const. (rel.)

$$D = \varepsilon_0 E + P = \varepsilon \varepsilon_0 E$$

$\Longrightarrow$

$$P = n_0 \alpha \left(E + P/3\varepsilon_0\right)$$

$$P = (\varepsilon - 1)\varepsilon_0 E$$

$$\varepsilon_0 (\varepsilon - 1) E = n_0 \alpha \left(E + \tfrac{1}{3}(\varepsilon - 1) E\right)$$

$$3\varepsilon_0 (\varepsilon - 1) E = n_0 \alpha (\varepsilon + 2) E$$

$$\therefore \quad \frac{\varepsilon - 1}{\varepsilon + 2} = \frac{n_0 \alpha}{3\varepsilon_0}$$

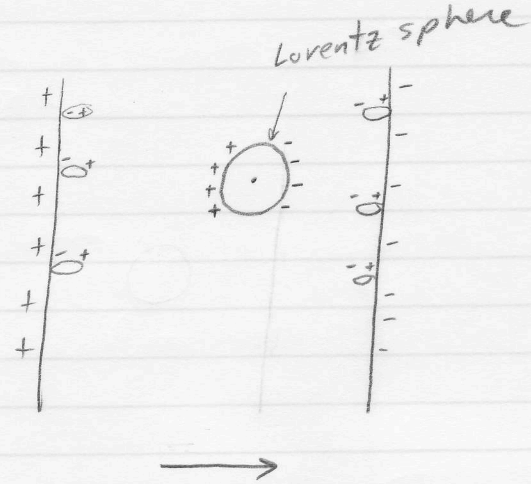
Claussius-Mossotti Relation

In Gaussian units

$$\frac{\varepsilon - 1}{\varepsilon + 2} = \frac{4\pi n_0 \alpha}{3} \qquad \text{(CM)}$$

Remarks about derivation:

Consider following set-up



$$E_{loc} = E_x + E_d + E_s + E''$$

E_x = field due to plates

E_d = depolarizing field due to bound charge at plates

E_s = field (in pos dir.) due to bound charge outside surface of sphere

E'' = field from dipoles inside sphere

The macroscopic field is $E = E_x + E_d$

So that

$$E_{loc} = E + E_s + E''$$

We have seen $E_s = \frac{1}{3\varepsilon_0} P$ (We called it E' before)

$E'' = 0$ this is the Lorentz calculation based on symmetry of sample (sphere)

Note: Lorentz calc $\not\Rightarrow$ zero contr. from all dip.

Thus $\boxed{E_{loc} = E + \frac{1}{3\varepsilon_0} P}$ which yields CM

CM works for other polarizable bodies on macro scale.
considered as expression for $\varepsilon^* =$ effective diel. const.
$\alpha =$ polarizability of individual bodies.

If entities are polarizable spheres of diel. const. ε_1 and radius a, then we have

$$\alpha = \frac{a^3(\varepsilon_1 - 1)}{(\varepsilon_1 + 2)}$$

Combining with CM yields

$$\frac{\varepsilon^* - 1}{\varepsilon^* + 2} = p_1 \frac{\varepsilon_1 - 1}{\varepsilon_1 + 2} \qquad p_1 = \text{vol frac. of spheres}$$

If spheres embedded in material ε_0 instead of free space ($\varepsilon = 1$),

$$\frac{\varepsilon^* - \varepsilon_0}{\varepsilon^* + 2\varepsilon_0} = p_1 \frac{\varepsilon_1 - \varepsilon_0}{\varepsilon_1 + 2\varepsilon_0}$$

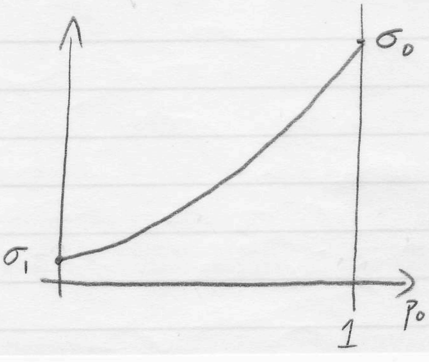
<u>NOTE</u>: This expression for ε^* <u>not</u> symmetric in ε_0 and ε_1.

Can write generalization to n types of spheres

$$\frac{\varepsilon^* - \varepsilon_0}{\varepsilon^* + 2\varepsilon_0} = \sum_{i=1}^{n} p_i \frac{\varepsilon_i - \varepsilon_0}{\varepsilon_i + 2\varepsilon_0}$$

<u>Note</u>: CM for effective conductivity yields

$$\sigma^* = \frac{(1 + 2p_1)\sigma_1 + 2p_0\sigma_0}{2 + p_1 + p_0 \frac{\sigma_1}{\sigma_0}} \qquad \begin{array}{l} p_1 \text{ vol frac } \varepsilon_1 \\ p_0 \text{ vol frac } \varepsilon_0 \end{array}$$



$\sigma_0 \gg \sigma_1$

<u>NO PERCOLATION THRESHOLD</u>

Remark: We get two different expressions for ε^*, depending on whether ε_0 is the host, or if ε_1 is the host, call them ε_0^* and ε_1^*

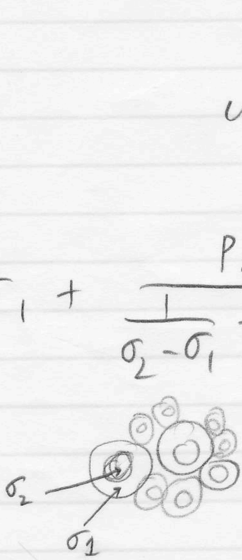
Observation: de Loor (1956) notes that for two component, isotropic composites,

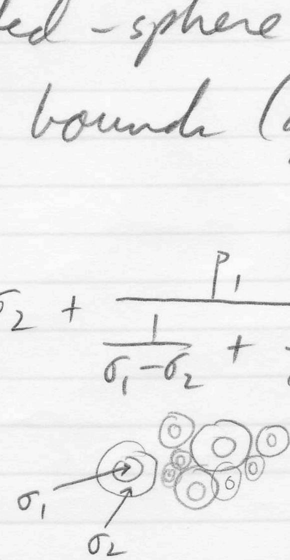
$$\varepsilon_1^*(p) \leq \varepsilon_{meas}^*(p) \leq \varepsilon_0^*(p) \qquad p = \text{vol frac.}$$

i.e., the measured values for ε^* for isotropic composites lie between the CM expressions.

Breakthrough: Hashin and Shtrikman (1962) prove that the two CM expressions form rigorous, optimal upper and lower bounds on ε^* for two-component isotropic media!
They generalize to n-component.
They construct coated-sphere geometries which attain the bounds (optimality).

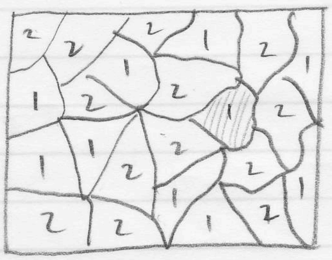
$$\sigma_1 + \frac{p_2}{\frac{1}{\sigma_2 - \sigma_1} + \frac{p_1}{d\sigma_1}} \leq \sigma^* \leq \sigma_2 + \frac{p_1}{\frac{1}{\sigma_1 - \sigma_2} + \frac{p_2}{d\sigma_2}} \qquad \sigma_1 \leq \sigma_2$$





Effective Medium Theories

Bruggeman's symmetrical EMT



σ_1, σ_2

let cross-hatched crystal be spherical

assume it is embedded in uniform medium w/ effective conductivity σ_m (the effective medium)

If field far from inclusion is E_0, then dipole moment associated w/ inclusion is

$$p = \frac{3}{4\pi} V \frac{\sigma_1 - \sigma_m}{\sigma_1 + 2\sigma_m} E_0 \quad , \qquad V = \text{vol of incl.}$$

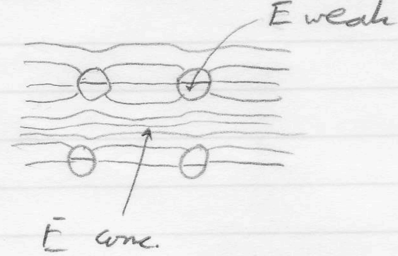
This polarization produces a deviation from E_0

The space integral of deviation is $-4\pi p$.

Now, the average deviation from E_0 must vanish

$$\langle E \rangle = E_0$$

fluctuations must avg. to zero.



Thus, the total polarization summed over the two types of inclusions must vanish

$$\langle P \rangle \overset{\text{assume}}{=} p_1 \frac{\sigma_1 - \sigma_m}{\sigma_1 + 2\sigma_m} + p_2 \frac{\sigma_2 - \sigma_m}{\sigma_2 + 2\sigma_m} = 0 \qquad (\star)$$

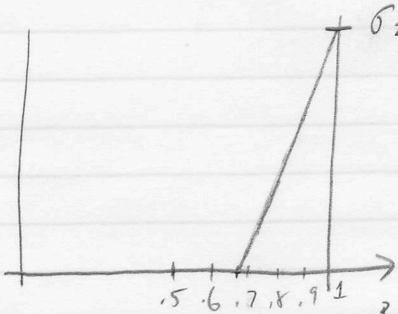
(This is where symmetry in σ_1 and σ_2 is introduced)

Quadratic equation for σ_m whose pos. sol. is

$$\sigma_m = \frac{1}{4}\left(\gamma + \sqrt{\gamma^2 + 8\sigma_1\sigma_2} \right) = \sigma_m(\sigma_1, \sigma_2, p_1, p_2)$$

where

$$\gamma = (3p_2 - 1)\sigma_2 + (3p_1 - 1)\sigma_1$$



$\Longrightarrow$ perc. threshold!

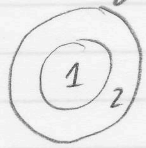
Can easily generalize to n components.

This is most commonly invoked approx in field

in d-dimensions $\quad p_1 \dfrac{\sigma_1 - \sigma_m}{\sigma_1 + (d-1)\sigma_m} + p_2 \dfrac{\sigma_2 - \sigma_m}{\sigma_2 + (d-1)\sigma_m} = 0$

Also called: Coherent Potential Approximation (CPA)
(from Solid State phys: estimating props of random alloys)

Remark: If apply EMT to coated spheres



then get H-S expression

$$\sigma^* = \sigma_2 + \frac{p_1}{\frac{1}{\sigma_1 - \sigma_2} + \frac{p_2}{d\sigma_2}}, \quad \sigma_1 \le \sigma_2$$

Thus EMT is exact for coated sphere geom.
sphere on all scales, fill space. (very special geom)

Can do EMT for ellipsoids (Sihvola, Kong 1988)
coated ellipsoids (Tinga, et. al., 1973)

EMT works well in many situations
it is the most widely invoke approximation in field.

HOWEVER range of validity unclear:
— Unclear what restrictions must have on geometry for EMT to work well

MILTON (1984): Produced class of hierarchical models for which EMT, in particular, the Bruggeman symm EMT (or CPA), is EXACT

Let's re-examine CPA. Consider again a granular aggregate two components σ_1, σ_2 w/ vol. frac. f_1, f_2, $f_1 + f_2 = 1$.

Spose the aggregate is injected w/ fluid of uniform conductivity σ_0, which forces grains apart get a suspension of well-separated grains

Let c be the vol. frac. of grains in fluid suspension

<u>Basic assump. of CPA</u>: If σ_0 is chosen to be σ^*, the eff. cond. of the aggregate, then σ_f^*, the eff. cond. of the fluid suspension, is almost invariant under injection as $c \to 0$

To examine, lets expand σ_f^* near $c=0$,

$$\sigma_f^* = \sigma_0 \left[1 + c P(\sigma_0) + o(c) \right],$$

where

$P(\sigma)$ is the avg. polarizability of grains in a matrix of conductivity σ. For well separated grains

$$P(\sigma) = \sum_{i=1}^{2} f_i \, p_i(\sigma)$$

p_i = individual polarizability of i^{th} type of grain

depends on σ_i, σ of fluid, and shape and orientation of grain.

<u>spherical grains:</u>

$$p_i(\sigma) = \frac{3\sigma_i - \sigma}{\sigma_i + 2\sigma}$$

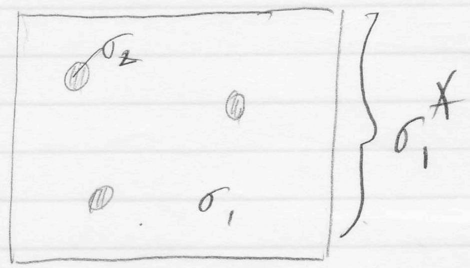
From expansion, the variation of σ_f^* in c $(c \ll 1)$, is minimal when $\sigma_0 = \sigma_m$, (the EMT expression) satisfying

$$P(\sigma_m) = 0, \qquad (\star)$$

which has unique sol.

Condition $(\star)$ makes σ_f^* nearly constant under injection, as $c \to 0$.

Consider following sequence of media



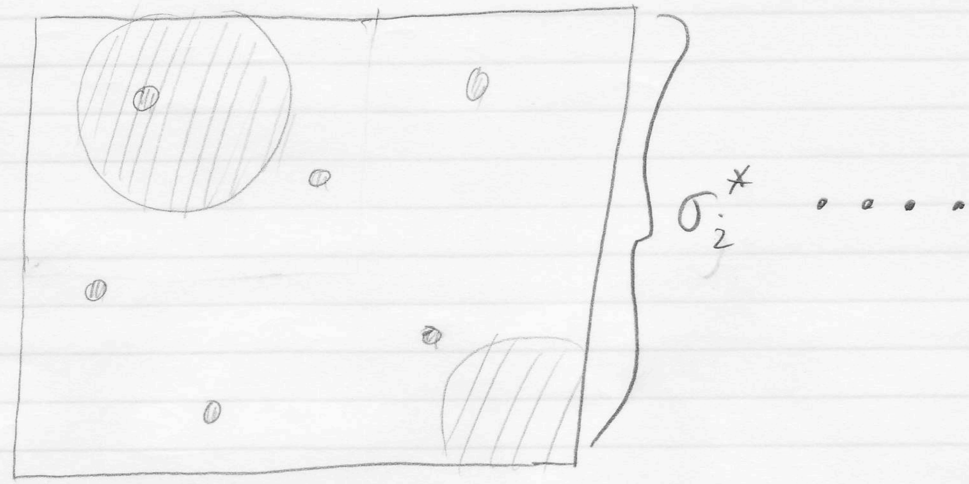
M_1

spheres of σ_2 in σ_1 host

rad $= r_1$

vol. frac $= c_1$

sph. centers sep $\geq 2 s_1$



M_2 = embed spheres of σ_2 in M_1 so that

rad $= r_2$

vol frac $= c_2$

sph. cents sep $\geq 2 s_2$

Keep iterating get hierarchical, self-similar fractal medium

spheres satisfy ① homogeneity condition to prevent macroscopic clustering

② The sequences $\{r_j\}$, $\{c_j\}$, $\{s_j\}$ satis

$$s_j \gg r_j \gg s_{j-1}$$

and such that only negligible vol frac of M_1 remains as $j \to \infty$

Under such conditions

$$\lim_{j \to \infty} \sigma_j^* = \sigma_m \text{ , the EMT (CPA) approximation}$$

The construction can be generalized to non-spherical grains

Note: for j large, the medium surrounding the largest spheres (are well-sep. and have vol frac. c_j ($\to 0$)) is behaving like the fluid

$j \to \infty \iff$ injection of more fluid!

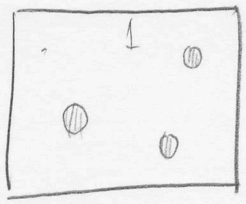
Fixed points of σ^* under transformation $j \to j+1$ are

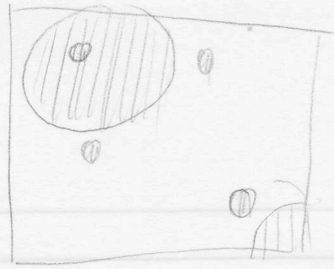
① ∞ (carving out spheres of ∞ cond mat. leaves eff cond. ∞)
② 0 (" " 0)
③ CPA

Idea of proof: Instead consider $\log \sigma^*$
then fixed points are $-\infty, \infty, \log$ CPA

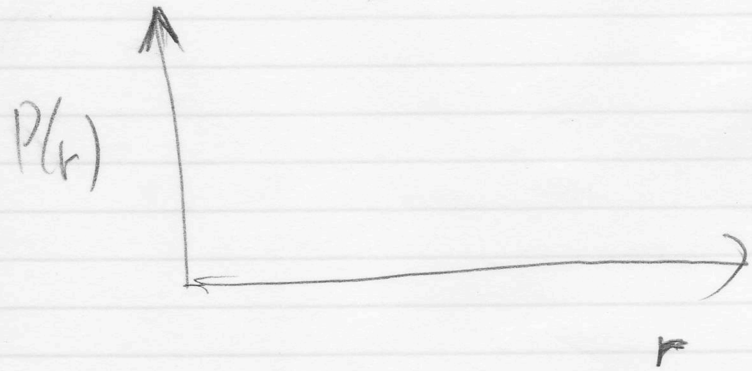
Prove transformation $j \to j+1$ is contraction with only finite fixed point $\log$ CPA!

7:45 → 11:10 #68
8:44 → 12:10 # 68.
→ 9:39 → 12:28 $96

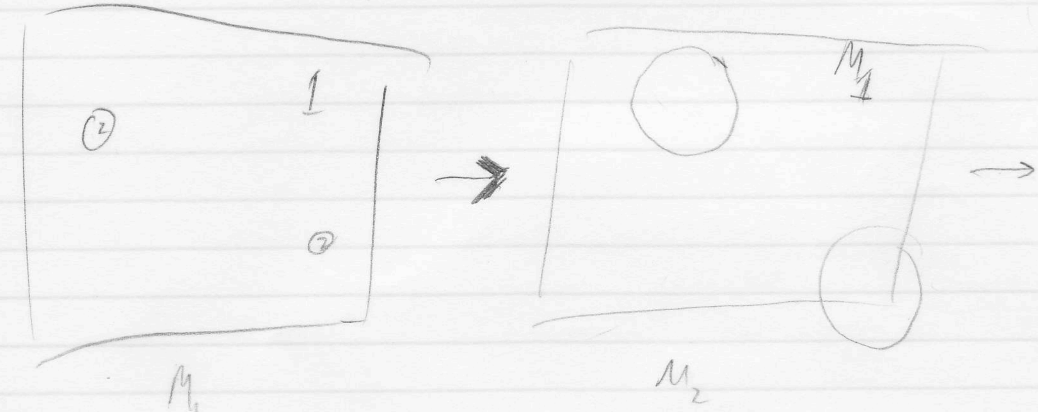




dist of sph size
dist of so wide &
that spheres of comp size
very far from each other



extremely broad
peak is very



holes/ref
r_i w/ sp s_i

eff med $(M_j) \xrightarrow[j\to\infty]{}$

low case of diff schm
diff sch → eff med. sch

holes in ref don't get info

indep of starting material

Fixed points ① ∞
② 0 same
③ CPA

take $\log \sigma^*$
contractions

$$\sigma_1 + \frac{p_2}{\frac{1}{\sigma_2-\sigma_1}+\frac{p_1}{d\sigma_1}} \le \sigma^* \le \sigma_2 + \frac{p_1}{\frac{1}{\sigma_1-\sigma_2}+\frac{p_2}{d\sigma_2}}$$

$\sigma_1 \le \sigma_2$

$\sigma_1 = 0$

$\sigma_2 = 1$

$$0 \le \sigma^* \le 1 + \frac{p_1}{-1+\frac{p_2}{d}}$$

CM exhibits no perc. thresh

H-S " " perc. thresh

Bruggem EMT <u>does</u> exhibit perc thre

Bruggeman

HS $\Longleftrightarrow$

Hill

CPA avg pol $= 0$ choose of med st.

H-S : choose of med so field in ext is unif.

$\ominus$ 0 polariz

538-8300

PERTURBATION EXPANSIONS

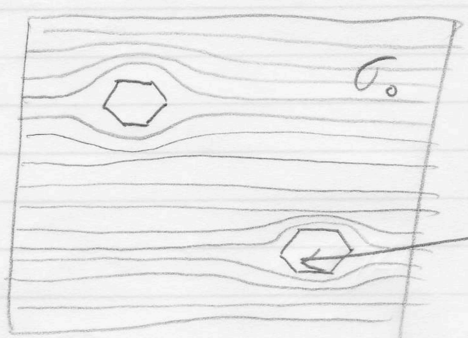
1. Volume Fraction Expansions (small p)
2. Expansion around Homogeneous Medium (small dev. in $\varepsilon(x)$ from homog)
3. "Almost Touching" Problems

1. Volume fraction expansions

Kozlov (1989)

Thorpe (1992)

Golden (1991), Bruno + Golden (1992)



Thorpe

holes (a few)

n-gons

Show
$$\frac{\sigma^*}{\sigma_0} = 1 - \alpha_n f + O(f^2)$$

$f =$ vol. frac. $= ns$

$n =$ # holes / unit area

$s =$ area of 1 hole.

$$\alpha_n = \frac{\tan(\pi/n)}{2\pi n}\,\Gamma^4\left(\tfrac{1}{n}\right)\Big/\Gamma^2\left(\tfrac{2}{n}\right)$$

$\alpha_n =$ 2.5811 triangles

2.1884 squares

2.0878 pentagons

⋮

$\alpha_n = 2$ as $n \to \infty$ (circle)

Idea: hole gets induced charge around perimeter
total induced charge = 0 →

get multipole distr.

for circle – induced charge only has dipole term
with potential that decays like $1/r$

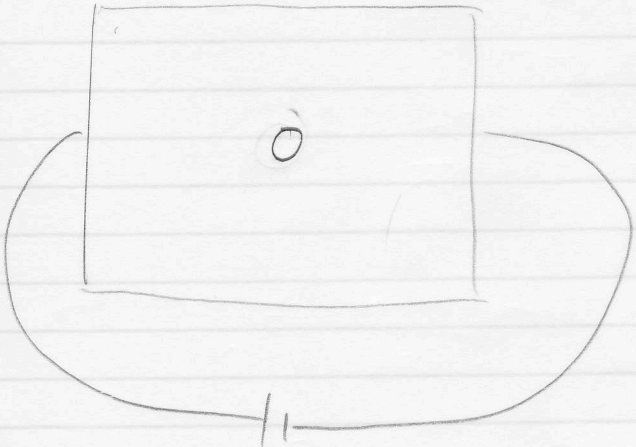
for other holes – have full multipole expansion
but only coef. of dipole term contr.
to f term

in $$\frac{\sigma}{\sigma_0} = 1 - \alpha f + O(f^2)$$

How small must f be to ignore higher order terms?

Answer: pert. caused by current flow around one hole cannot significantly
overlay with pert. around another one.

Now do for circle in 2 dimensions using conformal mapping



conductivity drops when
put in hole

Must solve Laplace equation $\Delta u = 0$ around hole w/ Neumann BC. - no flow into the hole

$$w = \frac{1}{2}\left(\frac{z}{a} + \frac{a}{z}\right), \quad a = \text{radius of hole}$$

In w-plane complex potential $u = -E_0 w$

$E_0 = E$ field at ∞

actual potential $= \mathrm{Re}[u]$

In z-plane

$$u = -E_0'\left(z + \frac{a^2}{z}\right)$$

$E_0' = E$ field at ∞ in z-plane

at distance R from circle

$$\mathrm{Re}[u] = -E_0' R\cos\theta\left(1 + \frac{a^2}{R^2}\right) = -E_0' R\cos\theta\,(1+f)$$

$f =$ area frac of hole $= \dfrac{\pi a^2}{\pi R^2}$

For large R, potential same with or without hole

$$\Rightarrow \quad E_0 = E_0'(1+f)$$

Now, relate to cond.

Joule heating inside large circle of rad R =

$\boxed{J=\sigma E}$

$$\int_{D_R} J\cdot E \, da = -\int_{\partial D_R} u(J\cdot ds)$$

(no current flows across inner surface)

Because $\sigma=0$ inside hole - don't need to know E inside hole - fortunately!

change in Joule heating upon introduction of hole is

$$\int_0^{2\pi} (E_0 R\cos\theta)\,\sigma_0 \left[E_0'\cos\theta\,(1-f) - E_0\cos\theta\right] R\,d\theta$$

$$= -2\sigma_0 E_0 E_0' \pi a^2$$

indep of R

Energy balance gives

$$\sigma E_0^2 \pi R^2 = \sigma_0 E_0^2 \pi R^2 - 2\pi\sigma_0 E_0 E_0' \pi a^2$$

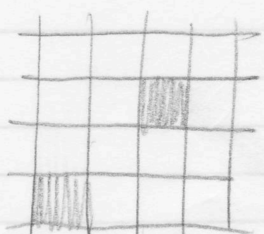
which yields

$$\frac{\sigma}{\sigma_0} = 1 - 2n\pi a^2 = 1-2f$$, to leading order in f

factor a^2 is coef. of dipole term $\frac{1}{z}$ in conf-map

Rigorous Results for Volume Fraction Expansion

Related model to Thorpe's : **chessboard**



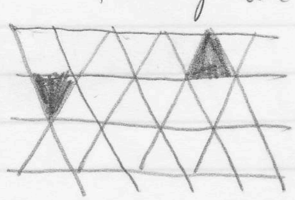
square

$$\sigma(x) = \begin{cases} 1 & 1-p \\ \delta \geq 0 & p \end{cases}$$

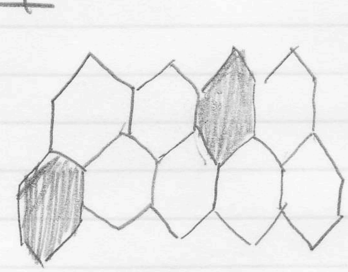
$n = 4$

Now treat small p

triangular



$n = 3$



hexagonal

$n = 6$

$\sigma_n^*(p, \delta)$ is eff. cond. for $n = 3, 4, 6$

$\sigma_n^*(p) = \lim_{\delta \to 0} \sigma_n^*(p, \delta)$

Theorem (Kozlov): For sufficiently small p,

$$|\sigma^*(p) - 1 + \alpha_n p| \leq C p^2$$

α_n as before, from Thorpe.

It follows that $\sigma_n^*(p)$ is diff at $p=0$ (one sided)

and $\left.\dfrac{d\sigma_n^*}{dp}\right|_{p=0} = -\alpha_n$

Proof is via stronger assertion

Thm $\exists$ pos consts. $\bar{p}, \bar{c}$ st.

$$|\sigma_n^*(p,\delta) - 1 + \alpha_n(\delta)p| \leq \bar{c}p^2, \quad 0 \leq p \leq \bar{p},$$

where $\lim_{\delta\to 0} \alpha_n(\delta) = \alpha_n$. The est. is valid $\forall\,\delta$.

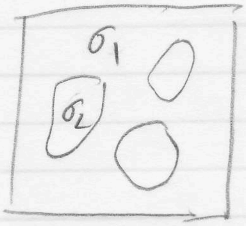
The consts. $\bar{c}, \bar{p}$ are indep of δ.

Full proof involves percolation theory as $\delta \to 0$.

Want to prove $\sigma^*(p,\delta)$ analytic in p for $\delta > 0$

Need pert. around homog. med.

Perturbation around homogeneous medium



$\sigma_1 = \sigma_2$ homog.

$$\sigma(x,\omega) = \sigma_1 \chi_1(x,\omega) + \sigma_2 \chi_2(x,\omega) \qquad \begin{matrix}\omega \in \Omega \text{ w/ } P \\ x \in \mathbb{R}^d\end{matrix}$$

$$J = \sigma E$$

$$\nabla \cdot J = 0 \qquad J, E \in L^2(\Omega, P)$$

$$\nabla \times E = 0$$

$$\langle E \rangle = e_k$$

$$\sigma^* \langle E \rangle = \langle J \rangle = \langle \sigma E \rangle$$

tensor

k,k diag. coef $\sigma^* = \sigma^*_{kk} = \langle \sigma E_k \rangle$

$$\sigma^* = \langle (\sigma_1 \chi_1 + \sigma_2 \chi_2) E_k \rangle$$

$$\frac{\sigma^*}{\sigma_2} = \left\langle \left(\frac{\sigma_1}{\sigma_2} \chi_1 + \chi_2 \right) E_k \right\rangle$$

$$m(h) = \langle (h\chi_1 + \chi_2) E_k \rangle$$

$$= \langle (h\chi_1 + 1 - \chi_1) E_k \rangle = 1 + \langle (h-1) \chi_1 E_k \rangle$$

Define $\quad F = 1 - m(h)$

$$F = \langle (1-h)\chi_1 E_k \rangle \qquad s = \frac{1}{1-h} = \frac{1}{1-\sigma_1/\sigma_2}$$

$$F(s) = \langle \frac{\chi_1}{s} E_k \rangle$$

Derive resolvent repr. for E.

$$\nabla\cdot(h\chi_1+\chi_2)E = 0$$

$$\nabla\cdot(h\chi_1+1-\chi_1)(e_k+G) = 0$$

$G \in L^2(\Omega) \cap$ curl free $\cap$ mean zero. $= \mathcal{H}$

$$\nabla\cdot(1-\tfrac{1}{s}\chi_1)(e_k+G) = 0$$

$$\nabla\cdot\left(e_k + G - \tfrac{1}{s}\chi_1 e_k - \tfrac{1}{s}\chi_1 G\right) = 0$$

$$\nabla\cdot\left(G - \tfrac{1}{s}\chi_1(e_k+G)\right) = 0$$

$$\nabla\cdot(sG - \chi_1(e_k+G)) = 0$$

$$s\nabla\cdot G - \nabla\cdot\chi_1 E = 0 \qquad \angle\; G = \nabla\varphi$$

$$s\Delta\varphi - \nabla\cdot\chi_1 E = 0$$

$$-s\varphi - (-\Delta)^{-1}\nabla\cdot\chi_1 E = 0$$

$$-sG - \underbrace{\nabla(-\Delta)^{-1}\nabla\cdot}_{\Gamma}\chi_1 E = 0$$

Γ = projection onto curl free fields

$$-sG + \Gamma\chi_1 E = 0$$

$$G + \tfrac{1}{s}\Gamma\chi_1 E = 0$$

$$E + \tfrac{1}{s}\Gamma\chi_1 E = e_k$$

$$sE + \Gamma \chi_1 E = s e_k$$

$$E = s(s+\Gamma\chi_1)^{-1} e_k$$

$$\therefore \quad F(s) = \left\langle \frac{\chi_1}{s} \cdot s\left((s+\Gamma\chi_1)^{-1} e_k\right) \cdot e_k \right\rangle$$

$$F(s) = \langle \chi_1 \, (s+\Gamma\chi_1)^{-1} e_k \cdot e_k \rangle$$

$\Gamma\chi_1$ is s.a. operator on $\mathcal{H}$ w/ χ_1 in inner product

w/ $\quad \|\Gamma\chi_1\| \leq 1$

for $|s| > 1$ expand in Neumann series

$$\frac{1}{s+\Gamma\chi_1} = \frac{1}{s\left(1+\frac{\Gamma\chi_1}{s}\right)} = \frac{1}{s}\left(1 - \frac{\Gamma\chi_1}{s} + \frac{(\Gamma\chi_1)^2}{s^2} - \cdots\right)$$

Note expanding around $s = \infty \Longleftrightarrow h = 1$ homog.

$$F(s) = \frac{\langle \chi_1 \rangle}{s} - \frac{\langle \chi_1 (\Gamma\chi_1 e_k \cdot e_k)\rangle}{s^2} + \frac{\langle \chi_1 (\Gamma\chi_1)^2 e_k \cdot e_k \rangle}{s^3} - \cdots$$

Let's do good applied math. : Apply (sophisticated) mathematical techniques to interesting + important physical problem (if do good job (get to essence) it will apply to other problems of similar (or not so similar) type)

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(see spectral thm, resolvent exp, pert theory, spectral measures, Dirac meas, int. eq. orthog. decomp, extremal probs)

$$\nabla\cdot(h\chi_1+\chi_2)E=0$$

(Goal: get bds on complex σ^* under fixed σ_1, σ_2 and geom constraints)

$$\nabla\cdot(h\chi_1+1-\chi_1)(e_k+g)=0$$

$$\nabla\cdot(1+(h-1)\chi_1)(e_k+g)=0$$

$$\nabla\cdot\left(e_k+g+(h-1)\chi_1(e_k+g)\right)=0$$

$$\nabla\cdot g+(h-1)\nabla\cdot\chi_1(e_k+g)=0$$

$g=\nabla\varphi$

$$\nabla\cdot\nabla\varphi+(h-1)\nabla\cdot\chi_1E=0$$

$$(-\Delta)^{-1}\Delta\varphi+(h-1)(-\Delta)^{-1}\nabla\cdot\chi_1E=0$$

$$\varphi+(1-h)(-\Delta)^{-1}\nabla\cdot\chi_1E=0$$

$$\nabla\varphi+(1-h)(-\Delta)^{-1}\nabla\cdot\chi_1E=0$$

$L^2(\mathbb{R}^n)=L^2_{\text{curl free}}+L^2_{\text{div free}}$

$$g+e_k+(1-h)\nabla(-\Delta)^{-1}\nabla\cdot\chi_1E=e_k$$

(Integral eq. for E)

projection onto curl free fields

$$\left(I+\tfrac{1}{s}\Gamma\chi_1\right)E=e_k$$

$$(s+\Gamma\chi_1)E=se_k$$

$$E=s(s+\Gamma\chi_1)^{-1}e_k$$

$\Gamma=\nabla(-\Delta)^{-1}\nabla\cdot$ = integral op

$$\Gamma^2=\nabla(-\Delta)^{-1}\nabla\cdot\left(\nabla(-\Delta)^{-1}\nabla\cdot\right)=\Gamma$$

$\Gamma\chi_1$ self adj in $\langle\chi_1 f\cdot g\rangle$

$$\sigma^*_{kk} = \langle \sigma E^k_k \rangle$$

$$\sigma^*_{kk} = \langle (\sigma_1 \chi_1 + \sigma_2 \chi_2) E^k_k \rangle$$

$$\frac{\sigma^*_{kk}}{\sigma_2} = \langle (h\chi_1 + (1-\chi_1)) E^k_k \rangle$$

$$= \langle ((h-1)\chi_1 + 1) E^k_k \rangle$$

$$\frac{\sigma^*}{\sigma_2} = 1 - \frac{1}{s} \langle \chi_1 E^k_k \rangle$$

$$1 - \frac{\sigma^*}{\sigma_2} = \frac{1}{s} \langle \chi_1 E^k_k \rangle$$

$$= \frac{1}{s} \langle \chi_1 e_k \cdot E^k \rangle$$

$$= \frac{1}{\cancel{s}} \langle \chi_1 e_k \cdot \cancel{s}(s + \Gamma\chi_1)^{-1} e_k \rangle$$

$$F(s) = \langle \chi_1 e_k \cdot (s + \Gamma\chi_1)^{-1} e_k \rangle \qquad f(A) = \frac{1}{s-A}$$

$$= \langle \chi_1 e_k \cdot f(A) e_k \rangle \qquad A = \Gamma\chi_1$$

analytic off $[0,1]$

product of projections

$$= (e_k \cdot f(A) e_k) \qquad \|A\| \le 1$$

$$= \int_{\sigma(A)} f(\lambda)\, d(e_k \cdot P_\lambda e_k)$$

$$= \int_0^1 \frac{d\mu(z)}{s - z} \qquad d\mu = d(e_k \cdot P_\lambda e_k) \geq 0$$

$$F(s) = \langle \chi_1 \ e_k \cdot (s + \Gamma \chi_1)^{-1} e_k \rangle$$

$$F(s) = \int_0^1 \frac{d\mu(z)}{s - z}$$

Need to inject geometry info μ

Resolvent Expansion (Neumann Series
Geom Series)

$$F(s) = \langle \chi_1 \ e_k \cdot \frac{1}{s + \Gamma \chi_1} e_k \rangle$$

$$= \frac{1}{s} \langle \chi_1 \ e_k \cdot \frac{1}{\left(1 + \frac{\Gamma \chi_1}{s}\right)} e_k \rangle$$

pert exp around homog. $\sigma_1 = \sigma_2$

$$= \frac{1}{s} \langle \chi_1 \ e_k \left(1 - \frac{\Gamma \chi_1}{s} + \frac{(\Gamma \chi_1)^2}{s^2} - \dots \right) e_k \rangle$$

$$= \frac{\langle \chi_1 \rangle}{s} + \frac{\langle e_k \cdot \chi_1 \Gamma \chi_1 e_k \rangle}{s^2} + \dots$$

$$= \frac{p_1}{s} + \frac{p_1 p_2 / d}{s^2} + \dots$$

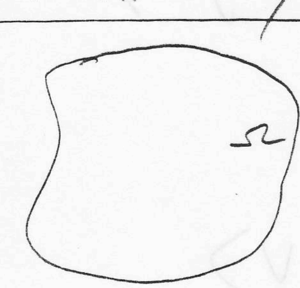
$$F(s) = \int_0^1 \left(\frac{1}{s} + \frac{z}{s^2} + \frac{z^2}{s^3} + \dots \right) d\mu = \frac{\mu_0}{s} + \frac{\mu_1}{s^2} + \dots$$

Dist fam prev Analytic cont of

4.30-5.30 1505 Thurs.

Application of Riesz to solution of Dirichlet problem

Ω open



$$\boxed{\begin{aligned} \Delta U &= 0 \quad \text{in } \Omega \\ U|_{\partial\Omega} &= f \end{aligned}}$$ old problem

extend f into Ω, look for

$v = U - f$ st

$\Delta U = 0 \Rightarrow$
$\Delta(v+f) = 0$
$\Delta v = -\Delta f$

New Problem
$$\boxed{\begin{aligned} \Delta v &= -w \quad \text{in } \Omega \\ v|_{\partial\Omega} &= 0 \end{aligned}} \quad (*)$$

with $w = \Delta f$ given

Now in $C^1(\bar\Omega)$ define $\langle u, v\rangle = \int_\Omega \nabla u \cdot \nabla v \, dx$

not inner product space since any $u = \text{const}$ has $\|u\| = 0$

denote $C_0^1(\bar\Omega) \subset C^1(\bar\Omega)$ st $u \in C_0^1(\bar\Omega)$ vanishes on $\partial\Omega$

Let $v \in C^2(\bar\Omega)$ be sol of $(*)$ where $w \in C^0(\bar\Omega)$

then $\forall u \in C_0^1(\bar\Omega)$

$$\langle u, v\rangle = \int \nabla u \cdot \nabla v \, dx = -\int_\Omega u \Delta v \, dx = \int u w \, dx$$

Then can find v sol of $(*)$ by repr.

$$\phi(u) = \int u w \, dx$$

as inner product $\langle u, v \rangle$

then $\phi(u) = \int u w \, dx = \langle u, v \rangle = -\int u \cdot \Delta v$

for any u in Hilbert space

to get Hilbert space must complete

$C_0^1(\bar{\Omega})$ under $\langle \, , \rangle$ into $H_0^1(\Omega)$ and prove

that ϕ is bdd lin. func. on $H_0^1(\Omega)$

<u>Bdd</u>: $\phi(u) \leq M \|u\|$

$\int u w \, dx \leq M \int \nabla u \nabla w$

Cauchy $\left(\int u w\right)^2 \leq \int u^2 \int w^2$

suffices to show $\int_\Omega |u|^2 dx \leq K \int_\Omega |\nabla u|^2$ Poincaré

Can extend ϕ as bdd func. to all of H_0^1

Then done

Remarks: $L^2(\mathbb{R})$ sep

once got weak sol. must show strong sol.

Lax-Milgram Theorem

$B(x,y)$ bilinear form on Hilbert space $\mathcal{H}$

$$\left(B(x_1+x_2, y) = B(x_1,y) + B(x_2,y) \right), \quad B(\alpha x, y) = \alpha B(x,y)$$

bounded if $\exists K$ $|B(x,y)| \le K\|x\|\|y\|$ $\quad \forall x,y \in \mathcal{H}$

coercive if $\exists \nu > 0$ s.t. $B(x,x) \ge \nu \|x\|^2 \quad \forall x \in \mathcal{H}$

Example: $B(x,y) = \langle x, y \rangle$

or $B(f,g) = \int_0^1 f(x) g(x)\, \omega(x)\, dx$ on $L^2[0,1]$

$0 < \omega(x) < \infty$ on $[0,1]$

Theorem: B is bdd, coercive bilinear form on $\mathcal{H}$

then for every bdd linear functional ϕ on $\mathcal{H}$

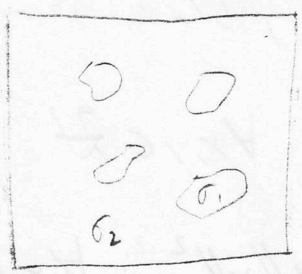
$\exists$ unique f s.t.

$$\phi(x) = B(x,f) \quad \forall x \in \mathcal{H}.$$

Application of Lax-Milgram to Existence + Uniqueness to effective cond prob

(w/ subsequent appl. to finding dir. / anal.)

$\rightarrow$



Ω

$$\sigma(x) = \sigma_1 \chi_1(x) + \sigma_2 \chi_2(x)$$

$$\chi_j := \begin{cases} 1 & x \in \text{med } j \\ 0 & x \notin \text{med } j \end{cases}$$

$$J = \sigma E$$

$$\nabla \cdot J = \nabla \cdot \sigma E = 0$$

$$\nabla \times E = 0$$

$$\langle E \rangle = \frac{1}{|\Omega|} \int_\Omega E \, dx = e_k$$

Please note there are technicalities I'm trying to get around

$$J(x) = \sigma(x) E(x)$$

$$\Downarrow$$

$$\langle J \rangle = \sigma^* \langle E \rangle \qquad \text{def 1}$$

$$\sigma^* e_k = \int_\Omega \sigma(x) E(x) \, dx$$

<u>or</u>

$$\sigma^* \langle E \rangle^2 = \langle \sigma E \cdot E \rangle \qquad \text{def 2}$$

Recall had weak sol to Dirichlet

when instead of $\Delta\varphi = -w$

we had φ st $\int u\Delta\varphi = -\int uw$

$\int \nabla u \cdot \nabla\varphi = \int uw$

this lin func repr
by inner product w/ φ
Riesz gives existence of φ

Now reformulate our problem

(Motivation: $E = e_k + g$, $\nabla \times g = 0$, $\langle g \rangle = 0$ mean 0 fluctuations)

Let $H = L^2(\Omega)$ vector fields

and $\mathcal{H} = \{ f \in H : \nabla \times f = 0 \text{ and } \langle f \rangle = 0 \}$

instead of $\nabla \cdot \sigma E = 0$

consider $\int_\Omega f \cdot \sigma E = 0 \quad \forall f \in \mathcal{H}$

find g s.t. $\int_\Omega f \cdot \sigma(e_k + g) = 0 \quad \forall f \in \mathcal{H}$

or $\int_\Omega \sigma f \cdot g = -\int \sigma f \cdot e_k \quad \forall \mathcal{H}$

this bdd linear funct. on $\mathcal{H}$
is repr. by Bilinear form
eval at g

Lax - Milgram $\Longrightarrow$

if $B(f_1, f_2) = \int_\Omega \sigma f_1 \cdot f_2$ is bdd + coercive

then $\exists!\, g^{\in \mathcal{H}}$ s.t. lin func. $\varphi(f) = -\int_\Omega \sigma f \cdot e_K$

$$\varphi(f) = B(f, g) \qquad \forall f \in \mathcal{H}$$

this gives existence + uniqueness (when coercive)

Question: when is it coercive$^{+\text{bdd}}$?

Exercise

$$\nabla \cdot \sigma E = 0$$

$$\nabla \cdot (\sigma_1 \chi_1 + \sigma_2 \chi_2) E = 0$$

$$\nabla \cdot \left(\underbrace{\frac{\sigma_1}{\sigma_2}}_{h} \chi_1 + \chi_2\right) E = 0$$

$$\nabla \cdot (h \chi_1 + \chi_2) E = 0$$

for which h is assoc. bilinear form bdd + coercive

obviously if h finite have bdd.

Equiv. B is $\quad B(f,g) = \int_\Omega (h x_1 + x_2) f \cdot g \quad$ on $\mathcal{H}$

when is $\quad |B(f,f)| \geq \alpha \|f\|^2 \quad \alpha > 0$

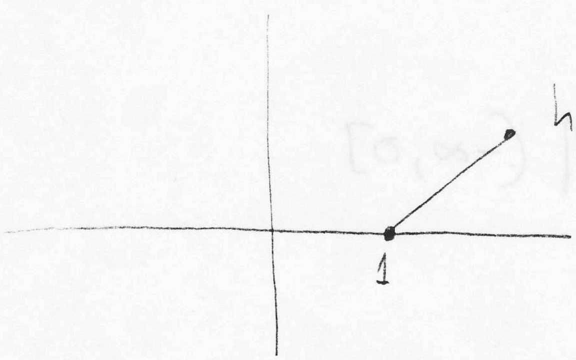
$$(*) \quad \left| \int_\Omega (h x_1 + x_2) f^2 \right| \geq \alpha \int f^2 \quad , \quad \alpha > 0$$

let $\quad \lambda = \dfrac{\int_\Omega x_1 f^2}{\int_\Omega f^2}$

$|\Omega| = 1$

and Note $\displaystyle\int_\Omega x_1 + x_2 = 1 \implies \frac{\int x_1 f^2}{\int f^2} + \frac{\int x_2 f^2}{\int f^2} = 1$

then $(*) \iff \quad |h\lambda + 1(1-\lambda)| \geq \alpha > 0$



coercive $\iff h \notin (-\infty, 0]$

How does σ^* depend on h

$$\sigma^* = \int_\Omega (\sigma_1 \chi_1 + \sigma_2 \chi_2) E \cdot E \quad \text{or} \quad \int_\Omega (\sigma_1 \chi_1 \cdot \sigma_2 \chi_2) E$$

$$m(h) = \frac{\sigma^*}{\sigma_2} = \int (h\chi_1 + \chi_2) E \cdot E$$

Consider m as analytic function of h

what is domain of analyticity

$h\chi_1 + \chi_2$ entire in h

all dep. on **h** in E

if E exist and unique m is analytic in h (☆)

furthermore $\operatorname{Im} h > 0 \Rightarrow \operatorname{Im} m > 0$
$(<) \qquad (<)$

We have

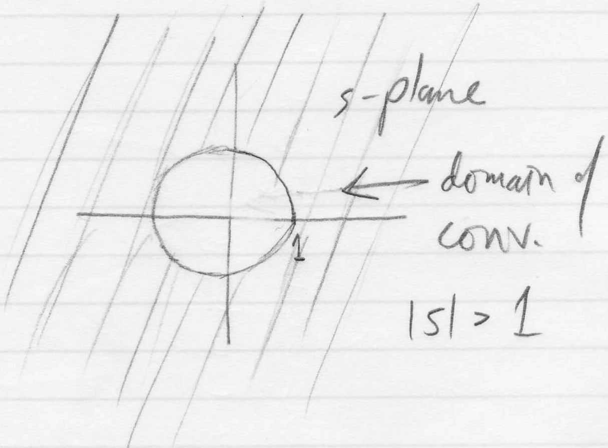
<u>Theorem</u>: ① $m(h)$ analytic off $(-\infty, 0]$
② $m(h) : U \to U$

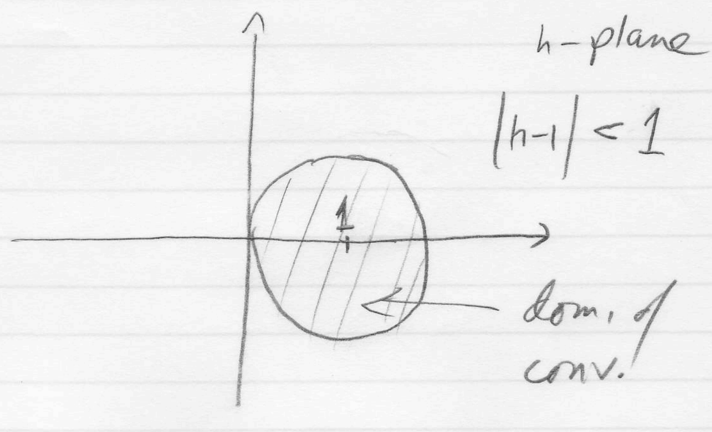
Exercise: Find domain of analyticity for 3 component med

<u>Extra</u>: Prove ☆.

$$= 1 - m(h) = m(1) + m'(1)(h-1) + \frac{m''(1)}{2!}(h-1)^2 + \dots$$

$$F(s) = \frac{a_1}{s} + \frac{a_2}{s^2} + \dots, \qquad |s| > 1$$





$$a_1 = \langle X_1 \rangle = p_1$$

$$a_2 = a_2^{kk} = -\langle X_1 \Gamma X_1 e_k \cdot e_k \rangle$$

$$= -\left\langle \left[X_1(0) \left(\Gamma X_1 e_k \right)(0) \right] \cdot e_k \right\rangle$$

$$= -\left\langle X_1(0) \left(\Gamma_{kk} X_1 \right)(0) \right\rangle$$

$$= -\left\langle X_1(0) \left[\frac{\partial}{\partial x_k} \int_{\mathbb{R}^d} g(x,y) \frac{\partial}{\partial y_k} \tilde{X}_1(y)\,dy \right](0) \right\rangle$$

$$= \left\langle X_1(0) \left[\frac{\partial}{\partial x_k} \int_{\mathbb{R}^d} \frac{\partial}{\partial y_k} g(x,y)\, \tilde{X}_1(y)\,dy \right](0) \right\rangle$$

$$= -\left\langle X_1(0) \left[\frac{\partial}{\partial x_k} \int_{\mathbb{R}^d} \frac{\partial}{\partial x_k} g(x,y)\, \tilde{X}_1(y)\,dy \right](0) \right\rangle$$

$$= -\left\langle X_1(0) \int_{\mathbb{R}^d} \frac{\partial^2}{\partial x_k^2} g(0,y)\, \tilde{X}_1(y)\,dy \right\rangle$$

$$\Gamma = \nabla (-\Delta)^{-1} \nabla \cdot$$

$$\Gamma_{kk} = \frac{\partial}{\partial x_k} (-\Delta)^{-1} \frac{\partial}{\partial x_k}$$

$$\left((-\Delta)^{-1} f \right)(x) = \int_{\mathbb{R}^d} g(x,y) f(y)\,dy$$

$$\Delta g(x) = -\delta_y(x)$$

$$\tilde{X}_1 = X_1 - p_1, \quad \langle \tilde{X}_1 \rangle = 0$$

$$a_2^{kk} = -\int_{\mathbb{R}^d} \frac{\partial^2}{\partial x_k^2} g(0,y)\, R(y)\, dy$$

$$R(y) = \langle \chi_1(0)\, \tilde{\chi}_1(y) \rangle$$
$$= \langle \chi_1(0)(\chi_1(y) - p_1) \rangle$$

$$Tr(a_2) = \sum_{k=1}^{d} \int_{\mathbb{R}^d} \frac{\partial^2}{\partial x_k^2} g(0,y) R(y)\, dy$$

$$= \int_{\mathbb{R}^d} \Delta g(0,y) R(y)\, dy = \int_{\mathbb{R}^d} \delta_0(y) R(y)\, dy = R(0)$$

$$Tr(a_2) = \langle \chi_1(0)(\chi_1(0) - p_1) \rangle = \langle \chi_1(0) \rangle - p_1 \langle \chi_1(0) \rangle$$
$$= p_1 - p_1^2 = p_1(1 - p_1)$$
$$= p_1 p_2$$

If material is statistically isotropic,

i.e. $\sigma^*_{ii} = \sigma^*_{jj}$, $\forall i,j = 1, \ldots, d$

so that $a_2^{ii} = a_2^{jj}$, $\forall i,j$

$$\Rightarrow \sum_{i=1}^{d} a_2^{ii} = p_1 p_2 \qquad \boxed{a_2 = \frac{p_1 p_2}{d}}$$

For general continuum systems, geometrical parameters derived from 3-point correlation functions have been investigated, Beran, M. 1965 Nuovo. Cim. 38, p. 771
Milton + Phan-Thien 1982 Proc. Roy. Soc. A380, p. 305, 333
and others

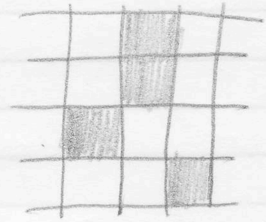
which determine a_3, similarly for a_4
These observations were used to obtain bounds better than Hashin-Shtrikman (1958)

Given a particular geometry, a_n can be calculated in principle, but very difficult in practice.

One class of situations, where it should be feasible to carry out the calculation of the a_n to a reasonable degree would be where the probability measure P on the space of realizations Ω is a product of Bernoulli measures.
Then correlation functions are "trivial".

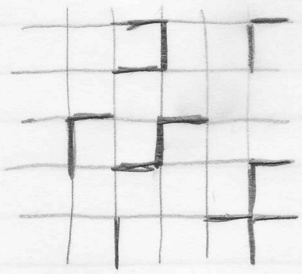
Examples: Cell Materials

Bernoulli meas per cell



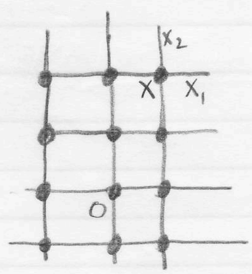
$$\sigma(x) = \begin{cases} \sigma_1 & \text{prob } 1-p \\ \sigma_2 & \text{prob } p \end{cases}$$

Lattices



$$\sigma(x) = \begin{cases} \sigma_1 \text{ — prob } 1-p \\ \sigma_2 \text{ — prob } p \end{cases}$$

Lets focus on <u>lattice</u> - <u>Random</u> <u>Resistor</u> <u>Network</u>



$$\Omega \simeq \{\sigma_1, \sigma_2\}^{d\mathbb{Z}^d}$$

e_i = unit vector in i^{th} direc.

$$T_i^+ = T_{+e_i} = \text{Translation from } x \text{ to } x+e_i$$

$$T_i^- = T_{-e_i}$$

then have forward and backward difference operators

$$D_i^+ = T_i^+ - I$$

$$D_i^- = I - T_i^-, \quad i=1,\dots,d$$

Let $J_i(x)$ be the current in the bond emanating from the node x in the direction e_i. Then

$$J_i = \sigma_i E_i$$

where $\sigma_i = \sigma_1 \chi_1 + \sigma_2 \chi_2$ is the conductivity in that bond

Kirchoff's Laws are: 1. sum of currents at one node $= 0$ (if no source at the node)

2. sum of potential drops around any closed path $= 0$

$$\sum_{i=1}^{d} D_i^- J_i = 0 \qquad (1.)$$

$$D_i^+ E_j - D_j^+ E_i = 0 \, , \ \forall i,j \qquad (2.)$$

$$\langle E \rangle = e_k$$

isotropic $\quad \sigma^* = \sigma^*_{kk} = \langle \sigma(x) E_k(x) \rangle$

Now $\Gamma = \nabla^+ (-\Delta)^{-1} \nabla^- \cdot \quad , \quad \nabla^{\pm} = (D_1^{\pm}, \dots, D_d^{\pm})$

$$(-\Delta)^{-1} f(x) = \sum_{y \in \mathbb{Z}^d} g(x,y) f(y)$$

$$\Delta g(x,y) = \begin{cases} -1 \, , & x = y \\ 0 \, , & x \neq y \end{cases}$$

or $$\Delta g(x,y) = -\delta(x-y)$$

Aside: Connection with random walks.

Let $P(x,y)$ be the transition probability for random walk in $\mathbb{Z}^2$, with

$$P(x,y) = \text{prob. that walker at } x \text{ makes next move to } y$$

Then the potential kernel $A(x,y) = a(x-y)$ of a recurrent aperiodic random walk in two dimensions satisfies

$$(\star) \qquad \sum_{y \in \mathbb{Z}^2} P(x,y)a(y) - a(x) = \delta(x,0), \qquad x \in \mathbb{Z}^2$$

Note: If $P_k(x,y)$ is the prob. that in k steps the walker moves from x to y, then

$$A(x,y) = \lim_{n \to \infty} \sum_{k=0}^{n} \left[P_k(0,0) - P_k(x,y) \right]$$

Special case: Standard nearest neighbor random walk.

$$P(0,y) = \begin{cases} \frac{1}{4}, & |y| = 1 \\ 0, & |y| \neq 1 \end{cases}$$

then $(\star)$ (in complex notation) $\iff$

$$\frac{1}{4}\left[a(z+1) + a(z-1) + a(z+i) + a(z-i)\right] - a(z) = \delta(z,0)$$

which is just $\quad \Delta a(x-y) = \delta(x-y)$

So that our $g(x,y)$ is just the $(-)$ potential kernel for the standard random walk in d-dimensions.

Some info. about $g(z)$ in $d=2$

	$y=0$	$y=1$	$y=2$	$y=3$
$x=0$	0			
	1	$4/\pi$		
	$4-8/\pi$	$-1+8/\pi$	$16/3\pi$	
	$17-48/\pi$	$92/3\pi - 8$	$8/3\pi + 1$	$92/15\pi$

McCrea + Whipple (1940)

Asymptotically, along the diagonal $z = n(1+i)$ as $n \to \infty$

$$a(z) \sim \frac{1}{\pi}\left[2\ln|z| + \ln 8 + 2\gamma\right]$$

$\gamma = 0.5572\ldots$ is Euler's const.

So it behaves asymptotically like continuum free space green's function $\frac{2}{\pi}\ln|r|$ in $d=2$.

$$F(s) = \frac{a_1}{s} + \frac{a_2}{s^2} + \dots \quad , \quad a_1 = p_1$$

Now lets calulate a_2 again, which is formally the same as in continuum.

$$a_2 = -\langle \chi_1 D_k^+ (-\Delta)^{-1} D_k^- (\chi_1 - p_1) \rangle$$

With manipulations as before, we have

$$a_2 = -\sum_{y \in \mathbb{Z}^d} D_k^+ D_k^- g(0,y) \langle \chi_1(0)(\chi_1(y) - p_1) \rangle$$

It is convenient (for later) to note that

$$\langle \chi_1(0)(\chi_1(y) - p_1) \rangle = \langle (\chi_1(0) - p_1)(\chi_1(y) - p_1) \rangle$$

which is a product of two mean-zero random variables

$$= R(0,y)$$

By independence (this is the advantage of the lattice)

$$R(0,y) = \begin{cases} B_2(p_1) = p_1 p_2 \quad , & y = 0 \\ 0 \quad , & y \neq 0 \end{cases}$$

Then

$$a_2 = -D_k^+ D_k^- g(0,0) \, B_2(p_1)$$

$g(x,y)$ is "isotropic"

$\Delta g = -\delta \Rightarrow -D_k^+ D_k^- g(0,0) = \frac{1}{d}$

$$= \frac{p_1 p_2}{d}$$

Lets look at a_3

$$a_3 = \sum_{j=1}^{d} \langle \chi_1\, D_k^+ (-\Delta)^{-1} D_j^- \chi_1\, D_j^+ (-\Delta)^{-1} D_k^- (\chi_1 - p_1) \rangle$$

After discrete int. by parts and similar manipulations

$$a_3 = \sum_{j=1}^{d} \sum_{y_1 \in \mathbb{Z}^d} \sum_{y_2 \in \mathbb{Z}^d} D_k^+ D_j^- g(0,y_1) D_j^+ D_k^- g(y_1,y_2) \langle \chi_1(0)\chi_1(y_1)(\chi_1(y_2)-p_1)\rangle$$

Center the correlation function again (so that we can eval. sums on g)

$$\langle \chi_1(0)\chi_1(y_1)(\chi_1(y_2)-p_2)\rangle = R(0,y_1,y_2) + p_1 \left(R(0,y_2) + R(y_1,y_2)\right)$$

where $R(0,y_1,y_2)$ is the centered three-point function

$$R(0,y_1,y_2) = \langle (\chi_1(0)-p_1)(\chi_1(y_1)-p_1)(\chi_1(y_2)-p_1)\rangle$$

so that $R(0,y_1,y_2) = 0$ unless $0 = y_1 = y_2$, when

$$R(0,0,0) = B_3(p_1) = p_1 - 3p_1^2 + 2p_1^3$$

After a fair bit of calculation

$$a_3 = \Big(\underbrace{\sum_{j=1}^{d} \left(D_k^+ D_j^- g(0,0)\right)^2}_{\text{can be calculated using table.}} \Big) B_3(p_1) - \underbrace{\left(D_k^+ D_k^- g(0,0)\right)}_{= 1/d} p_1 B_2(p_1)$$

= third order poly in p.

a_4 is a fourth order poly. in p_1, the coeffs. involve infinite lattice sums of discrete derivs. of lattice Green's function $g(x,y)$.

Let's use the fact that a_n is an n^{th} order polynomial in p to prove analyticity of $\sigma^*(p)$ in p. Do it for lattice, but proof will hold for cell materials and their generalization

Consider the <u>d-dim bond lattice</u>

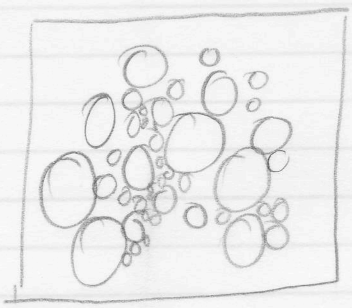
$$\text{w/ conductivity} \quad \sigma(x) = \begin{cases} 1 & \text{prob } p \\ \varepsilon > 0 & \text{prob } 1-p \end{cases}$$

<u>Theorem</u> (Golden): For every $\varepsilon > 0$, there exists an open neighborhood V_ε in the complex p-plane such that $[0,1] \subset V_\varepsilon$ and $\sigma^*(p,\varepsilon)$ is analytic (in p) in V_ε.

Connections between Volume Fraction and Perturbation Expansions:

Bruno's Infinitely Interchangeable Media.

To start, let's consider a cell material, for example



spheres of all sizes

filling all space

$$\text{sphere} \longrightarrow \begin{cases} \sigma_1 & 1-p \\ \sigma_2 & p \end{cases}$$

Then $\sigma^* = \sigma^*(\sigma_1, \sigma_2, p)$ (p, σ_1, σ_2 completely det σ^*)

By homogeneity of σ^*, take $\sigma_1 = 1$, $\sigma_2 = z$

$$m(z,p) = \sigma^*(1, z, p)$$

Vol Frac Exp: $$m(z,p) = \sum_{i=0}^{\infty} l_i(z)\, p^i$$

Pert. Exp. (around homog med) $$m(z,p) = \sum_{i=0}^{\infty} a_i(p)\,(z-1)^i$$

where $a_i(p) = \left.\dfrac{d^i m}{dz^i}\right|_{z=1}$

<u>Bruno's Thesis</u> : relate the a_i's to the l_i's in particular, he found explicit algorithm to derive $a_0, a_1, \ldots, a_{2k+1}$ from the coefficients $l_0, \ldots, l_k$

Method applies to class of inf. int. media, which include all cell materials — this is a generalization of when P on Ω is a product of Bernoulli measures.

<u>Basic Idea</u>: Consider above cell material

Spose rel. vol. fracs are $\sigma_1 \sim 1/3$, $\sigma_2 \sim 2/3$. (assigned at random)

☆ The σ_2 component can be viewed as a random composite <u>itself</u>, composed of two materials, z_2 and z_3, that have also been assigned at random, that occupy a vol. frac of $1/3$ each, such that the values of z_2 and z_3 happen to coincide with σ_2, i.e., $z_2 = z_3 = \sigma_2$

So the material can really be described by a conductivity function of a three-component mixture

$$s = s(z_1, z_2, z_3). \quad \text{w/} \quad \begin{array}{ll} z_1 & 1/3 \\ z_2 & 1/3 \\ z_3 & 1/3 \end{array}$$

with

$$\sigma^*(\sigma_1, \sigma_2, 2/3) = s(\sigma_1, \sigma_2, \sigma_2).$$

Note that s is a <u>symmetric</u> function of its arguments,

i.e., $s(z_1, z_2, z_3) = s(z_i, z_j, z_k)$, for any permutation of i, j, k

i.e., s is the conductivity of an interchangeable material.

<u>Definition</u>: A family of composites of conductivities $\sigma^*(\sigma_1, \sigma_2, p)$ is said to infinitely interchangeable iff for each integer n, $\exists$ a function $s_n(z_1, \ldots, z_n)$ such that

(i) s_n is the cond. func. of an n-phase composite material

(ii) s_n is symmetric in its coordinates, i.e.

$$s_n(z_1, \ldots, z_n) = s_n(z_{p_1}, \ldots, z_{p_n})$$

for any permutation of its coordinates

(iii) For each integer $k \le n$, we have

$$\sigma^*(\sigma_1, \sigma_2, (n-k)/n) = s_n(\underbrace{\sigma_1, \ldots, \sigma_1}_{k}, \underbrace{\sigma_2, \sigma_2, \ldots, \sigma_2}_{n-k})$$

<u>Remark</u>: All examples of cell materials in literature are infinitely interchangeable.

Sketch of method for deriving relations

For an inf. int. material,

$$m\left(z, \frac{n-k}{n}\right) = s_n(1, \dots, 1, \underbrace{z, \dots, z}_{n-k})$$

Since s_n is symmetric

$$\frac{dm}{dz}\left(1, \frac{(n-k)}{n}\right) = (n-k)\, s_n^1 ,$$

where

$$s_n^1 = \frac{\partial s_n}{\partial z_1}(1, 1, \dots, 1)$$

Also,

$$\frac{d^2 m}{dz^2}\left(1, \frac{n-k}{n}\right) = (n-k)\left(s_n^{11} + (n-k-1)\, s_n^{12}\right)$$

where

$$s_n^{11} = \frac{\partial^2 s_n}{\partial z_1^2}(1, 1, \dots, 1) \qquad s_n^{12} = \frac{\partial^2 s_n}{\partial z_1 \partial z_2}(1, \dots, 1)$$

To get pert. coeffs, need to compute the $s_n^1, s_n^{11}, \dots$

Get linear equations for them:

Ingredients: 1. diff ident. $s_n(1, \dots, 1, z, \dots, z) = z\, s_n\left(\frac{1}{z}, \dots, \frac{1}{z}, 1, \dots, 1\right)$

not enough, get rank deficient system.

Need more info, this is done by considering $1^{st}, 2^{nd}, \dots$ derivs. of $s_n(1, \dots, 1, z)$, $s_n(1, \dots, 1, z, z)$ can be related to low vol. frac. info.

Example $\quad d=2$ bond lattice

To illustrate, rederive elementary result $a_1(p) = p$

by def, $a_1\left(\frac{n-k}{n}\right) = \frac{dm}{dz}\left(1, \frac{n-k}{n}\right) = (n-k)\, s_n^1$

where

$$s_n^1 = \frac{\partial s_n}{\partial z_1}(1, 1, \dots, 1)$$

To get s_n^1, note

$$s_n(z, \dots, z) = z$$

so that $\quad n s_n^1 = 1 \quad$ or $\quad s_n^1 = \frac{1}{n}$

Thus

$$a_1\left(\frac{n-k}{n}\right) = \frac{(n-k)}{n}, \quad \text{or} \quad a_1(p) = p \quad \forall p, \text{ by continuity.}$$

Further calculations yield

$$a_2 = \frac{-p(1-p)}{d}$$

$$a_3 = \frac{1}{d^2}\, p(1-p)\left[1 + (d-2)p\right]$$

Using Keller interchange equality in $d=2$

$$m(z,p)\, m\left(\tfrac{1}{z}, p\right) = z \quad \text{or} \quad \sigma^*(\sigma_1, \sigma_2)\, \sigma^*(\sigma_2, \sigma_1) = \sigma_1 \sigma_2$$

get

$$a_4 = \frac{1}{8}\, p(1-p)(p^2 - p - 1)$$

Duality Keller-Dykhne Interchange Theorem

Consider conduction in $d=2$:

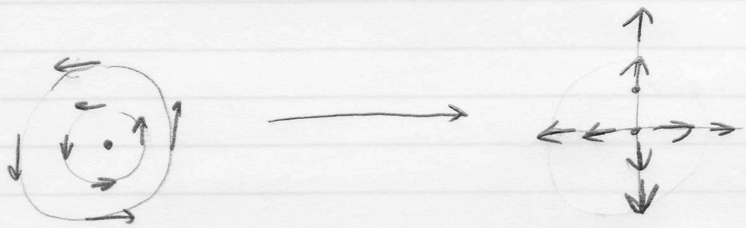
$$J(x) = \sigma(x) E(x) \qquad \langle J \rangle = \sigma^* \langle E \rangle$$

$$\nabla \cdot J = 0$$

$$\nabla \times E = 0$$

Observation:

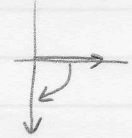
pointwise rotation by $90°$ converts curl-free fields $\rightarrow$ div-free fields



the duality transformation

$\nabla \times E = 0$ $\nabla \cdot R_\perp E = 0$

$$R_\perp = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \qquad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$



$$(R_\perp^{-1}) = R_\perp^T$$

$$J'(x) = R_\perp E(x) \qquad E'(x) = R_\perp J(x)$$

Then

$$\nabla \cdot J' = 0 \qquad \nabla \times E' = 0$$

Pf: $\nabla \cdot J' = \dfrac{\partial j_1'}{\partial x_1} + \dfrac{\partial j_2'}{\partial x_2} = \dfrac{\partial e_2}{\partial x_1} - \dfrac{\partial e_1}{\partial x_2} = 0$

$\nabla \times E' = \dfrac{\partial e_2'}{\partial x_1} - \dfrac{\partial e_1'}{\partial x_2} = \dfrac{-\partial j_1}{\partial x_1} - \dfrac{\partial j_2}{\partial x_2} = 0$

Now, how are J' and E' related:

$$J' = \sigma' E'$$

from $J = \sigma E \Rightarrow \quad R^T E' = \sigma R^T J'$

$$\text{or} \quad J' = \underbrace{R \tfrac{1}{\sigma} R^T}_{\sigma'} E' \qquad \sigma' = R \tfrac{1}{\sigma} R^T$$

i.e., J' and E' solve the conduction equations in dual material whose local conductivity given by σ', which can be quite different from σ. If isotropic

$$\sigma'(x) = \frac{1}{\sigma(x)}$$

so that high cond $\rightarrow$ low cond and vice versa.

Due to this isomorphism, eff. cond. σ^* for $\sigma(x)$ is related to σ^* for dual material.

$\langle J' \rangle = R \langle E \rangle \qquad \langle J \rangle = \sigma^* \langle E \rangle$

$\langle E' \rangle = R \langle J \rangle \qquad R\langle J \rangle = R\sigma^* \langle E \rangle$

$$\langle E' \rangle = R\sigma^* R^T \langle J' \rangle$$

$$\text{or} \quad \langle J' \rangle = \underbrace{R(\sigma^*)^{-1} R^T}_{(\sigma^*)'} \langle E \rangle$$

$$\langle J' \rangle = (\sigma^*)' \langle E' \rangle$$

$$(\sigma^*)' = R \frac{1}{\sigma^*} R^T$$, so eff tensor transformed same way as $\sigma(x)$

Now apply duality to two-component media:

$$\sigma(x) = \sigma_1 \chi_1(x) + \sigma_2 \chi_2(x)$$

consider σ^* as func of σ_1 and σ_2 then

$$\sigma^*\left(\frac{1}{\sigma_1}, \frac{1}{\sigma_2}\right) = (\sigma^*)' = R\left[\sigma^*(\sigma_1, \sigma_2)\right]^{-1} R^T \qquad (\star)$$

σ^* for σ'

From homogeneity $\sigma^*\left(\frac{1}{\sigma_1}, \frac{1}{\sigma_2}\right) = \frac{1}{\sigma_1\sigma_2}\sigma^*(\sigma_2, \sigma_1)$

inserting this in $(\star)$ yields

$$\sigma^*(\sigma_2, \sigma_1)\, R\, \sigma^*(\sigma_1, \sigma_2) R^T = \sigma_1 \sigma_2\, I$$

For isotropic Materials

$$\sigma^*(\sigma_1, \sigma_2)\, \sigma^*(\sigma_2, \sigma_1) = \sigma_1 \sigma_2$$

Keller-Dykhne Interchange Theorem

For particular class of microgeometries : symmetric materials (interchange invariant)

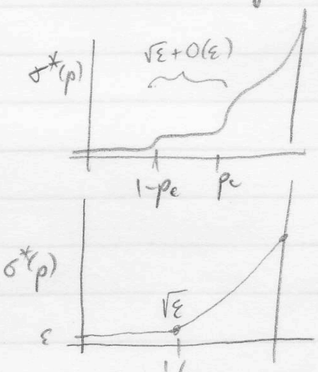
i.e, materials for which $\sigma^*(\sigma_1, \sigma_2) = \sigma^*(\sigma_2, \sigma_1)$, Then

$$\det \sigma^* = \sigma_1 \sigma_2$$

for isotropic $\sigma^* = \sqrt{\sigma_1 \sigma_2}$ exact formula (Dykhne)

<u>Example</u>: checkerboards

resistor networks



for $p \in (1-p_c, p_c)$ "spectral backbone" is interchange invariant

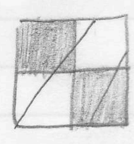
at $p = 1/2$, lattice is interchange invariant

duality $\Rightarrow$ convexity in p around $p = 1/2$

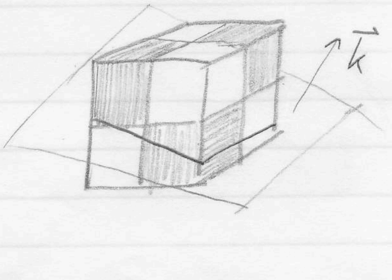
(although $\sigma^*(p)$ is <u>not</u> strictly convex function of p)

<u>example</u>: quasi-periodic media in $d=2$

first $d=1$ a) $\sigma(x) = 3 + \cos x + \cos kx$

(b) 

$$\sigma^* = \begin{cases} \frac{1}{2} & k \text{ irrat'l.} \\ \frac{1}{2} - \frac{1}{2pq} & k = p/q \quad p,q \text{ odd rel pr.} \\ \frac{1}{2} & k = p/q \text{, otherwise} \end{cases}$$

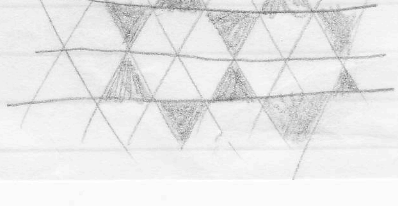
$d=3$ (c) 

$\vec{k}$ irrational

$\Rightarrow$ interchange invariance

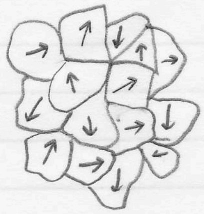
$\Rightarrow \det(\sigma^*) = \sigma_1 \sigma_2$

part k, rat'l.



NOT interchange inv.

<u>polycrystals</u>: duality gives exact result for $\underline{\underline{\sigma}}^*$ for isotropic polycrystal in $d=2$.



granular aggregate

each grain has conductivity tensor

$$\sigma_0 = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

For polycrystal, local cond tensor is

$$\sigma(x) = R(x)\,\sigma_0\,R^T(x)$$

where $R(x)$ is rotation matrix, giving orientation of the crystal at each point x. In practice $R(x)$ is piecewise const. (can consider systems where $R(x)$ is smoothly varying)

<u>dual material</u>:

$$\sigma'(x) = R(x)\left\{R_\perp \sigma_0 R_\perp^T\right\}^{-1} R^T(x)$$

where $R_\perp$ is rotation by $90°$, as before.

Also

$$R_\perp\,\sigma_0\,R_\perp^T = \begin{pmatrix} \lambda_2 & 0 \\ 0 & \lambda_1 \end{pmatrix} = \lambda_1\lambda_2 \begin{pmatrix} 1/\lambda_1 & 0 \\ 0 & 1/\lambda_2 \end{pmatrix}$$

or

$$R_\perp\,\sigma_0\,R_\perp^T = \det(\sigma_0)\,\sigma_0^{-1}$$

so that

$$\sigma'(x) = \frac{\sigma(x)}{\det(\sigma_0)}$$

Now recall $(\sigma^*)' = R_\perp (\sigma^*)^{-1} R_\perp^T$

Plugging in a relation analogous to $R_\perp \sigma_0 R_\perp^T = \det(\sigma_0)\, \sigma_0^{-1}$

for $(\sigma^*)'$ yields

$$(\sigma^*)' = \frac{\sigma^*}{\det(\sigma^*)}$$

(also recall $\sigma'(x) = \frac{\sigma(x)}{\det(\sigma_0)}$)

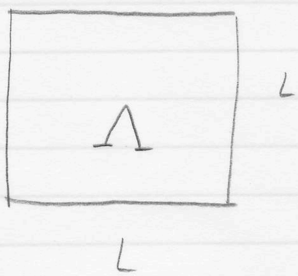
Homogeneity then implies

$$\det(\sigma^*) = \det(\sigma_0)$$

Isotropy $\Longrightarrow$ $\boxed{\sigma^* = \sqrt{\det(\sigma_0)}\; I}$

indep. of details of polycrystalline microstructure.

Variational Formulation of Effective Properties



energy dissipated in conducting med per unit vol.

$$U = \frac{1}{2|\Lambda|}\int_{\Lambda} J\cdot\bar{E}\,dx = \frac{1}{2|\Lambda|}\int \sigma(x)E(x)\cdot\bar{E}(x)\,dx$$

if homogeneous $\quad U = \dfrac{\sigma E\cdot\bar{E}}{2|\Lambda|}$

if $\langle E\rangle = e_k$

$$\frac{\sigma^* e_k\cdot\bar{e}_k}{2} = U = \frac{1}{2|\Lambda|}\int_{\Lambda}\sigma(x)E(x)\cdot\bar{E}(x)\,dx$$

or $$\sigma^* = \frac{1}{|\Lambda|}\int_{|\Lambda|}\sigma(x)E(x)\cdot\bar{E}(x)\,dx \qquad \left(\begin{array}{c}\text{then take}\\ |\Lambda|\to\infty\end{array}\right)$$

Now get variational form

field eqs. are $\quad \nabla\cdot J = 0$

$\quad \nabla\times E = 0$

Now, do variation of energy integral subject to condition $\nabla\times E = 0$, and obtain that minimum solves $\nabla\cdot J = 0$

vary $\quad U = \frac{1}{2|\Lambda|}\int_\Lambda \sigma E\cdot E\,dx \quad$ s.t. $\quad \nabla\times E = 0$

For simplicity assume σ smoothly varying

$$\nabla\times E = 0 \implies E = \nabla\varphi$$

$$\star \qquad U = \frac{1}{2|\Lambda|}\int_\Lambda \sigma\, \nabla\varphi\cdot\nabla\varphi\, dx$$

assume variation of φ vanishes on boundary $\partial\Lambda$

$\varphi + \delta\varphi$

Variation of $\star \implies$

$$\delta U = \frac{1}{2|\Lambda|}\int_V 2\sigma\,\nabla\varphi\cdot\delta\nabla\varphi\,dx$$

Note $\delta\nabla\varphi = \nabla(\delta\varphi)$

Divergence thm. gives

$$\int_\Lambda [\nabla\delta\varphi]\,\sigma\,\nabla\varphi\,dx = -\int_\Lambda \delta\varphi\,\nabla\cdot[\sigma\nabla\varphi]\,dx + \int_{\partial\Lambda}\hat{n}\cdot(\sigma\nabla\varphi\,\delta\varphi)\,dS$$

Since $\delta\varphi = 0$ on $\partial\Lambda$, we have

$$\delta U = -\frac{1}{|\Lambda|}\int \delta\varphi\,\nabla\cdot[\sigma\nabla\varphi]\,dx$$

$$\delta U = 0 \implies \nabla\cdot(\sigma\nabla\varphi) = 0 \text{ or } \nabla\cdot J = 0$$

Thus. $\quad U = \min\limits_{\nabla\times F = 0} \frac{1}{|\Lambda|}\int_{|\Lambda|} \sigma F\cdot F\,dx \quad$ sol. satisfies $\nabla\cdot\sigma F = 0$

Dual variational principle

$$\text{vary} \quad U = \frac{1}{2|\Lambda|}\int_{|\Lambda|} \frac{1}{\sigma} J \cdot \bar{J}\, dx \quad \text{subject to} \quad \nabla \cdot J = 0$$

$U = \frac{1}{\sigma^*}\langle J\rangle \cdot \langle J\rangle$

minimum satisfies $\nabla \times \left(\frac{J}{\sigma}\right) = 0$

Thus

$$\boxed{\begin{aligned} \sigma^* &= \min_{\nabla \times E = 0} \frac{1}{|\Lambda|}\int_{\Lambda} \sigma(x)\, E(x) \cdot \bar{E}(x)\, dx \qquad (1) \\ \frac{1}{\sigma^*} &= \min_{\nabla \cdot J = 0} \frac{1}{|\Lambda|}\int_{\Lambda} \frac{1}{\sigma(x)} J(x) \cdot \bar{J}(x)\, dx \qquad (2) \end{aligned}}$$

Get bounds

stick in trial fields $E = e_k$ in (1)

$J = e_k$ in (2)

$(1) \Rightarrow \sigma^* \le \langle \sigma \rangle$

$(2) \Rightarrow \frac{1}{\sigma^*} \le \left\langle \frac{1}{\sigma} \right\rangle$

$$\frac{1}{\left\langle \frac{1}{\sigma} \right\rangle} \le \sigma^* \le \langle \sigma \rangle$$

Arithmetic + Harmonic Mean Bounds