

Theory of Inhomogeneous Materials

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

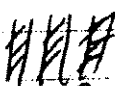
① atmosphere : air w/ water droplets or molecules
air w/ density fluctuations

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.

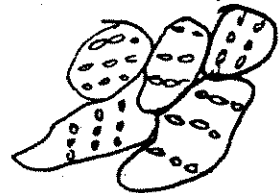
⑤ porous media : sandstones - composite of air and rock
or rock air + liquid
such as oil or brine
(fractal structure)

⑥ sea ice : ice, brine + air

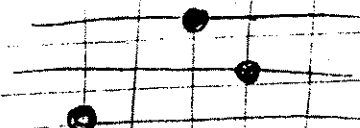
composite on two levels

polycrystal

but the individual crystals are themselves composites



⑦ doped semiconductors



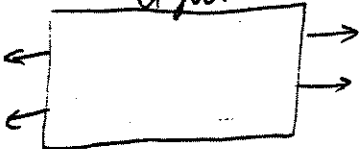
random impurities
hopping conduction

⑧ turbulent fluid

Properties of composites can be different from constituents:

①

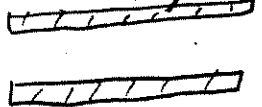
weak, cheap
light



concrete breaks
apart under tension

+

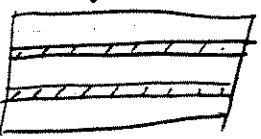
strong, expensive
heavy



steel rods

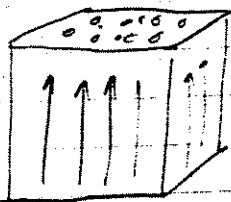
=

strong, cheap
light



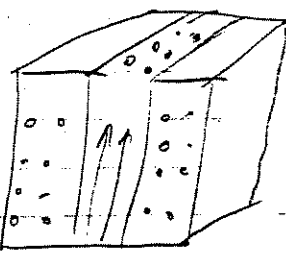
(in skis also)

②



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

→

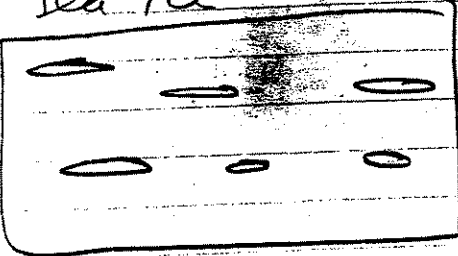


plywood
strong in two (or all)
directions

introduces problem of interfaces
(also in polycrystals)

③

sea ice

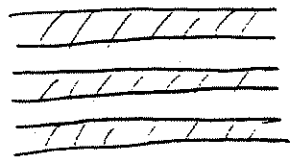


E field

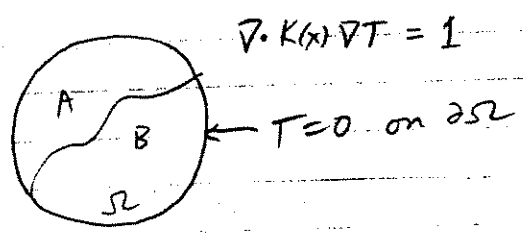
anomalous dielectric effect
effect of interfaces

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

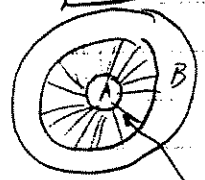
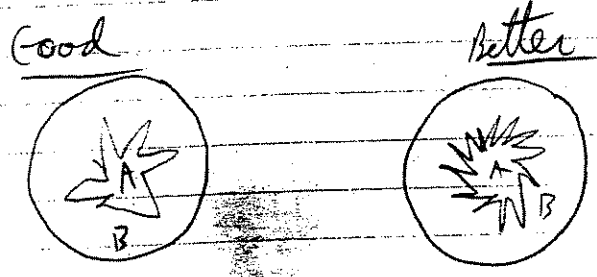


2) Example of Tartar and Murat



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

Which configuration minimizes
avg. temp. $\int_{\Omega} T(x) dx$
optimal



infinitely fine
(problem of existence)

G-dense (Lurie + Cherkakov)

Types of Inhomogeneities

periodic, quasiperiodic, random (translation invariant)

Equations of Interest

$$J = \sigma E \quad \nabla \cdot J = \rho \quad \overset{\text{source}}{\rho} \quad E = \nabla u \quad \nabla \cdot \sigma \nabla u = \rho$$

Problem	J	E	σ
elec. cond.	elect. current J	elec. field E	cond. tensor $\underline{\sigma}$
dielectrics	displacement D	" E	permittivity $\underline{\epsilon}$
magnetism	mag. ind. B	mag. field H	permeability $\underline{\mu}$
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 $\underline{\kappa}$

Homog. eqs:

$$J = \sigma E$$

$$\downarrow$$

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

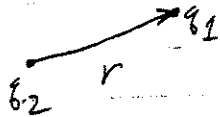
Material Properties

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

Focus on electromagnetic fields:

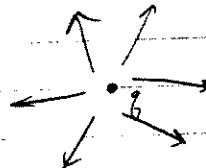
Force on q_1 due to q_2

$$\vec{F}_{21} = \frac{q_1 q_2}{4\pi\epsilon_0} \frac{\vec{r}}{|\vec{r}|^3} \quad \text{Coulomb}$$



Electric field $\vec{E} = \lim_{q \rightarrow 0} \frac{\vec{F}_q}{q}$

E due to point charge



$$\vec{E}(\vec{r}) = \frac{q}{4\pi\epsilon_0} \frac{\vec{r}}{|\vec{r}|^3}$$

$$\vec{E} = -\nabla\phi, \quad \phi(\vec{r}) = \frac{1}{4\pi\epsilon_0} \frac{q}{|\vec{r}|} \quad (\nabla \times \vec{E} = 0)$$

materials are $\begin{cases} \text{conductors} \\ \text{insulators (dielectrics)} \end{cases}$

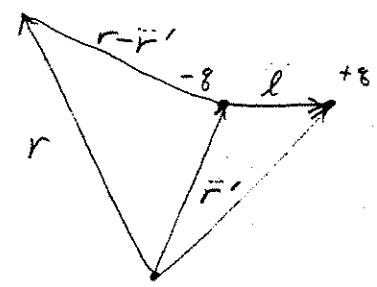
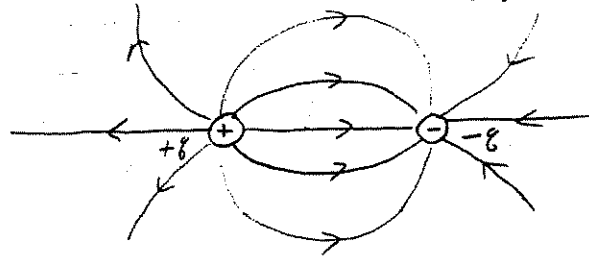
conductors: have large numbers of free charge carriers (like metals) they move (and carry current) when subjected to E field

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, $\phi(r) = \frac{1}{4\pi\epsilon_0} \frac{\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3}$, $\mathbf{p} = q\mathbf{l}$

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

$$\Delta \mathbf{p} = \int_{\Delta V} \mathbf{r} d\mathbf{q}$$

electric dipole moment per unit volume

$$\mathbf{P} = \lim_{\Delta V \rightarrow 0} \frac{\Delta \mathbf{p}}{\Delta V}$$

electric polarization

or $\mathbf{P} = \frac{1}{\Delta V} \sum_m \mathbf{p}_m$, $\mathbf{p}_m = \int_{\text{molecules}} \mathbf{r} d\mathbf{q}$

For isotropic media

$$\mathbf{P} = \chi(\mathbf{E}) \mathbf{E}$$

χ = electric susceptibility

Now define electric displacement

$$D = \epsilon_0 E + P$$

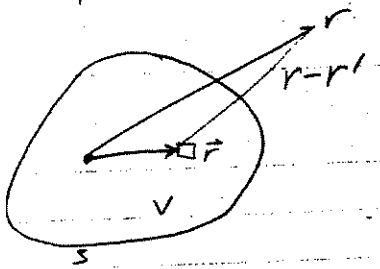
so that $\epsilon_0 E = D - P$

$$= \epsilon_0 E + \chi E$$

$$\boxed{D = \epsilon E}, \quad \epsilon = \epsilon_0 + \chi = \text{permittivity}$$

equation for D :

potential due to dielectric medium

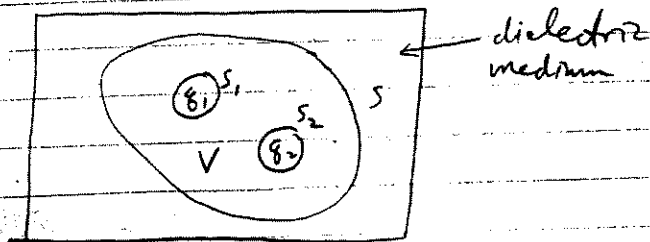


$$\phi(r) = \frac{1}{4\pi\epsilon_0} \int_V \frac{P(r') \cdot (r - r')}{|r - r'|^3} dV$$

$$= \frac{1}{4\pi\epsilon_0} \int_S \frac{P \cdot n}{|r - r'|} dA + \frac{1}{4\pi\epsilon_0} \int_V \frac{-\nabla \cdot P}{|r - r'|} dV$$

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

Now consider



Gauss $\int_S E \cdot n dA = \frac{1}{\epsilon_0} (Q + Q_p)$

$Q = q_1 + q_2$ 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 theorem on vol. int. in Q_p , we get

$$Q_p = - \int_S \mathbf{P} \cdot \mathbf{n} dA$$

thus

$$\epsilon_0 \int_S \mathbf{E} \cdot \mathbf{n} dA + \int_S \mathbf{P} \cdot \mathbf{n} dA = Q$$

or

with $\boxed{\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}}$

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

or

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

thus

$$\mathbf{D} = \epsilon \mathbf{E} = (\epsilon_0 + \chi) \mathbf{E}$$

$\epsilon = K \epsilon_0$, K is dielectric constant (dimensionless)

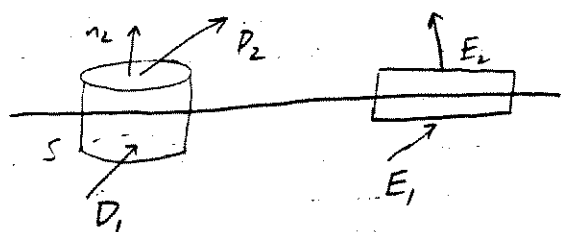
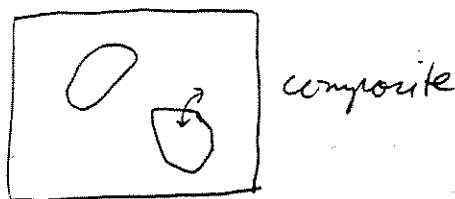
$$K = \frac{\epsilon}{\epsilon_0} = 1 + \frac{\chi}{\epsilon_0}, \quad \epsilon_0 = \text{permittivity of free space.}$$

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



$$\nabla \cdot D = \rho \Rightarrow D_{2n} - D_{1n} = \sigma$$

σ = surface density of free charge

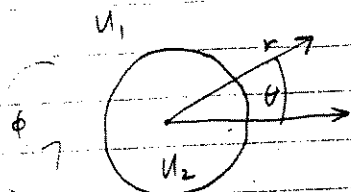
$$\nabla \times E = 0 \Rightarrow E_{1t} = E_{2t}$$

Fundamental Example: Dielectric sphere in uniform electric field

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

$$\Delta u = 0, \quad u \text{ indep. of } \phi$$

(r, θ, ϕ)



two lowest order spherical harmonics are enough

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

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

$\frac{1}{r}$ not necessary since it corresponds to net charge on sphere

Use following conds to det coeff:

- ① $u_1 \rightarrow -E_0 r \cos \theta$ as $r \rightarrow \infty$
- ② cont. of u across interface
- ③ cont. of D_n

$$\Rightarrow A_1 = -E_0, \quad A_2 = \frac{-3E_0}{K+2}, \quad C_2 = 0 \quad (\text{otherwise macro dipole, } \infty \text{ field})$$

$$C_1 = \frac{(K-1) a^3 E_0}{K+2}$$

$$E_2 = \frac{3}{K+2} E_0$$

$K > 1$

Resonance in K plane at $K = -2$



$$|E_{2t}| < |E_0|$$

lines of D are cont. (no surface charge)
lines of E are discont. (due to polarization chrgs)

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

$$I = \int_S \mathbf{J} \cdot \mathbf{n} dA$$

$$\mathbf{J} = \text{current density} \\ = N q \mathbf{v}$$

N = # charge carriers per unit volume

q = charge
 $\mathbf{v}$ = drift velocity of each carrier.

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

$$I = - \int_S \mathbf{J} \cdot \mathbf{n} dA = - \int_V \nabla \cdot \mathbf{J} dV$$

at

I = rate at which charge is being transported into V

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

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

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

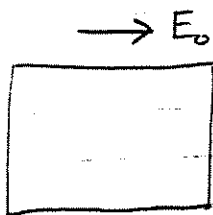
Resistivity $\tau = \frac{1}{\sigma}$

τ meas. in $\frac{\text{volt} \cdot \text{m}}{\text{amp}}$
or ohm meters

$$1 \text{ ohm} = \frac{1 \text{ volt}}{1 \text{ amp}}$$

<u>Material</u>	<u>Resistance τ (ohm.m)</u>	
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 $\tau(T)$.)
Silicon ($10^{-4} \cdot 0^\circ\text{As}$)	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

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

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

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

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

Similarly if $D = D_0 e^{i(\omega t - s)}$ then $D = (1 + \frac{\chi}{\epsilon_0}) \epsilon_0 E$
 can be written as $D = \epsilon \epsilon_0 E$, $\epsilon = \epsilon' + i\epsilon''$, $\epsilon_{\text{space}} = 1 + i0$

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

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

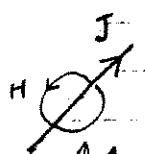
We will derive them from the experimentally determined laws of electricity and magnetism: (Written in Gaussian units: $\epsilon_0 = \mu_0 = 1$)

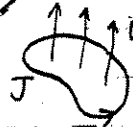
Coulomb's law: $\nabla \cdot D = 4\pi \rho$

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

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

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

 Current causes magnetic field

 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))

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, however, in general, we have

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

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

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

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 $\nabla \times H = \frac{1}{c} \frac{\partial D}{\partial t}$ suggest mutual production of E and B (waves)...

1. ... 1st Maxwell's equation:

Maxwell's Equations:

in Gaussian ($\epsilon_0 = \mu_0 = 1$)

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

in rationalized MKS

$$\epsilon_0 = \frac{10^{-7}}{4\pi c^2} (\text{I}^2 \text{t}^4 \text{m}^{-1} \text{s}^{-3})$$

$$\mu_0 = 4\pi \times 10^{-7} (\text{mI}^2 \text{s}^{-2})$$

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}, \quad \mathbf{H} = \frac{1}{\mu_0} \mathbf{B} - \mathbf{M}$$

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

Plane Waves in Homogeneous, Nonconducting Medium

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

$$\begin{aligned} \nabla \cdot \mathbf{E} &= 0 & \nabla \times \mathbf{E} &= -\frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} \\ \nabla \cdot \mathbf{B} &= 0 & \nabla \times \mathbf{B} &= \frac{\mu \epsilon}{c} \frac{\partial \mathbf{E}}{\partial t} \end{aligned} \quad (\text{in Gaussian})$$

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

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

$$v = \frac{c}{\sqrt{\mu \epsilon}}$$

in free space $\mu = \epsilon = 1$
 $\Rightarrow v = c$

our eq. has well known plane wave solutions

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

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

propagation in x -direction, fund. sol. is

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

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

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

Then medium is dispersive, i.e., if $\mu \epsilon$ is function of freq.,

for each freq. component the plane waves are still solutions,

at reconstructing the (x, t) dep, $*$ 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

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

$$F = -m\omega_0^2 x \quad (k = m\omega_0^2, \omega_0 = \sqrt{\frac{k}{m}})$$

$x = \text{displacement}$

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

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

Then induced dipole moment is

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

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

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

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

Then the average dipole moment is

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

Now consider oscillating case.

For simplicity, neglect difference between applied and local field
 $\Rightarrow$ model only valid for substances of low density.

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

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

γ measures damping force

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

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

Then dipole moment for one electron is

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

Now suppose 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 dielectric const. $\epsilon = 1 + 4\pi N e^2$ is

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

where $\sum_j f_j = Z$

Anomalous Dispersion and Resonant Absorption

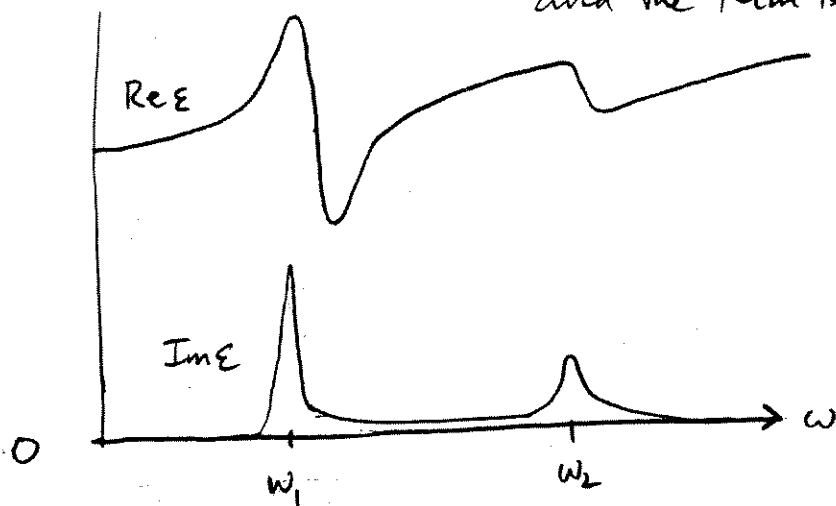
Generally $\gamma_j \ll \omega_j \Rightarrow \epsilon(\omega)$ approx real for most ω

$\frac{1}{\omega_j^2 - \omega^2}$ 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 $\epsilon(\omega) > 1$. As ω incs, and get more and more neg. terms, eventually, $\epsilon(\omega) < 1$.

Resonance: ω near ω_j

Real part of denom in (*) vanishes and the term is large and imaginary



Normal Dispersion: inc. in $\text{Re } \epsilon(\omega)$ with ω (occurs everywhere except in nbhd. of resonance)

Anomalous Dispersion: dec. in $\text{Re } \epsilon(\omega)$ with ω

Resonant Absorption: $\text{Im } \epsilon$ large and pos. - wave loses energy

($\text{Im } \epsilon < 0 \Rightarrow$ enery. given to wave by med. - laser)

Attenuation of plane wave. Write wave number as

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

α = absorption coeff. or attenuation const.

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

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

$$\beta^2 - \frac{\alpha^2}{4} = \frac{\omega^2}{c^2} \text{Re} \epsilon$$

$$\beta \alpha = \frac{\omega^2}{c^2} \text{Im} \epsilon$$

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

$$\alpha \approx \frac{\text{Im} \epsilon(\omega)}{\text{Re} \epsilon(\omega)} \beta, \quad \beta = \sqrt{\text{Re} \epsilon} \omega / c$$

Low Frequency Behavior:

As $\omega \rightarrow 0$, 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 free ($\omega_0=0$)

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

Now separate out free electron behavior, from (*)

$$\begin{aligned}\epsilon(\omega) &= 1 + C \sum_j f_j \frac{1}{(\omega_j^2 - \omega^2 - i\omega\gamma_j)} \quad , \quad C = \frac{4\pi N e^2}{m} \\ &= \hat{\epsilon} - C \frac{f_0}{\omega(i\gamma_0 + \omega)} \quad < \omega_0 = 0, \quad \hat{\epsilon} = \text{contr. from non-zero res.} \\ &= \hat{\epsilon} + i \frac{C f_0}{\omega(\gamma_0 - i\omega)} \quad (**)\end{aligned}$$

Let's 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 $\hat{\epsilon}$ ($D = \hat{\epsilon} E$)
Assume harmonic time dependence for fields $e^{-i\omega t}$

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

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

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

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

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/ $f_0 N = \# \text{ free elec. / unit vol.}$

(Assume $f_0 = O(1)$)
Measurements of conductivity of copper give $\gamma_0 \sim O(10^{13})$

$\Rightarrow$ At frequencies well beyond microwave region
 $\omega \lesssim 10^{11} \text{ sec}^{-1}$, 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.

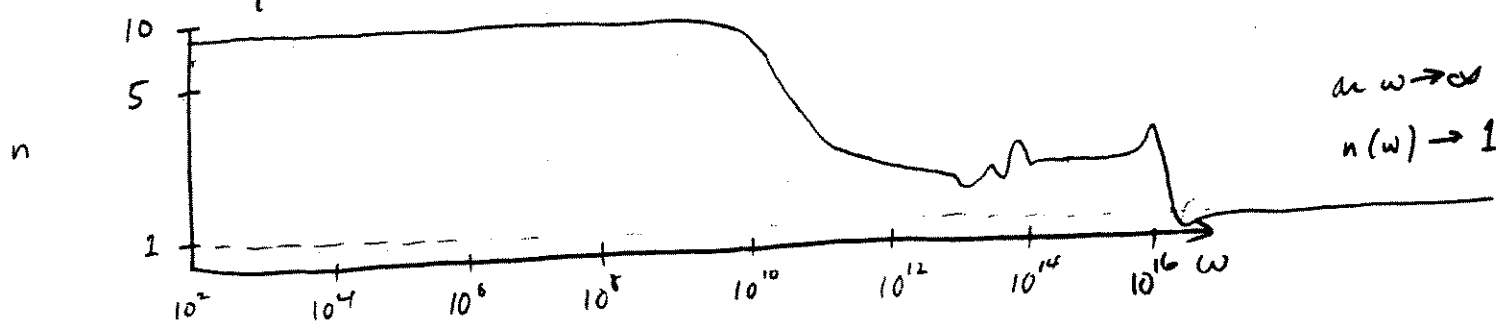
Let's look at water (its ubiquitous)

Index of refraction $n(\omega) = \text{Re} \sqrt{\mu \epsilon}$

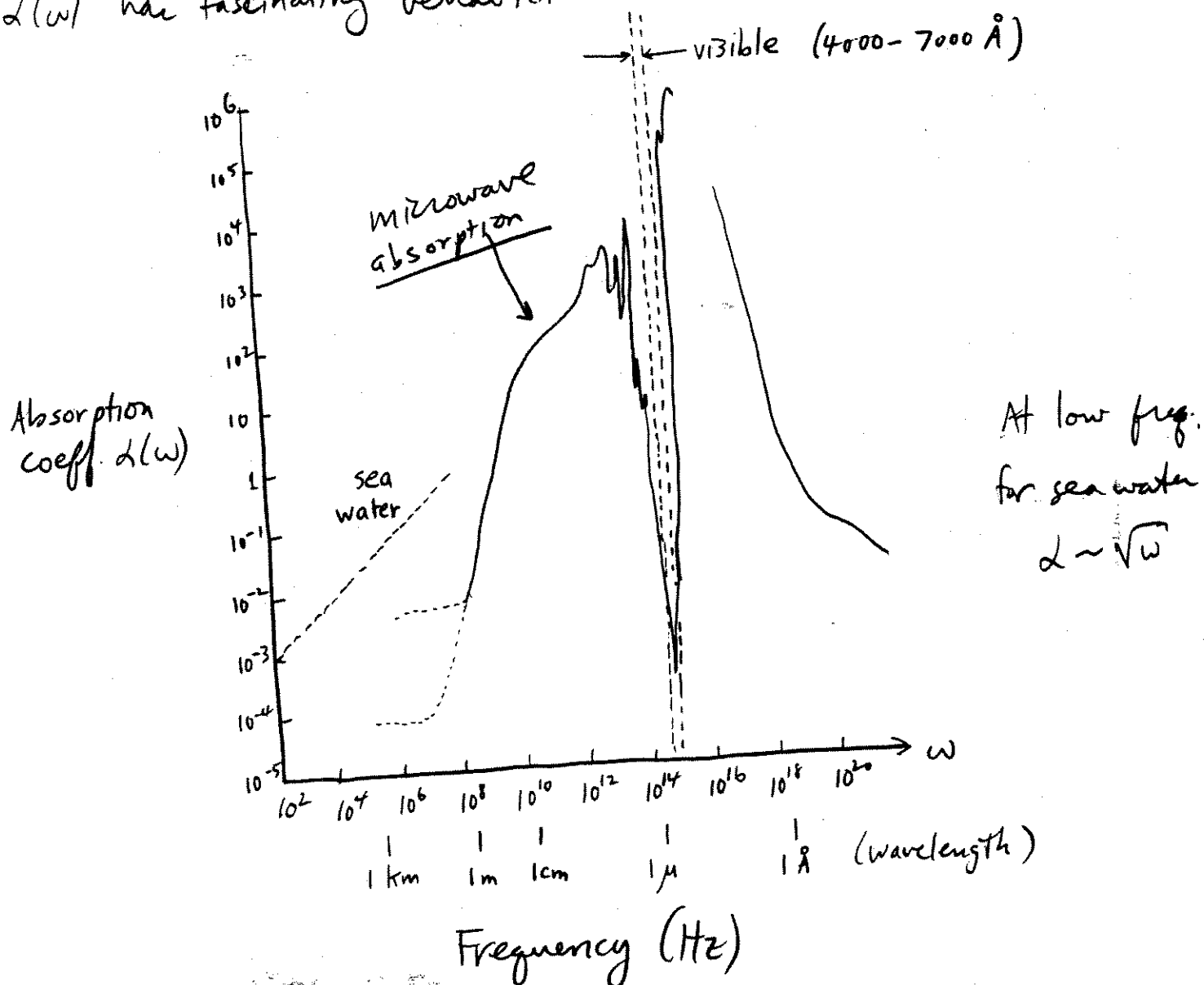
Absorption coeff $\alpha(\omega) = 2 \text{Im} \sqrt{\mu \epsilon} \frac{\omega}{c}$

At low frequencies ($< 10^{10}$ Hz) $n(\omega) \approx 9$ ($\epsilon \approx 81$)

which arises from partial orientation of permanent dipole moments of water molecules.



$\alpha(\omega)$ has fascinating behavior



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)

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

α = molecular, atomic, or ionic polarizability

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

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

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

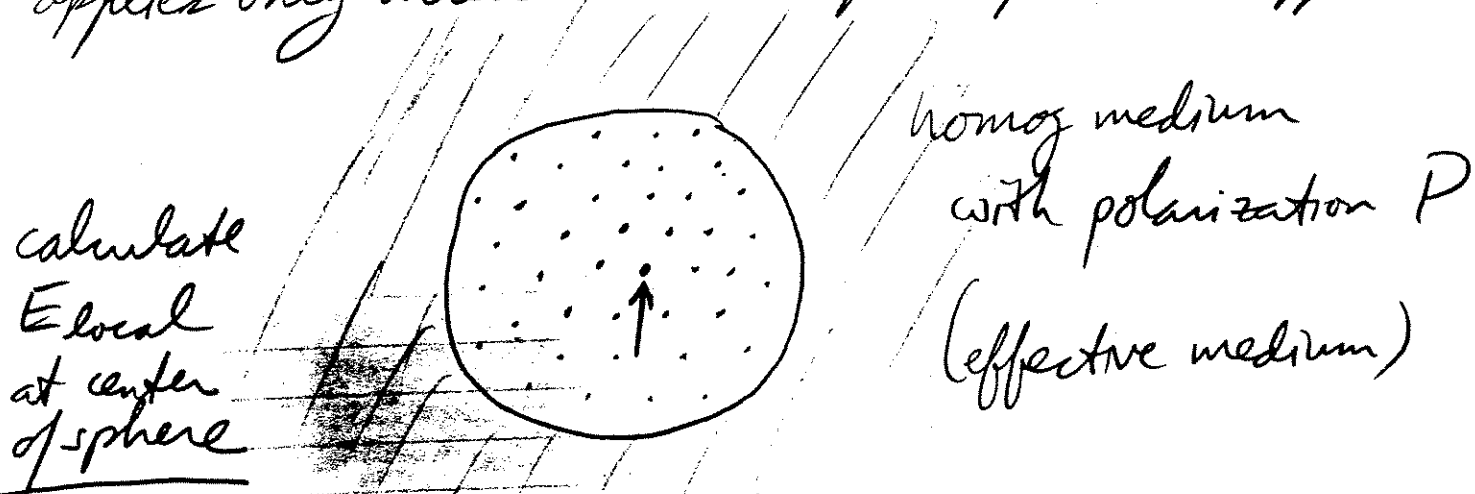
$$E_{\text{local}} = E + E_{\text{con.}}$$

Note: even though $E_{\text{dipole}} \sim \frac{1}{r^3}$, 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_{con} (Lorentz)

applies only when induced dipoles parallel to appl. E .

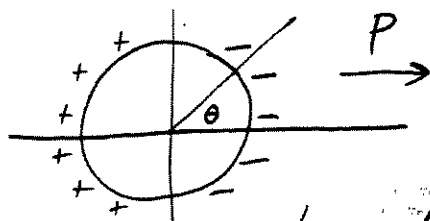


homog med. produces contribution $= E'$
net field strength of "nearby" dipoles $= E'$
(radius of sphere is large compared to intermolecular distances)

Then write

$$E' + E'' = E_{\text{con}}$$

To calculate E'



only contribution is from bound surface charge density
density (with - sign since we want contr.)
from outside sphere

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

Integrating, $E' = \frac{1}{3\epsilon_0} P$,

where P is actual polarization in medium.

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

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

(27)

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

$$E_{\text{con}} = E' = \frac{1}{3\epsilon_0} P$$

$$\Rightarrow E_{\text{local}} = E + E_{\text{con}} = E + P/3\epsilon_0$$

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

$\epsilon = \text{dielect. const. (rel.)}$

$$D = \epsilon_0 E + P = \epsilon \epsilon_0 E$$

$$\Rightarrow P = n_0 \alpha (E + P/3\epsilon_0)$$

$$\epsilon_0 (\epsilon - 1) E = n_0 \alpha \left(E + \frac{1}{3} (\epsilon - 1) E \right) \quad \left\{ \begin{array}{l} P = (\epsilon - 1) \epsilon_0 E \end{array} \right.$$

$$3\epsilon_0 (\epsilon - 1) E = n_0 \alpha (\epsilon + 2) E$$

$$\therefore \frac{\epsilon - 1}{\epsilon + 2} = \frac{n_0 \alpha}{3\epsilon_0}$$

Clausius-Mossotti Relation

In Gaussian units

$$\frac{\epsilon - 1}{\epsilon + 2} = \frac{4\pi n_0 \alpha}{3}$$

(CM)

Remarks about derivation:

Consider following set-up

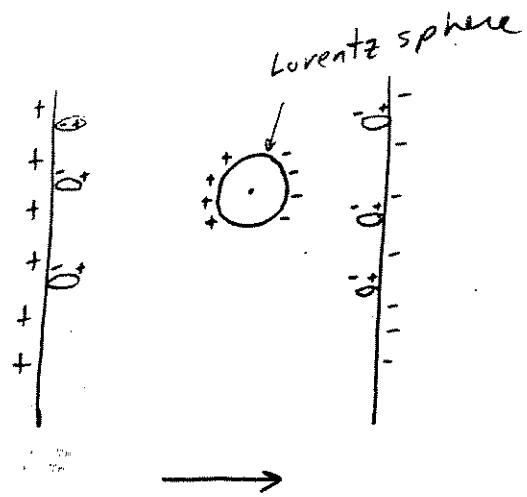
$$E_{loc} = E_x + E_d + E_s + E''$$

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 $E_s = \frac{1}{3\epsilon_0} P$ (we called it E' before)

$$E'' = 0$$

this is the Lorentz calculation based on symmetry of sample (sphere)
Note: Lorentz calc $\neq$ zero contr. from all dipoles

Thus $E_{loc} = E + \frac{1}{3\epsilon_0} P$ which yields CM

CM works for other polarizable bodies on macro scale, considered an expression for ϵ^* = effective diel. const

α = polarizability of individual bodies.

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

$$\alpha = \frac{a^3(\epsilon_1 - 1)}{(\epsilon_1 + 2)}$$

Combining with CM yields

$$\frac{\epsilon^* - 1}{\epsilon^* + 2} = p_1 \frac{\epsilon_1 - 1}{\epsilon_1 + 2} \quad p_1 = \text{vol frac. of spheres}$$

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

$$\frac{\epsilon^* - \epsilon_0}{\epsilon^* + 2\epsilon_0} = p_1 \frac{\epsilon_1 - \epsilon_0}{\epsilon_1 + 2\epsilon_0}$$

NOTE: This expression for ϵ^* not symmetric in ϵ_0 and ϵ_1 .

Can write generalization to n types of spheres

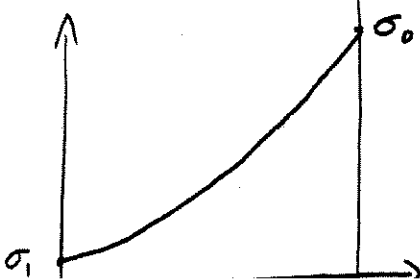
$$\frac{\epsilon^* - \epsilon_0}{\epsilon^* + 2\epsilon_0} = \sum_{i=1}^n p_i \frac{\epsilon_i - \epsilon_0}{\epsilon_i + 2\epsilon_0}$$

Note: CM for effective conductivity yields

$$\sigma^* = \frac{(1 + 2p_1)\sigma_1 + 2p_0\sigma_0}{2 + p_1 + p_0 \frac{\sigma_1}{\sigma_0}}$$

p_1 vol frac ϵ_1
 p_0 vol frac ϵ_0

$$\sigma_0 \gg \sigma_1$$



NO PERCOLATION THRESHOLD

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,

$$\epsilon_1^*(p) \leq \epsilon_{\text{meas}}^*(p) \leq \epsilon_0^*(p) \quad p = \text{vol frac.}$$

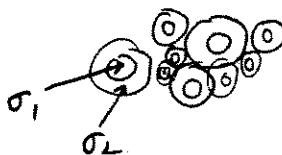
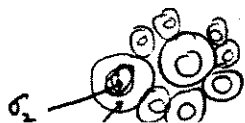
i.e., the measured values for ϵ^* for isotropic composites lie between the CM expressions.

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.

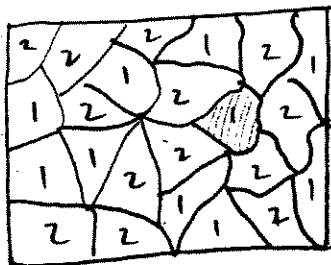
They construct coated-sphere geometries which attain the bounds (optimality).

$$\sigma_1 + \frac{P_2}{\frac{1}{\sigma_2 - \sigma_1} + \frac{P_1}{d\sigma_1}} \leq \sigma^* \leq \sigma_2 + \frac{P_1}{\frac{1}{\sigma_1 - \sigma_2} + \frac{P_2}{d\sigma_2}} \quad \sigma_1 \leq \sigma_2$$



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

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

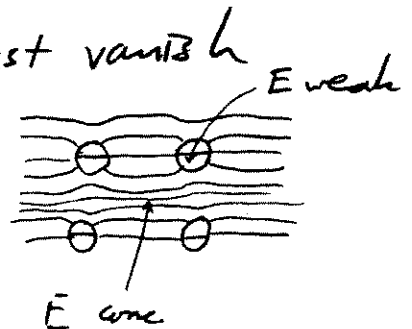
This polarization produces a deviation from E_0 .

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.

assume

$$\langle P \rangle' = p_1 \frac{\sigma_1 - \sigma_m}{\sigma_1 + 2\sigma_m} + p_2 \frac{\sigma_2 - \sigma_m}{\sigma_2 + 2\sigma_m} = 0$$



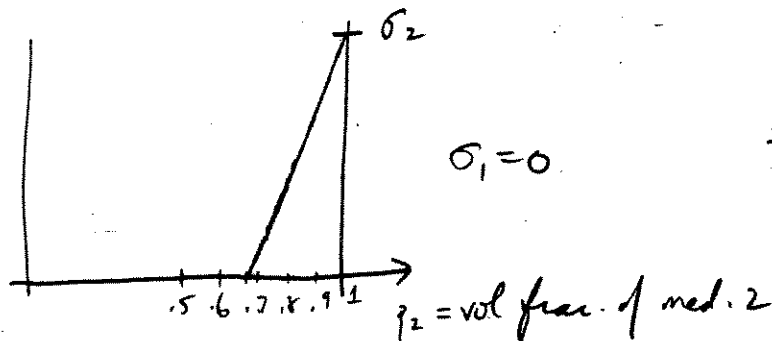
(This is where symmetry in σ_1 and σ_2 is introduced)

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

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



$\Rightarrow$ perc. threshold!

Can easily generalize to n components.

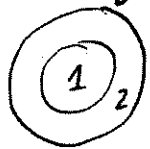
This is most commonly invoked approx in field

in d -dimensions

$$p_1 \frac{\sigma_1 - \sigma_m}{\sigma_1 + (d-1)\sigma_m} + p_2 \frac{\sigma_2 - \sigma_m}{\sigma_2 + (d-1)\sigma_m} = 0$$

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

$$\sigma^* = \sigma_2 + \frac{P_1}{\frac{1}{\sigma_1 - \sigma_2} + \frac{P_2}{2\sigma_2}}, \quad \sigma_1 \leq \sigma_2$$

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

Can do EMT for ellipsoids
coated ellipsoids

(Sihvola, Kong 1988)
(Tinga, et al., 1973)

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

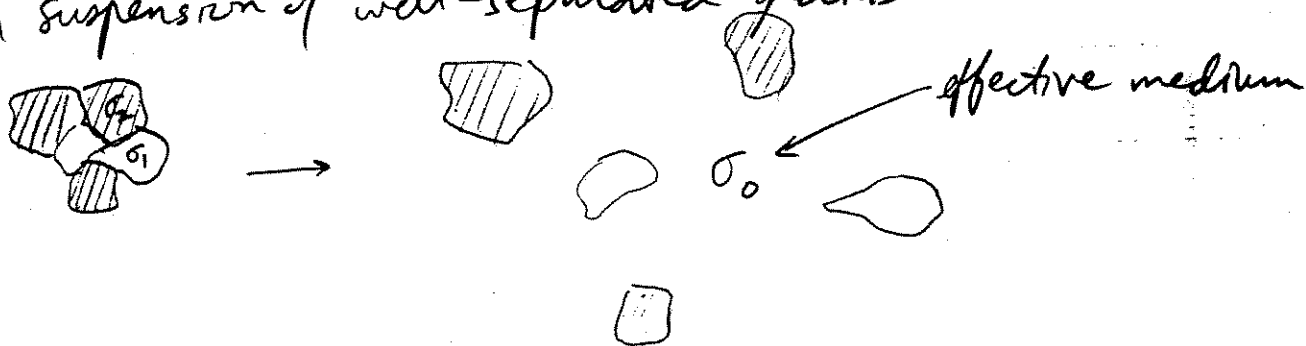
HOWEVER range of validity unclear:

— 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 , $f_1 + f_2 = 1$.

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



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

Basic assumption of CPA: 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 $c \rightarrow 0$

To examine, let's expand σ_f^* near $c=0$,

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

here

$P(\sigma)$ 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

Spherical grains:

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

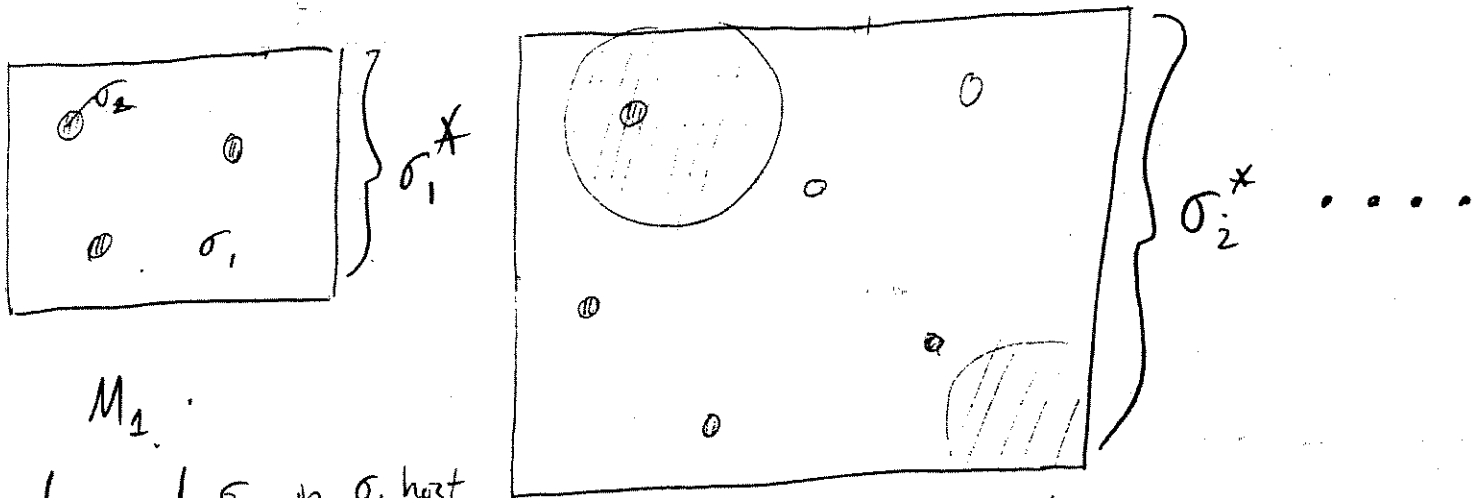
From expansion, the variation of σ_f^* in c ($c \ll 1$), is minimal when $\sigma_0 = \sigma_m$, (the FMT expression) satisfying

$$P(\sigma_m) = 0, \quad (*)$$

which has unique sol.

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

Consider following sequence of media



M_1

spheres of σ_2 in σ_1 host

rad = r_1

vol. frac = c_1

h. centers sep $\geq 2s_1$

M_2 = embed spheres of σ_2 in M_1 so

that

rad = r_2

vol. frac = c_2

sph. centers sep $\geq 2s_2$

keep iterating

get hierarchical, self-similar
fractal medium

spheres satisfy ① homogeneity condition to prevent
macroscopic clustering

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

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

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

Under such conditions

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

the construction can be generalized to non-spherical grains

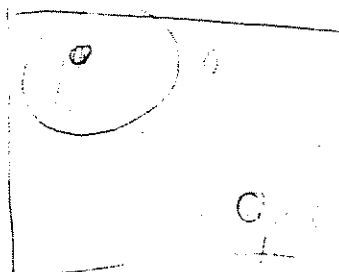
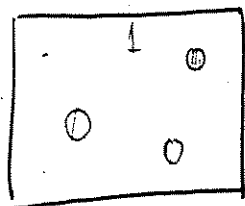
Note: for j large, the medium surrounding the largest spheres (are well-sep. and have vol frac. $c_j \rightarrow 0$), is behaving like the fluid

$j \rightarrow \infty \Leftrightarrow$ injection of more fluid!

Fixed points / transformation $j \rightarrow j+1$ are

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

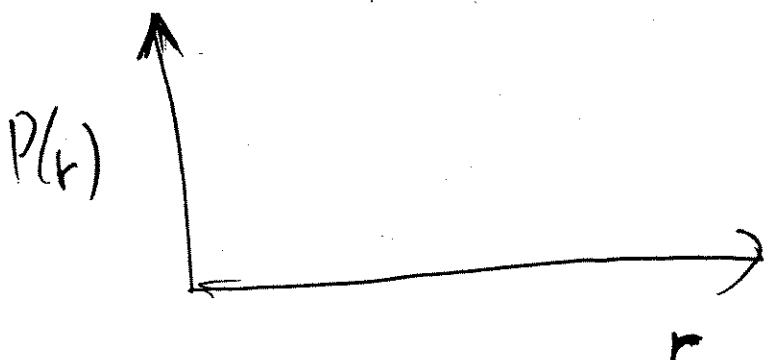
Idea of proof: Instead consider $\log \sigma^*$
then fixed points are $-\infty, \infty, \log \text{CPA}$
Prove transformation $j \rightarrow j+1$ is contraction
with only finite fixed point $\log \text{CPA}$!



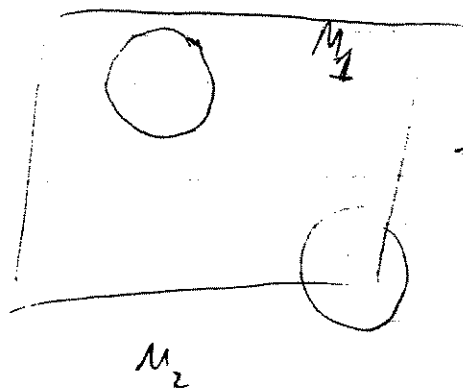
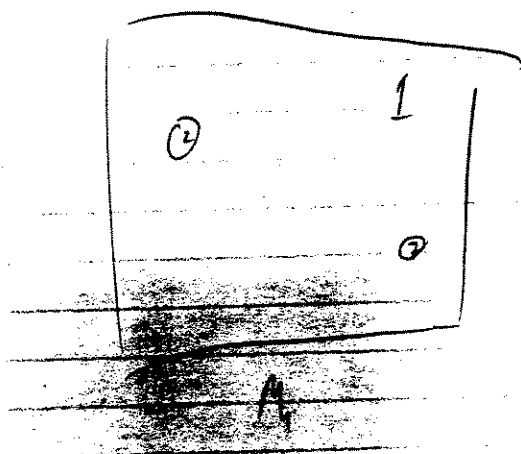
$7:45 \rightarrow 11:10$ F68
 $8:44 \rightarrow 12:10$ ÷ 68
 $\rightarrow 9:39 \rightarrow 12:28$ 596



1/2 s/h size
 dist'd so wide &
 that spheres of comp size
 very far from each other



extremely broad
 peak is very narrow



hole / vol
 V_i w/ sp S_i

M_j

eff vol $(M_i) \rightarrow$

low conc of diff soln
 diff soln $\rightarrow$ eff vol all

Indep of starting material

to be $\log \sigma^*$
 contractions
 Fixed points ① ∞
 ② 0
 ③ OA

hole
 in vol
 vol per
 inf.

same

$$+ \frac{P_2}{\frac{1}{\sigma_2 - \sigma_1} + \frac{P_1}{d\sigma_1}} \leq \sigma^* \leq \sigma_2 + \frac{P_1}{\frac{1}{\sigma_1 - \sigma_2} + \frac{P_2}{d\sigma_2}}$$

$$\sigma_1 \leq \sigma_2$$

$$\sigma_1 = 0$$

$$\sigma_2 = 1$$

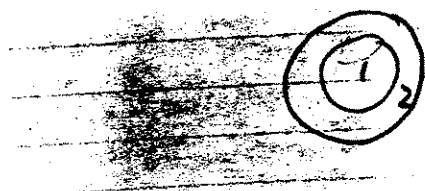
$$0 \leq \sigma^* \leq 1 + \frac{P_1}{-1 + \frac{P_2}{d}}$$

CM exhibits no perc. threat

H-S " " perc. threat

Bruggem EMT does exhibit perc threat

Bruggem



H-S $\Leftrightarrow$

Hill



CPA avg pol ≥ 0 choice of med st.

H-S: choice of med so fold in ext to unimp.
 $\Rightarrow$ 0 polarize.

558-8300

PERTURBATION EXPANSIONS

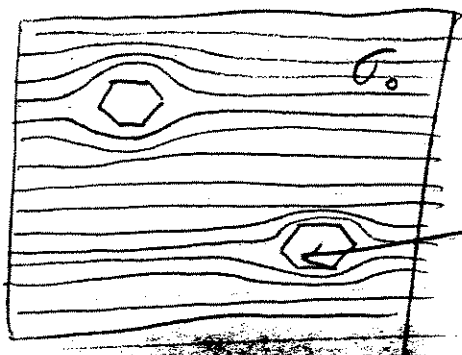
- 1) Volume Fraction Expansions (small p)
- 2) Expansion around Homogeneous Medium (small dev. in $\epsilon(x)$ homog)
- 3) "Almost Touching" Problems.

1) Volume fraction expansions

Kozlov (1989)

Thorpe (1992)

Golden (1991), Bruna + Golden (1992)



Thorpe
holes (a few)
n-gons

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

$f = \text{vol. frac.}$

$$= nS$$

$n = \# \text{ holes / unit area}$
 $S = \text{area of 1 hole.}$

$$d_n = \frac{\tan(\pi/n)}{2\pi n} \Gamma^4\left(\frac{1}{n}\right) / \Gamma^2\left(\frac{2}{n}\right)$$

$$d_n = \begin{array}{ll} 2.5811 & \text{triangles} \\ 2.1884 & \text{squares} \\ 2.0878 & \text{pentagons} \end{array}$$

$$d_n = 2 \text{ as } n \rightarrow \infty \text{ (circle)}$$

Idea: hole gets induced charge around perimeter
total induced charge = 0 $\rightarrow$



get multipole distr.

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

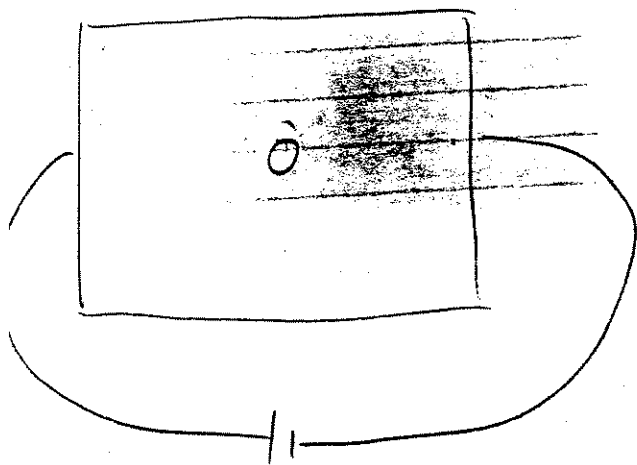
for other holes - have full multipole expansion
but only coef. of dipole term contr.
to f term

$$\sigma/\sigma_0 = 1 - 2f + O(f^2)$$

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.

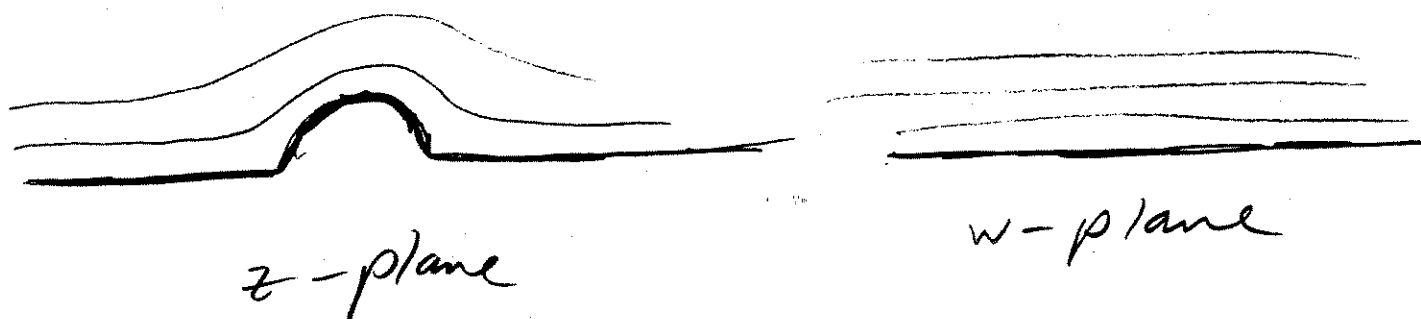
Now do for circle in 2 dimensions using conformal
mapping



conductivity drops when
put in hole.

(40)

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 = $\text{Re}[u]$

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

$$\text{Re}[u] = -E'_0 R \cos \theta \left(1 + \frac{a^2}{R^2} \right) = -E'_0 R \cos \theta (1 + f)$$

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

large R , potential same with or without hole
 $\Rightarrow E_0 = E'_0 (1+f)$

low, relate to cond.

only heating inside large circle of rad $R =$

$$\boxed{=\sigma E} \quad \int_{D_R} \mathbf{J} \cdot \mathbf{E} \, da = - \int_{\partial D_R} u(\mathbf{J} \cdot d\mathbf{s}) \quad \left(\begin{array}{l} \text{no current} \\ \text{flows across} \\ \text{inner surface} \end{array} \right)$$

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

E inside hole - fortunately!

change in Joule heating upon introduction of hole is

$$\int_0^{2\pi} (E_0 R \cos \theta) \sigma_0 [E'_0 \cos \theta (1-f) - E_0 \cos \theta] R \, d\theta$$

$$= -2\sigma_0 E_0 E'_0 \pi a^2$$

indep of R

Energy balance gives

$$\sigma E_0^2 \pi R^2 = \sigma_0 E_0^2 \pi R^2 - 2\pi \sigma_0 E_0 E'_0 \pi a^2$$

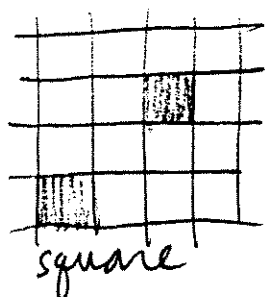
which yields

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

factor $a^2 R$ incl. dipole term $\frac{1}{2}$ in conf-map

Rigorous Results for Volume Fraction Expansion

Related model to Thorpe's : chessboard



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

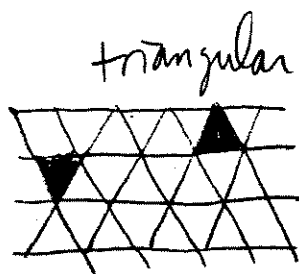
$$1-p$$

$$p$$

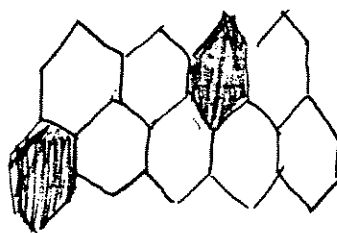


$$n=4$$

Now treat small p



$$n=3$$



$$n=6$$

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

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

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

proof is via stronger assertion

lim $\exists$ 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 $\lim_{\delta \rightarrow 0} \alpha_n(\delta) = \alpha_n$. The est. is valid $\forall \delta$.

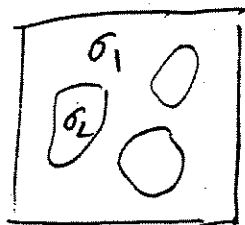
The consts. $\bar{c}, \bar{p}$ are indep. of δ .

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

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

Need pert. around homog. med.

Perturbation around homogeneous medium



$$\sigma_1 = \sigma_2 \quad \text{homog.}$$

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

$$\omega \in \Omega \quad \omega \neq P$$

$$x \in \mathbb{R}^d$$

$$J = \sigma E$$

$$\nabla \cdot J = 0$$

$$\nabla \times E = 0$$

$$\langle E \rangle = e_k$$

$$J, E \in L^2(\Omega, P)$$

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

tensor

$$k \text{ diag. wof } \sigma^* = \sigma_{kk}^* = \langle \sigma E_k \rangle$$

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

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

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

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

Define $F = 1 - m$

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

$$s = \frac{1}{1-h} = \frac{1}{1-\sigma_1/\sigma_2}$$

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

give resolvent repr. for E .

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

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

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

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

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

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

$$s \nabla \cdot G - \nabla \cdot \chi_1 E = 0$$

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

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

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

Γ = projection onto unid free fields

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

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

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

$G \in L^2(\Omega) \cap$ unid
free
 $\cap$ mean
zero.
= ~~2~~

$$\angle G = \nabla \varphi$$

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

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

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

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

$P\chi_1$ is s.a. operator on $\mathcal{H} \cap \chi_1$ in inner product

$$\text{w/ } \|P\chi_1\| \leq 1$$

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

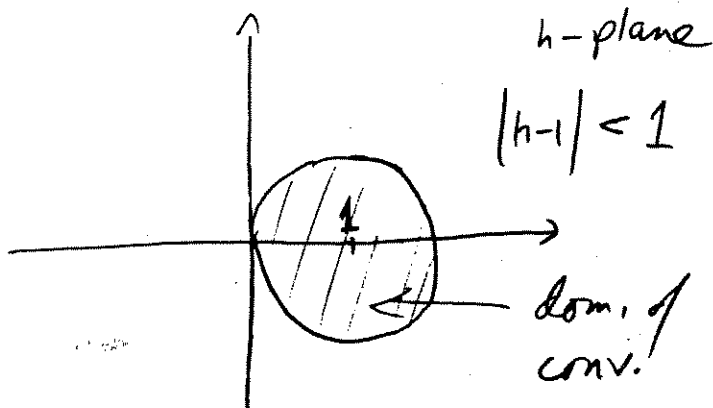
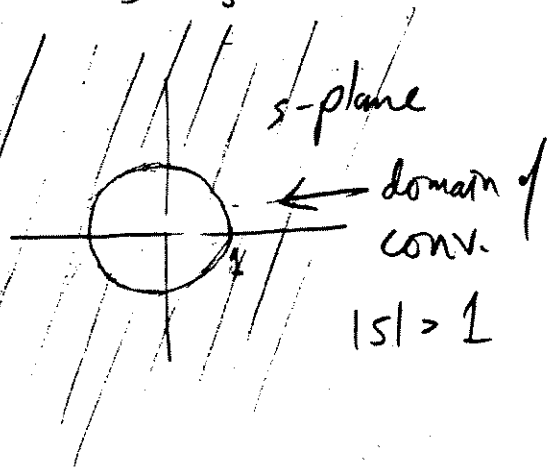
$$\frac{1}{s + P\chi_1} = \frac{1}{s(1 + \frac{P\chi_1}{s})} = \frac{1}{s} \left(1 - \frac{P\chi_1}{s} + \frac{(P\chi_1)^2}{s^2} - \dots \right)$$

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

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

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

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



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

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

$$= -\left\langle [X_1(0) (\Gamma X_1 e_k)(0)] \cdot e_k \right\rangle \left\{ \begin{array}{l} \Gamma = \nabla (-\Delta)^{-1} \nabla \cdot \\ \Gamma_{kk} = \frac{\partial}{\partial x_k} (-\Delta)^{-1} \frac{\partial}{\partial x_k} \end{array} \right.$$

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

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

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

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

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

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

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

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

$$\begin{aligned} R(y) &= \langle x_1(0) \tilde{x}_1(y) \rangle \\ &= \langle x_1(0) (x_1(y) - p_1) \rangle \end{aligned}$$

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

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

$$\begin{aligned} \text{Tr}(a_2) &= \langle x_1(0) (x_1(0) - p_1) \rangle = \langle x_1(0) \rangle - p_1 \langle x_1(0) \rangle \\ &= p_1 - p_1^2 = p_1(1 - p_1) \\ &= p_1 p_2 \end{aligned}$$

If material is statistically isotropic,

i.e. $\overset{*}{O}_{ii} = \overset{*}{O}_{jj}, \forall i, j = 1, \dots, d$

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

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

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, 33:
and others

which determine q_3 , similarly for q_4
These observations were used to obtain bounds better than Hashin-Shtrikman (1958)

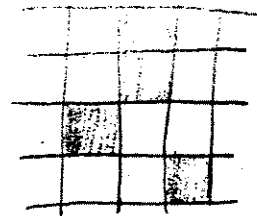
Given a particular geometry, q_n can be calculated in principle, but very difficult in practice.

One class of situations, where it should be possible to carry out the calculation of the q_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".

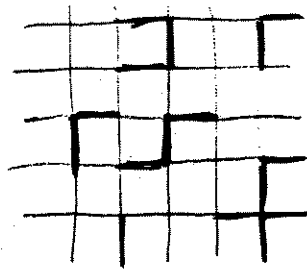
examples: Cell Materials

Bernoulli meas per cell



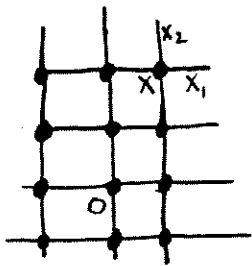
$$\sigma(x) = \begin{cases} \sigma_1 & \square \text{ prob } 1-p \\ \sigma_2 & \square \text{ prob } p \end{cases}$$

Lattices



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

focus on lattice - Random Resistor Network



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

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

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

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

$$\langle E \rangle = e_k$$

Isotropic $\sigma^* = \sigma_{kk}^* = \langle \sigma(x) E_k(x) \rangle$

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

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

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

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

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

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

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

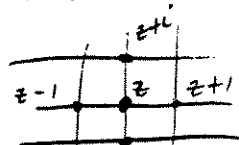
$$A(x, y) = \lim_{n \rightarrow \infty} \sum_{k=0}^n [P_k(0, 0) - P_k(x, y)]$$

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) $\Leftrightarrow$

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



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

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	$\frac{4}{\pi}$		
	$4 - \frac{8}{\pi}$	$-1 + \frac{8}{\pi}$	$\frac{16}{3\pi}$	
	$17 - \frac{48}{\pi}$	$\frac{92}{3\pi} - 8$	$\frac{8}{3\pi} + 1$	$\frac{92}{15\pi}$

McCrea
+ Whipple (1940)

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

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

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

So it behaves asymptotically like continuum free space green's function $\frac{1}{\pi} \ln |z|$ in $d=2$.

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

Now let's calculate 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)

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

Then

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

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

$$\left\langle \begin{array}{l} g(x, y) \text{ is "isotropic"} \\ \Delta g = -\delta \Rightarrow -D_K^+ D_K^- g(0, 0) = \frac{1}{d} \end{array} \right.$$

to look at a_3

$$a_3 = \sum_{j=1}^d \langle X_1 D_k^+ (-\Delta)^{-1} D_j^- X_1 D_j^+ (-\Delta)^{-1} D_k^- (X_1 - p_1) \rangle$$

after discrete int. by parts and similar manipulations

$$a_3 = \sum_{j=1}^d \sum_{Y_1 \in \mathbb{Z}^d} \sum_{Y_2 \in \mathbb{Z}^d} D_k^+ D_j^- g(0, Y_1) D_j^+ D_k^- g(Y_1, Y_2) \langle X_1(0) X_1(Y_1) (X_1(Y_2) - p_1) \rangle$$

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

$$\langle X_1(0) X_1(Y_1) (X_1(Y_2) - p_1) \rangle = R(0, Y_1, Y_2) + p_1 (R(0, Y_2) + R(Y_1, Y_2))$$

where $R(0, Y_1, Y_2)$ is the centered three-point function

$$R(0, Y_1, Y_2) = \langle (X_1(0) - p_1) (X_1(Y_1) - p_1) (X_1(Y_2) - p_1) \rangle$$

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

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

a_4 is a fourth order poly. in p , 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 move analyticity of $\sigma^*(p)$ in p . Do it for lattice, but proof will hold for cell materials and their generalization

Consider the d-dim bond lattice

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

Theorem (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 .

runo's Thesis : relate the a_i 's to the l_i 's

in particular, he found explicit algorithm to derive $a_0, a_1, \dots, a_{2k+1}$ from the coefficients $l_0, \dots, l_k$

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.

Basic Idea: Consider above cell material

Space rel. vol. frac 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 itself, 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

6

a conductivity function of a three-component mixture

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

with

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

Note that s is a symmetric 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.

Definition: A family of composites of conductivities $\sigma^*(\sigma_1, \sigma_2, p)$
is said to be infinitely interchangeable iff for each integer n ,
 $\exists$ a function $s_n(z_1, \dots, z_n)$ 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.

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

for any permutation of its coordinates

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

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

Remark: All examples of cell materials in literature
are infinitely interchangeable.

(61)

Sketch of method for deriving relations

For an inf.-int. material,

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

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,

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

where

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

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

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

Get linear equations for them:

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

not enough, get rank deficient system.

Need more info, this is done by considering

1st, 2nd, ... derivs. of $s_n(1, \dots, 1, z), s_n(1, \dots, 1, z, z)$

can be related to low vel frac. info.

Example $d=2$ 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

$$s_n^1 = \frac{2s_n}{2z} (1, 1, \dots, 1)$$

To get s_n^1 , note

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

so that

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

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

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

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

Using Keller interchange equality in $d=2$

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

get

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

Duality Keller-Dykhne Interchange Theorem

Consider conduction in $d=2$:

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

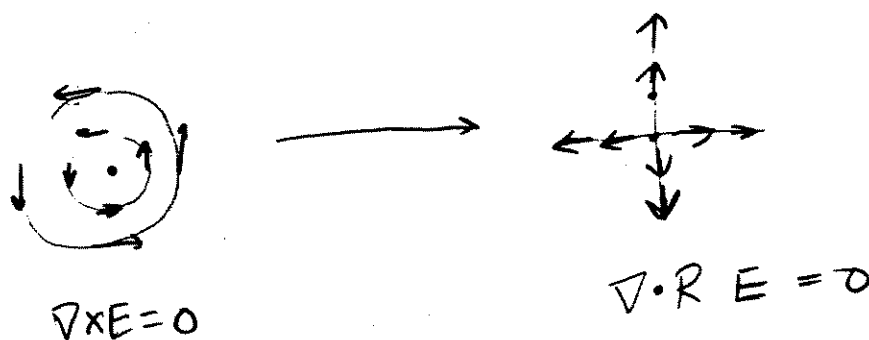
$$\langle J \rangle = \sigma^* \langle E \rangle$$

$$\nabla \cdot J = 0$$

$$\nabla \times E = 0$$

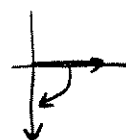
Observation:

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



the duality transformation

$$R = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$



$$(R^{-1}) = R^T$$

$$J'(x) = R E(x)$$

$$E'(x) = R J(x)$$

Then

$$\nabla \cdot J' = 0$$

$$\nabla \times E' = 0$$

If: $\nabla \cdot J' = \frac{\partial j'_1}{\partial x_1} + \frac{\partial j'_2}{\partial x_2} = \frac{\partial e_2}{\partial x_1} - \frac{\partial e_1}{\partial x_2} = 0$

$$1 \quad 2e' \quad 2e' \quad -2j_1 \quad -2j_2 \quad -\lambda$$

Now, how are J' and E' related:

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

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

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

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.

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

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

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

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

$$\langle J' \rangle = \sigma^{*'} \langle E' \rangle$$

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

we 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

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

σ^* for σ'

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

inserting this in (*) 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)

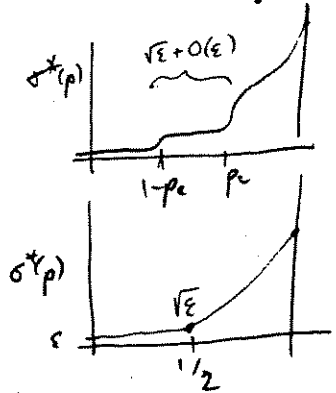
i.e. materials for which $\sigma^*(\sigma_1, \sigma_2) = \sigma^*(\sigma_2, \sigma_1)$, then

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

for Botvinnik

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

sample: checkerboards
resistor networks



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

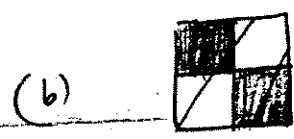
at $p = 1/2$, lattice
is interchange invariant

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

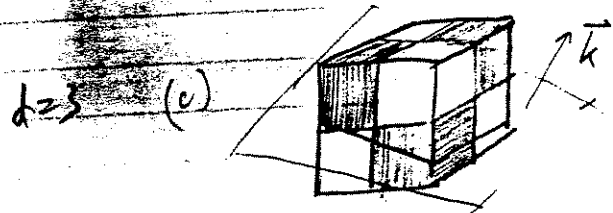
sample: quasi-periodic media in $d=2$

(although $\sigma^*(p)$ is not
strictly convex function of p)

first $d=1$ a) $\sigma(x) = 3 + \cos 2\pi x + \cos 4\pi x$



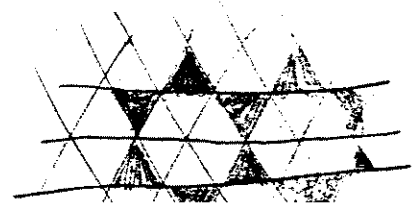
$$\sigma^* = \begin{cases} \frac{1}{2} & k \text{ irrat.} \\ \frac{1}{2} - \frac{1}{2\sqrt{1-k^2}} & k = \frac{p}{q} \text{ } p, q \text{ odd rel. pr.} \\ \frac{1}{2} & k = p/q, \text{ otherwise} \end{cases}$$



$\vec{k}$ irrational
 $\Rightarrow$ interchange invariance

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

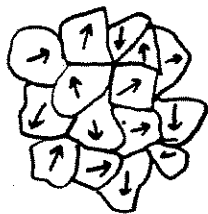
part
 K irrat.



NOT interchange inv.

polycrystals

duality gives exact result for $\underline{\sigma}^*$ 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,

dual material:

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

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

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

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

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

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

$$\left(\begin{array}{l} \text{also} \\ \text{recall} \end{array} \quad \sigma'(x) = \frac{\sigma(x)}{\det(\sigma_0)} \right)$$

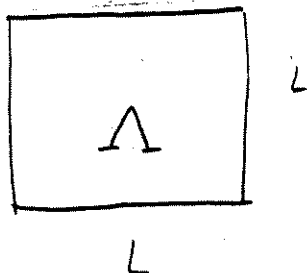
homogeneity then implies

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

$$\text{Isotropy} \Rightarrow \boxed{\sigma^* = \sqrt{\det(\sigma_0)} \mathbf{I}}$$

indep. of details
of polycrystalline
microstructure.

Variational Formulation of Effective Properties



energy dissipated in conducting med
per unit vol.

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

if homogeneous $U = \frac{\sigma \mathbf{E} \cdot \bar{\mathbf{E}}}{2|\Lambda|}$

if $\langle \mathbf{E} \rangle = \mathbf{e}_k$

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

or $\sigma^* = \frac{1}{|\Lambda|} \int_{\Lambda} \sigma(x) \mathbf{E}(x) \cdot \bar{\mathbf{E}}(x) \, dx$ (then take $|\Lambda| \rightarrow \infty$)

Now get variational form

field eqs are $\nabla \cdot \mathbf{J} = 0$

$\nabla \times \mathbf{E} = 0$

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

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

For simplicity assume σ smoothly varying

$$\nabla \times E = 0 \Rightarrow E = \nabla \phi$$

* $U = \frac{1}{2|\Lambda|} \int \sigma \nabla \phi \cdot \nabla \phi dx$

assume variation of ϕ
vanishes on boundary $\partial\Lambda$
 $\phi + \delta\phi$

Variation of * $\Rightarrow$

$$\delta U = \frac{1}{2|\Lambda|} \int 2\sigma \nabla \phi \cdot \delta \nabla \phi dx$$

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

Divergence thm. gives

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

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

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

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

Thus. $U = \min_{\nabla \times F = 0} \frac{1}{|\Lambda|} \int \sigma F \cdot \bar{F} dx$ sol. satisfies $\nabla \cdot \sigma F = 0$

(71)

Dual variational principle

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

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

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

Thus

$$\sigma^* = \min_{\nabla \times E = 0} \frac{1}{|A|} \int_A \sigma(x) E(x) \cdot \bar{E}(x) \, dx \quad (1)$$

$$\frac{1}{\sigma^*} = \min_{\nabla \cdot \bar{J} = 0} \frac{1}{|A|} \int_A \frac{1}{\sigma(x)} J(x) \cdot \bar{J}(x) \, dx \quad (2)$$

Get bounds

$$\text{stick in trial fields } E = e_k \quad \text{in } (1)$$

$$J = e_k \quad \text{in } (2)$$

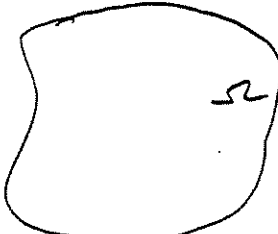
$$(1) \Rightarrow \sigma^* \leq \langle \sigma \rangle$$

$$(2) \Rightarrow \frac{1}{\sigma^*} \leq \langle \frac{1}{\sigma} \rangle$$

$$\langle \frac{1}{\sigma} \rangle \leq \sigma^* \leq \langle \sigma \rangle$$

Arithmetic +
Harmonic Mean Bound

Application of Riesz to solution of Dirichlet problem

Ω open  Ω

$$\begin{aligned} \Delta u &= 0 \quad \text{in } \Omega \\ u|_{\partial\Omega} &= f \end{aligned}$$

old problem

extend f into Ω , look for

$$v = u - f \quad \text{s.t.}$$

$$\begin{aligned} \Delta u &= 0 \Rightarrow \\ \Delta(v + f) &= 0 \\ \Delta v &= -\Delta f \end{aligned}$$

New Problem

$$\begin{aligned} \Delta v &= -w \quad \text{in } \Omega \\ v|_{\partial\Omega} &= 0 \end{aligned}$$

(*)

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 $C_0^1(\bar{\Omega}) \subset C^1(\bar{\Omega})$ s.t. $u \in C_0^1(\bar{\Omega})$ vanishes on $\partial\Omega$

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

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

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

Then can find v sol of (*) by rep.

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

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

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

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 $H_0^1(\Omega)$

Bdd: $\phi(u) \leq M \|u\|$

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

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

$$\text{suppose to show } \int_{\Omega} |u|^2 \, dx \leq K \int_{\Omega} |\nabla u|^2 \quad \text{Poincaré}$$

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

Then done

remark: $L^2(\Omega)$ sep

inner product is not defined on $L^2(\Omega)$

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Lax-Milgram Theorem

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

$$(B(x_1 + x_2, y) = B(x_1, y) + B(x_2, y), B(ax, y) = aB(x, y))$$

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

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

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

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

$0 < \omega(x) < \infty \quad \text{on } [0, 1]$

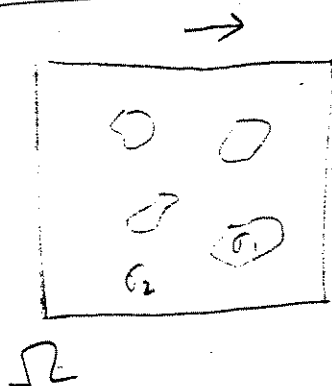
Theorem: B is bdd, coercive bilinear form on $\mathcal{H}$

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 of av. vel.)



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

$$\chi_j = \begin{cases} 1 & x \in \text{mat} \\ 0 & x \in \text{void} \end{cases}$$

$$J = \sigma E$$

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

$$\nabla \times E = 0$$

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

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



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

def 1

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

$$\sigma^* \langle E \rangle^2 = \langle \sigma E \cdot \bar{E} \rangle$$

def 2

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

or

Recall had weak sol to Dirichlet

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

we need of st
$$\int u \Delta \phi = - \int u w$$

$$\int \nabla u \cdot \nabla \phi = \int u w$$

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

Now reformulate our problem

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

Motivation:
 $E = e_k + g$ $\begin{matrix} \nabla \times g = 0 \\ \langle g \rangle = 0 \end{matrix}$
↑ mean 0 fluctuations

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

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

↑ this bdd linear funct. on $\mathcal{H}$
lin Bilinear form

(83)

Lax-Milgram $\Rightarrow$ if $B(f_1, f_2) = \int_{\Omega} \sigma f_1 \cdot f_2$ is bdd + coercivethen $\exists! g \in \mathcal{H}$ s.t. lin form. $\varphi(f) = - \int_{\Omega} \sigma f \cdot e_k$

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

this gives existence + uniqueness
(when coercive)Question: when is it coercive^{+ bdd}?

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

$$\nabla \cdot (\sigma_1 X_1 + \sigma_2 X_2) E = 0$$

$$\nabla \cdot \left(\underbrace{\begin{pmatrix} \sigma_1 \\ \sigma_2 \end{pmatrix}}_L X_1 + X_2 \right) E = 0$$

$$\nabla \cdot (L X_1 + X_2) E = 0$$

for which L is assoc. bilinear form bdd + coercive
obviously if L finite have bdd.

Equiv. B is $B(f, g) = \int_{\Omega} (h\chi_1 + \chi_2) f \cdot g$ on $\mathcal{H}$

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

$$(*) \quad \left| \int_{\Omega} (h\chi_1 + \chi_2) f^2 \right| \geq \alpha \int f^2, \quad \alpha > 0$$

$$\text{let } \lambda = \frac{\int_{\Omega} \chi_1 f^2}{\int_{\Omega} f^2}$$

$$|\lambda| = 1$$

$$\text{and Note } \int_{\Omega} \chi_1 + \chi_2 = 1 \Rightarrow \frac{\int \chi_1 f^2}{\int f^2} + \frac{\int \chi_2 f^2}{\int f^2} = 1$$

$$\text{then } (*) \Leftrightarrow |h\lambda + 1(1-\lambda)| \geq \alpha > 0$$



$$\text{coercive} \Leftrightarrow h \notin (-\infty, 0]$$

How does σ^* depend on h

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

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

Consider m as analytic function of h

what is domain of analyticity

$h \chi_1 + \chi_2$ entire in h

and dep. on h in E

if E exists and is unique m is analytic in h (*)

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

We have

Theorem: ① $m(h)$ analytic on $(-\infty, 0]$
 ② $m(h): U \rightarrow U$

Exercise: Find domain of analyticity for 3 component case

Let's do good applied math.

(see spectral thm, need vexp, p.d. theory, spectral measures, Dirac measures, int. eg. orthog. decomp, extended states)

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

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

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

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

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

$$g = \nabla \varphi$$

$$\nabla \cdot \nabla \varphi + (h-1)\nabla \cdot \chi_1 E = 0$$

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

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

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

$$g + e_k + (1-h)\nabla(-\Delta)^{-1} \nabla \cdot \chi_1 E = e_k \quad \left(\text{Integral eq. for } E \right)$$

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

projection onto
curl-free fields

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

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

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

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

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

$$\Gamma \chi_1 \text{ self adj. in } \langle \chi, f \cdot g \rangle$$

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$$\sigma_{kk}^* = \langle \sigma E_k^k \rangle$$

$$\sigma_{kk}^* = \langle (\sigma_1 \chi_1 + \sigma_2 \chi_2) E_k^k \rangle$$

$$\begin{aligned} \frac{\sigma_{kk}^*}{\sigma_2} &= \langle h \chi_1 + (1 - \chi_1) E_k^k \rangle \\ &= \langle ((h-1)\chi_1 + 1) E_k^k \rangle \end{aligned}$$

$$\frac{\sigma_{kk}^*}{\sigma_2} = 1 - \frac{1}{s} \langle \chi_1 E_k^k \rangle$$

$$1 - \frac{\sigma_{kk}^*}{\sigma_2} = \frac{1}{s} \langle \chi_1 E_k^k \rangle$$

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

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

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

$$f(A) = \frac{1}{s - A}$$

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

$$A = \Gamma \chi_1$$

↑
product of
projections

$$= (e_k \cdot f(A) e_k)$$

$$\|A\| \leq 1$$

$$= \int f(\lambda) d(e_k \cdot P_\lambda e_k)$$

$$= \int_{\sigma(A)}^1 \frac{d\mu(z)}{z - \bar{z}}$$

$$d\mu = d(e_k \cdot P_\lambda e_k) \geq 0$$

analytic
off
[0,1]

$$F(s) = \langle X_1 e_k \cdot (s + \Gamma X_1)^{-1} e_k \rangle$$

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

Need to inject geometry info μ

Resolvent Expansion (

Neumann Series
Geom Series)

$$F(s) = \langle X_1 e_k \cdot \frac{1}{s + \Gamma X_1} e_k \rangle$$

$$= \frac{1}{s} \langle X_1 e_k \cdot \frac{1}{(1 + \frac{\Gamma X_1}{s})} e_k \rangle$$

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

$$= \frac{1}{s} \langle X_1 e_k \left(1 - \frac{\Gamma X_1}{s} + \left(\frac{\Gamma X_1}{s} \right)^2 - \dots \right) e_k \rangle$$

$$= \frac{\langle X_1 \rangle}{s} + \frac{\langle e_k \cdot X_1 \Gamma X_1 e_k \rangle}{s^2} + \dots$$

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

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

Int for power Analytic cond of

Percolation and Homogenization in Composite Media

Professor Kenneth M. Golden

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Abstract

Composite random media appear throughout science and engineering. Calculating their bulk, or homogenized material properties is a formidable mathematical problem, but has wide ranging applications. We shall focus on those media whose behavior depends critically on the connectedness, or percolation properties of a particular phase. For example, sandstones are permeable to water when there is a high enough volume fraction of pores that they connect and form pathways, and the electromagnetic properties of an insulating polymer film with conducting carbon black particles vary dramatically near the critical volume fraction where the particles begin to form a connected matrix. This critical volume fraction is called the percolation threshold, and near this point the effective transport coefficients typically display scaling behavior characterized by critical exponents. There is an extensive literature on these types of problems built up over the past 40 years by researchers in the physics, engineering, materials science, geophysics, and mathematics communities, although many fundamental questions remain unanswered. Mathematical progress in this area has been notoriously difficult. After giving a general introduction to homogenization and the effective properties of composite random media, we will concentrate on lattice and continuum percolation models and their bulk transport properties, as well as applying these models to materials such as sea ice and composite conductors.

Topics to be covered:

1. Introduction to composite media and homogenization
2. Lattice and continuum percolation models
3. Integral representations and bounds on transport coefficients
4. Connections to phase transitions in statistical mechanics
5. Applications to matrix-particle composites and sea ice
6. Inverse homogenization and the recovery of microstructural parameters

1 Introduction to composite media and homogenization

Composite and inhomogeneous media are pervasive. Examples include:

- plywood – a laminated structure
- concrete reinforced with steel rods
- rocks – aggregates of individual grains
- metals and other polycrystals – aggregates of crystals with different orientations
- fiber composites used in skis, bullet proof vests and helmets
- honeycomb structures used in aviation
- solid rocket propellants and other powders and granular media
- biological materials – muscle, bones, heart and lung tissue
- atmosphere – air with water droplets or dust particles
- turbulent fluid – inhomogeneous velocity field

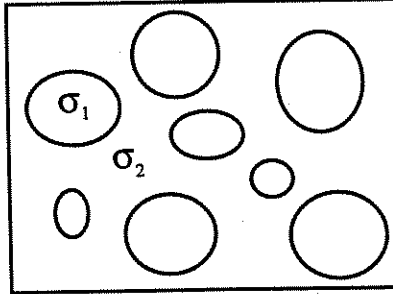
The bulk properties of many important examples depend on the connectedness properties of a given phase:

- sandstones and soils
- thin silver films
- polymerization
- vanadium dioxide
- doped semiconductors
- fractures
- matrix-particle composites and radar absorbing materials
- sea ice
- glacial firn

Properties of composites can be different from constituents:

- wood strong in one direction, plywood strong in all directions
- properly placed holes in metal sheet significantly reduces weight, but retains strength
- anomalous dielectric effect – dielectric properties larger than either constituent due to interfacial effects

Composites arise as solutions in optimization problems.



Transport in random media

- effective conductivity and permittivity, and magnetic permeability (transport of **current** and **EM waves**)
- effective diffusivity (transport of **heat** and **tracers**)
- effective fluid permeability for Darcy flow through a **porous medium**
- effective diffusivity for convection enhanced diffusion in a **turbulent fluid**

Electrical conduction in two phase random media

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

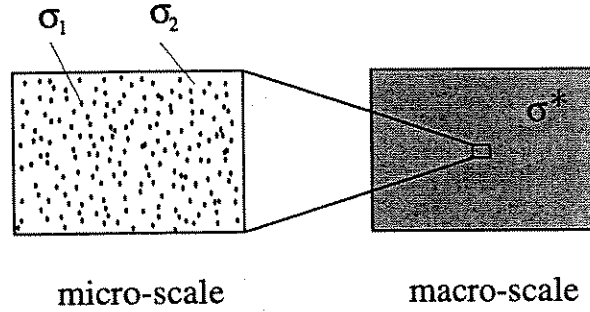
- stationary random field in $x \in R^d$ and $\omega \in \Omega$
- Ω is the set of realizations of the random medium
- $\chi_j(x, \omega)$ is the characteristic function of σ_j

Let $E(x, \omega)$ and $J(x, \omega)$ be stationary random electric and current fields satisfying

$$J = \sigma E \quad \langle E \rangle = e_k$$

$$\nabla \cdot J = 0$$

$$\nabla \times E = 0$$



HOMOGENIZED Transport Coefficient:

Effective conductivity tensor σ^*

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

$$\sigma^* = e_k \cdot \sigma^* e_k = \sigma_{kk}^* = \langle (\sigma_1 \chi_1 + \sigma_2 \chi_2) E_k \rangle$$

$$m(h) = \frac{\sigma^*}{\sigma_2} = \langle (h \chi_1 + \chi_2) E_k \rangle \quad h = \frac{\sigma_1}{\sigma_2}$$

Variational Formulation for $\sigma(x)$ in box Λ :

Energy dissipated in conducting medium per unit volume

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

If homogeneous with $\sigma(x) = \sigma^*$, $U = \frac{1}{2} \sigma^* e_k \cdot \bar{e}_k$, or

$$\sigma^* = \frac{1}{|\Lambda|} \int_{\Lambda} \sigma E \cdot \bar{E} \, dx$$

Variation of energy integral subject to condition $\nabla \times E = 0$ gives minimum satisfying $\nabla \cdot \sigma E = 0$, with

$$\sigma^* = \min_{\nabla \times E = 0} \frac{1}{|\Lambda|} \int_{\Lambda} \sigma E \cdot \bar{E} \, dx.$$

Variation of dual integral for J subject to condition $\nabla \cdot J = 0$ gives minimum satisfying $\nabla \times (J/\sigma) = 0$, with

$$\frac{1}{\sigma^*} = \min_{\nabla \cdot J = 0} \frac{1}{|\Lambda|} \int_{\Lambda} \frac{1}{\sigma} J \cdot \bar{J} \, dx.$$

Insertion of trial fields $E = e_k$ and $J = e_k$ into these equations yields **arithmetic and harmonic mean bounds**:

$$\left\langle \frac{1}{\sigma} \right\rangle^{-1} \leq \sigma^* \leq \langle \sigma \rangle.$$

These bounds are **optimal**: there are actual composites which attain the bounds. The upper bound is attained by a laminated or layered structure parallel to the applied field, and the lower bound is attained by a laminated structure perpendicular to the applied field.

REMARK: We will also be interested in effective complex permittivity for electromagnetic wave propagation, where $J(x) = \sigma(x)E(x)$ is replaced by $D(x) = \epsilon(x)E(x)$, with $\nabla \cdot D = 0$ and $\nabla \times E = 0$, and the homogenized or effective complex permittivity satisfies

$$\langle D \rangle = \epsilon^* \langle E \rangle.$$

The real part of ϵ corresponds to the polarizability of the medium and the imaginary part corresponds to the conductivity (controlling absorption or losses), as in $\epsilon = \epsilon' + i\sigma/\nu$, where ν is angular frequency and ϵ' is the real permittivity. Recall that in the static case, $\epsilon = \epsilon' = 1 + \chi/\epsilon_0$, is the relative permittivity or dielectric constant, with ϵ_0 the permittivity of free space and χ the dielectric susceptibility in $P = \chi E$, where P is the polarization field.

Classical results in homogenization [1]

1. Homogenization on molecular scale – approximate formula of Claussius and Mossotti (CM) for the permittivity ϵ of a homogeneous medium with n molecules per unit volume, each with polarizability α

$$\frac{\epsilon - 1}{\epsilon + 2} = \frac{n\alpha}{3\epsilon_0}.$$

2. CM can be applied to polarizable bodies on macro-scale, such as spheres of radius a and permittivity ϵ_1 embedded in host of permittivity ϵ_2 , which have polarizability $\alpha = a^3(\epsilon_1 - \epsilon_2)/(\epsilon_1 + 2\epsilon_2)$ (from a standard single sphere calculation). CM formula for this system is

$$\frac{\epsilon^* - \epsilon_2}{\epsilon^* + 2\epsilon_2} = p_1 \frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + 2\epsilon_2},$$

where p_1 is the volume fraction of spheres. Remark: this formula does **not** exhibit a percolation threshold, and is not symmetric in ϵ_1 and ϵ_2 , i.e., gives two different results ϵ_1^* and ϵ_2^* if the host medium is ϵ_1 or ϵ_2 , respectively.

3. Hashin and Shtrikman [2] prove using variational principles that the CM expressions for ϵ_1^* and ϵ_2^* form rigorous, optimal, upper and lower bounds on ϵ^* for two component isotropic composites,

$$\epsilon_2 + p_1 \left(\frac{1}{\epsilon_1 - \epsilon_2} + \frac{p_2}{d\epsilon_2} \right)^{-1} \leq \epsilon^* \leq \epsilon_1 + p_2 \left(\frac{1}{\epsilon_2 - \epsilon_1} + \frac{p_1}{d\epsilon_1} \right)^{-1},$$

when ϵ_1 and ϵ_2 are real with $\epsilon_1 \geq \epsilon_2$. They construct coated sphere geometries which attain the bounds.

4. Effective Medium Theories – Bruggeman's symmetrical EMT, most commonly invoked approximation [3, 4]. For cell-type material, consider a single inclusion embedded in a uniform medium of of (an as yet undetermined) effective permittivity ϵ_m (the effective medium). Polarization of this inclusion creates a deviation in the applied field E_0 . Since $\langle E \rangle = E_0$, i.e., the fluctuations must average out to 0, assume the total polarization summed over the two types of inclusions vanishes,

$$\langle P \rangle = p_1 \frac{\epsilon_1 - \epsilon_m}{\epsilon_1 + 2\epsilon_m} + p_2 \frac{\epsilon_2 - \epsilon_m}{\epsilon_2 + 2\epsilon_m} = 0.$$

Solve the quadratic equation for ϵ_m , then resulting formula for $\epsilon^* = \epsilon_m$ in $d = 2$ is

$$\epsilon^* = \frac{1}{4} \left(\gamma + \sqrt{\gamma^2 + 8\epsilon_1\epsilon_2} \right), \quad \gamma = (3p_2 - 1)\epsilon_2 + (3p_1 - 1)\epsilon_1,$$

which is symmetric in ϵ_1 and ϵ_2 and exhibits a percolation threshold (and is realizable). This scheme is also called the coherent potential approximation (CPA).

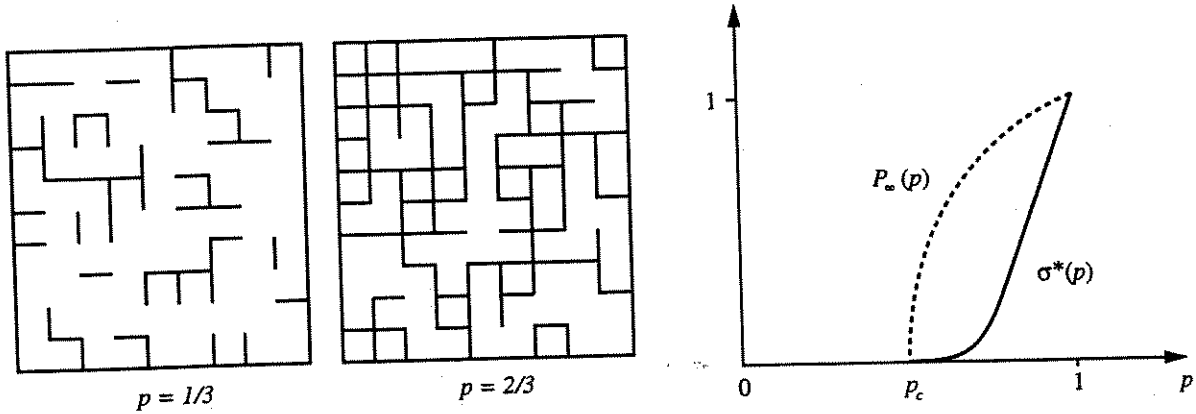


Figure 1: Typical configurations of the two dimensional lattice in bond percolation, below ($p=1/3$) and above ($p=2/3$) the percolation threshold $p_c = 1/2$, and graphs of the infinite cluster density $P_\infty(p)$ and effective conductivity $\sigma^*(p)$.

2 Lattice and continuum percolation models

In high contrast composites with $h = \sigma_1/\sigma_2 \rightarrow 0$ or $h \rightarrow \infty$ **connectedness dominates transport properties**. Classical methods of homogenization, including bounds, approximate formulas, and perturbation methods give little information on the effective behavior. Percolation theory was initiated in 1957 by Broadbent and Hammersley [5] to address such situations, with the introduction of a simple lattice model to study the flow of air through permeable sandstones used in miners' gas masks. In subsequent decades, this theory has been used to successfully model a broad array of disordered materials and processes, including flow in porous media like rocks and soils [6, 7], fractures [8], doped semiconductors [9], and various types of disordered conductors [10, 11] like piezoresistors, thermistors [12], radar absorbing composites [13], thin metal films [14], and polar film [15]. The original percolation model and its generalizations have been the subject of intensive theoretical investigations, particularly in the physics [16, 17] and mathematics [18, 19] communities. One reason for the broad interest in the percolation model is that it is perhaps the simplest, purely probabilistic model which exhibits a type of phase transition.

We now describe the original percolation model in its simplest form. Consider the d -dimensional integer lattice $\mathbf{Z}^d$, and the square (or cubic) network of bonds joining nearest neighbor lattice sites. To each bond, with probability p , $0 \leq p \leq 1$, we assign a 1, meaning it is open, so that fluid can flow through it, and with probability $1-p$ we assign a 0, meaning it is closed. Groups of connected open bonds are called open clusters, and the size or mass of a cluster is just the number of open bonds it contains. The average cluster size $\chi(p)$ clearly increases with p : for $p = 0$, $\chi(p) = 0$, and for $p = 1$, $\chi(p) = \infty$, since then all the bonds are open. The remarkable feature of the percolation model is that there is a critical probability p_c , $0 < p_c < 1$, called the percolation threshold, at which $\chi(p)$ first diverges and an infinite cluster appears, rendering this discrete medium permeable to fluid. For the two dimensional bond lattice, $p_c = 1/2$, and in $d = 3$, $p_c \approx 0.31$. Typical open cluster configurations in $d = 2$ for $p = 1/3$ and $p = 2/3$ are shown in Figure 1. For $p \geq p_c$, one may define an infinite cluster density $P_\infty(p)$ as the probability that the origin (or any point, by translation invariance)

is contained in the infinite cluster, or $P_\infty(p) = \lim_{L \rightarrow \infty} M_\infty(L, p)/L^d$, where $M_\infty(L, p)$ is the mass of the infinite cluster contained in a box of side L . At the percolation threshold, the infinite cluster has a self-similar, fractal structure, with $M_\infty(L, p_c) \sim L^{d_f}$ as $L \rightarrow \infty$, where $d_f \leq d$ is the fractal dimension. The graph of $P_\infty(p)$ for $d = 2$ is shown in Figure 1. In the neighborhood of p_c , $P_\infty(p)$ is believed to exhibit the scaling behavior $P_\infty(p) \sim (p - p_c)^\beta$, where β is the percolation critical exponent, which satisfies $\beta \leq 1$, and in $d = 2$ it is believed that $\beta = \frac{5}{36}$. It should be remarked that we have described the bond problem, but one can also formulate the so-called site problem, where one assigns a 0 or 1 to a lattice site itself, rather than the bonds between them. This changes the values of p_c , but not the critical exponents like β , which are universal, and depend only on dimension, even if one changes the lattice from square to, say, triangular or hexagonal. It should also be mentioned that while the percolation model is very simply stated, some of the most basic questions concerning its behavior remain unanswered. A simple example is the continuity of $P_\infty(p)$ at p_c , i.e., whether $P_\infty(p) \rightarrow 0$ as $p \rightarrow p_c^+$. While nobody would question that the answer is yes, which has been proven in two dimensions, a rigorous proof in three dimensions has eluded the best efforts of some of the world's leading probabilists for many years!

An important quantity is the pair connectedness function $\tau_p(x, y)$, which is the probability that two lattice sites x and y are contained in the same open cluster. For $p < p_c$, $\tau_p(x, y) \sim \exp(-|x - y|/\xi(p))$ as $|x - y| \rightarrow \infty$, which defines a very important quantity called the correlation length $\xi(p)$. Essentially, it measures the scale over which points are connected. As $p \rightarrow p_c^-$, $\xi(p) \sim (p - p_c)^{-\nu}$, which defines the correlation length critical exponent, which is again universal, with $\nu = \frac{4}{3}$ in $d = 2$. The correlation length also measures the separation of "independent crossings". In Figure 1, for $p = 2/3$, while there are many possible starting points on the left boundary for paths which cross the box, there are only two independent crossings (which do not cross each other). For p near p_c , with $p > p_c$, the scale of separation of these independent paths is measured by the correlation length (appropriately defined for above p_c).

The percolation model discussed above deals only with the geometrical aspects of connectedness in disordered media. However, we are interested in the transport of fluids, heat, and electromagnetic waves through such media as well. As an illustrative example, we consider electrical conduction through the percolation model, which is then called the random resistor network. It should be noted, though, that in the limit of low Reynolds number fluid flow, the corresponding random pipe model is equivalent to the random resistor network [20, 6]. Now, to each bond, with probability p we assign an electrical (or fluid) conductance of 1, and with probability $1 - p$ we assign a conductance of $h \geq 0$. We are interested in the effective conductivity of the network, defined by $\sigma^*(p, h) = \lim_{L \rightarrow \infty} L^{2-d} \sigma_L(p, h)$, where $\sigma_L(p, h)$ is the conductance of a box of side L , which is equal to the current that flows through the network (as determined by Kirchhoff's laws) when there is a unit potential gradient across the box. When $h = 0$, clearly, for $p < p_c$, $\sigma^*(p, 0) = 0$. In the neighborhood of p_c , with $p > p_c$, it is believed that $\sigma^*(p, 0) \sim (p - p_c)^t$, where t is the conductivity critical exponent, which is believed to be universal within the class of lattice models. In $d = 2$, $t \approx 1.3$, and in $d = 3$, $t \approx 2.0$, which are the generally accepted values based on numerical estimates. The graph of $\sigma^*(p, 0)$ for $d = 2$ is shown in Figure 1. The reason why $P_\infty(p)$ is larger than $\sigma^*(p, 0)$ is that only a very small part of the infinite cluster, called the backbone, carries current. Most of the infinite cluster near p_c consists of "dead ends" for the current.

While there have been many famous attempts to relate t to the pure percolation exponents like β and ν , none of these relations seem to be exactly true [16, 11], although there are rigorous inequalities relating t to percolation exponents [23]. Assuming a node-link-blob hierarchical structure for the conducting backbone, it has been proven that $1 \leq t \leq 2$ in $d = 2, 3$ and $2 \leq t \leq 3$ in $d \geq 4$ [21, 22]. Another important transport exponent δ is defined at criticality by $\sigma^*(p_c, h) \sim h^{1/\delta}$, $h \rightarrow 0^+$, and for the $d = 2$ bond lattice, $\delta = 2$. The effective fluid permeability $\kappa^*(p, h)$ for a random pipe network is defined in a similar manner to $\sigma^*(p, h)$ (except with a different scaling factor L^{1-d} replacing L^{2-d} above), with $\kappa^*(p, 0) \sim (p - p_c)^e$. For lattice models the critical exponents for permeability and electrical conductivity are the same [24, 7], $e = t$, although this is not generally true for continuum systems [24]. Further review of the relation between conductivity and permeability is contained in [25], and a rigorous expression relating them in the continuum has been found in [26].

In general, percolation models in the continuum can display transport behavior which is more complicated than in the lattice, due to geometric effects. For example, the random checkerboard with conducting and insulating (conductivity h) squares, displays two percolation thresholds as one increases the volume fraction of the conducting squares – the first when they percolate by corners, so that the current has to pass through corner connections, and the second when they percolate by edges [27, 28]. For small h , $\sigma^*(p, h)$ has three separate regimes of asymptotic behavior, separated by the two percolation thresholds. An important breakthrough occurred in the study of transport in percolating systems when it was discovered that in the continuum, t can exhibit nonuniversal behavior with a value different than in the lattice case. In particular, for a Swiss cheese model, which is a conducting host with discs or spheres (possibly overlapping) removed, t is equal to its lattice value in $d = 2$ but is different in $d = 3$ [29, 24].

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